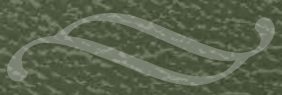
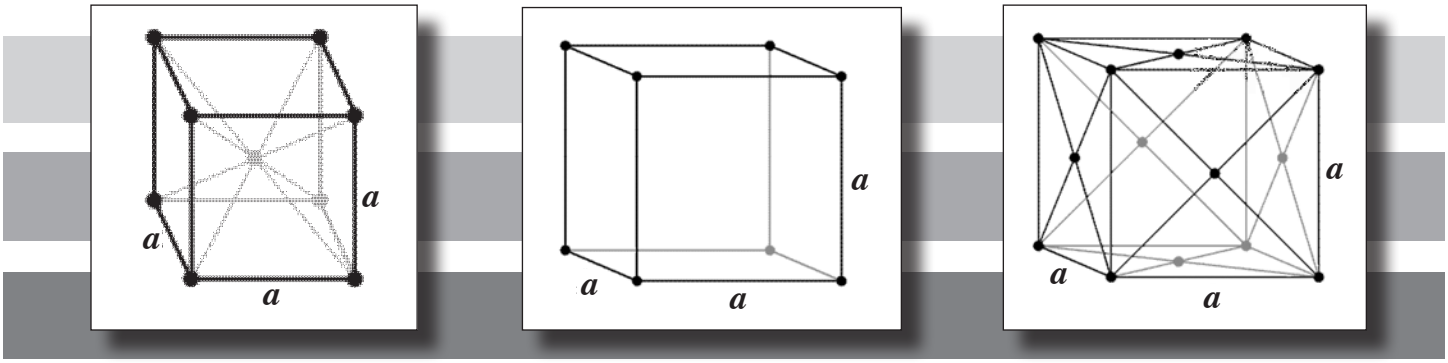
Selected Values of the Crystallographic Properties of Elements



John W. Arblaster

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JOHN W. ARBLASTER

ASM International
Materials Park, Ohio 44073-0002
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First printing, March 2018

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Prepared under the direction of the ASM International Technical Book Committee (2017–2018), Craig Schroeder, Chair.

ASM International staff who worked on this project include Scott Henry, Senior Content Engineer; Karen Marken, Senior Managing Editor; Madrid Tramble, Manager of Production

Library of Congress Control Number: 2018933957

ISBN-13: 978-1-62708-154-2
ISBN-10: 1-62708-154-2
EISBN: 978-1-62708-155-9

SAN: 204-7586

ASM International®
Materials Park, OH 44073-0002
www.asminternational.org

Printed in the United States of America

Preface

A unique and comprehensive review on the crystallographic properties of all of the elements. A general reference book for metallurgists and crystallographers. The book evaluates the crystallographic properties of all of the elements at ambient pressure in order to provide a base line for high pressure studies.

The book presents lattice parameters of the elements as a function of temperature. It also provides related properties, for example, thermal expansion coefficients, molar volumes and densities. This book is the first to include this data for all of the elements; it condenses all of the data in to a single volume with special attention given to ensure that the selected values correspond to the latest values of atomic weights and the fundamental constants.

The author, John Arblaster, spent his career as a metallurgical chemist analysing a wide variety of ferrous and non-ferrous metals and alloys in a number of commercial laboratories. He first became interested in crystallography in order to solve the dispute over whether osmium or iridium was the densest metal in the room temperature region. He showed, by proper application of up to date input data, that it was in fact osmium. He then produced comprehensive reviews on the crystallographic properties of the six platinum group of metals and has now extended this work to all of the elements. Background notes relating to this book can be obtained from the author at the e-mail address: jwarblaster@yahoo.co.uk

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A. INTRODUCTION

The main purpose of this book is to evaluate the crystallographic properties of all of the elements at ambient pressure in order to provide a base line for high pressure studies. The exception is of course helium which cannot be obtained as a solid at ambient pressure and is therefore considered on a temperature-pressure-volume basis. Allotropic modifications are considered for boron, carbon, oxygen, phosphorus, sulfur and selenium and separate isotopic evaluations are given for hydrogen, helium, lithium, boron, carbon, nitrogen, neon and silicon.

Compilations on the thermodynamic properties of the elements at the U.S. Bureau of Mines were introduced in 1934 (Kelley 1960) but the first comprehensive review on all of the elements appears to be that of Stull and Sinke 1956. However, until the present evaluation there does not appear to have been a similar detailed review on the crystallographic properties of the elements, although various aspects of such a review were contained in three *tours de force*, on the thermal expansion of the metallic elements by Touloukian et al. 1975, on the non-metallic elements by Touloukian et al. 1977, and on the crystal structures of the elements by Donohue 1974. Not only did Touloukian et al. 1975, 1977 contain extensive bibliographies but they also included a significant amount of data which was originally given only in the form of graphs. They also gave representative equations, graphs and tables of both selected values and original thermal expansion and length change values. Although new data has resulted in many of the equations becoming obsolete there are still several which cannot be improved upon and have been accepted in the present publication with full acknowledgement. Donohue 1974 also included an extensive bibliography and, especially for the room temperature region, included all of the reported lattice parameter measurements available for each element. Values already rejected by Donohue 1974 were not included in the present evaluation. Although published over forty years ago, many of the room temperature lattice parameter values selected by Donohue 1974 are very close to values selected here once wavelength corrections are taken into account. A further very useful service provided in the review of Donohue 1974 was the correct description of axis sequencing for anisotropic structures which eliminated much confusion that had existed in the literature.

Other reviews included tables of thermal expansion for many elements by Kirby at al 1972 but without references. Goldak et al. 1966 reviewed the crystallographic properties of alpha zirconium, and Lloyd and Barrett 1966 reviewed alpha uranium. Wang and Reeber 1998 selected thermal expansion values for the body-centered cubic refractory metals vanadium, niobium, tantalum, molybdenum and tungsten, Reeber and Wang 1996a diamond, Reeber and Wang 1996b silicon and germanium, Wang and Reeber 1996 copper and Wang and Reeber 2000 aluminum. Lu et al. 2005 reviewed the thermal expansion of several metallic elements but appeared ultimately to have relied on the thermal expansion values given by Kirby et al. 1972 and Touloukian et al. 1975, as did Zhang et al. 2013 who carried out an assessment of the thermal expansion coefficients for forty two pure metals using a Debye-Grüneisen model.

B. NOTATION

T = Temperature in kelvins

t = Temperature in degrees Celsius

RT = Room temperature

α = Thermodynamic thermal expansion coefficient in units of K^{-1}

α^* = Thermal expansion coefficient relative to 293.15 K in units of K^{-1}

$\varepsilon_T = (l_T - l_{293.15\ K})/\ l_{293.15\ K}$

$\varepsilon_0 = (l_T - l_{0\ K})/\ l_{0\ K}$

$L_T = 1 + \varepsilon_T$ or $1 + \varepsilon_0$

$\alpha_m = \varepsilon_T / (T - 293.15\ K)$

$100\Delta\varepsilon = 100\varepsilon_T$ experimental $- 100\varepsilon_T$ calculated or $100\varepsilon_0$ experimental $- 100\varepsilon_0$ calculated

For anisotropic structures ε_T avr $= (V_T / V_{293.15})^{⅓} - 1$ where V_T is the molar volume of the phase at temperature T and $V_{293.15}$ is the molar volume of the reference phase at 293.15 K. For anisotropic structures based on a baseline of 0 K then ε_0 avr $= (V_T / V_0)^{⅓} - 1$ where V_0 is the molar volume of the reference phase at 0 K.

C. CONSTANTS

C1. Reporting of Accuracy

A short hand method is adopted, i.e. 236.42 (2) is used to represent 236.42 ± 0.02 while 2.364 (4) x 10^{10} is used to represent (2.364 ± 0.004) x 10^{10} and 21.2 (1.2) is used to represent 21.2 ± 1.2

C2. Avogadro Constant

This is required to calculate molar volumes and densities. The accepted value is that selected by Mohr et al. 2016a, 2016b for the 2014 CODATA fundamental physical constants: $N_A = 6.022140857\ (74) \times 10^{23}\ mol^{-1}$. At the level of accuracy given no molar volume or density values would be affected by correcting to the 2017 CODATA value of $N_A = 6.02214076 \times 10^{23}\ mol^{-1}$ exactly (Newell et al. 2018)

C3. Atomic Weights

Atomic weights are required to calculate density values from lattice parameter data. However, it is unfortunate that for the 2009 atomic weights ten elements, hydrogen, lithium, boron, carbon, nitrogen, oxygen, silicon, sulfur, chlorine and thallium, were no

longer given as single atomic weight values but only as a range of extreme values (Wieser and Coplen 2011). This is a highly unsatisfactory situation since the actual extreme values represent only a small fraction of the total and therefore cannot be considered as being fully representative of these elements. However, it was noted that in the graphical representations of the isotopic ratios that the 2007 atomic weights (Wieser and Berglund 2009) with their assigned accuracies would be representative of the vast majority of any materials likely to be encountered. Therefore, these values were used to calculate the density values. For the 2011 atomic weights (Wieser et al. 2013) only bromine and magnesium were treated in this manner and therefore the 2009 atomic weights were used for these elements. No further corrections of this type were included in the 2013 atomic weights (Meija et al. 2016) or in the 2015 atomic weights (CIAAW 2015) but were included for argon and lead in the 2017 atomic weights (Meija 2017). For the elements with no stable or very long lived isotopes, as well as for individual stable isotopes such as deuterium, helium 3, lithium 6 and 7, boron 10 and 11, carbon 13, nitrogen 15, neon 20 and 22 and silicon 28, atomic masses were selected from the review by Wang et al. 2017.

C4. The Effect of Ambient Pressure on Selected Molar Volume and Density Values

Molar volume and density values calculated from lattice parameter measurements are necessarily those values obtained in a vacuum. However, at the level of accuracy assigned to these values the differences from values that would be obtained at ambient pressure (atmospheric pressure) are entirely negligible and the quoted values could be considered as equally applying in both vacuum and ambient pressure conditions. The density values selected for beta rhombohedral boron, alpha white phosphorus and germanium are based on directly determined ambient pressure values. An exception would be the ultra precision lattice parameter measurements for silicon 28 except that all values associated with silicon 28 experiments are determined in vacuum conditions.A further exception is of course helium where all values are subject to pressure and temperature effects.

C5. Wavelength Scales

The traditional value for the conversion factor from kX to ångstroms at 1.00202 has long been superseded as indicated by the 2014 CODATA fundamental physical constants conversion factors for the primary X-ray wavelength standards (Mohr et al. 2016a, 2016b).

Wavelength	Definition	Conversion Factor	Equivalent Value nm
Cu $K\alpha_1$	1.537400 kX	0.100207697 (28)	0.154059313 (43)
Mo $K\alpha_1$	0.707831 kX	0.100209952 (53)	0.070931711 (38)
W $K\alpha_1$	0.2090100 Å*	0.100001495 (90)	0.020901312 (19)

Values given in kX units without wavelength standards were converted to nm using the above conversion factor for Cu $K\alpha_1$ while values given in ångstroms without wavelength standards were converted using the default ratio 0.100207697/1.00202. Bearden 1964 carried out a review of wavelengths where published values were adjusted so as to be

equivalent to the Mo $K\alpha_1$ definition of 707.831 x units. On this scale, Cu $K\alpha_1$ is equal to 1537.370 x units. Bearden 1967 returned to using Cu $K\alpha_1$ with the above definition 1537.400 x units. Therefore, all of the values given in Bearden 1964 which were related to Cu $K\alpha_1$ were converted to nm using the ratio 0.100207697 x 1.537400/1537.370 which is 1.00209652 x 10^{-4} which was used to construct the table of wavelength standards below, except for Cu $K\alpha_2$ which Bearden 1964 originally selected as 1541.198 x units which should have converted to 1.544398 Å* but was instead given as 1.544390 Å* which is equivalent to the value 1541.1905 x units which is used as a basis below. The only exception is Mo$K\alpha_2$ which is directly related to Mo$K\alpha_1$. The value of $K\alpha$ is defined as being equal to $(2\ K\alpha_1 + K\alpha_2)/3$.

Element	$K\alpha_1$ nm	$K\alpha_2$ nm	$K\alpha$ nm	$K\beta$ nm
V	0.250361	0.250744	0.250489	0.228445
Cr	0.228975	0.2293653	0.229105	0.208491
Mn	0.2101863	0.210583	0.204064	0.198025
Fe	0.1936082	0.1940020	0.1937395	0.175665
Co	0.1789002	0.1792887	0.1790297	0.162082
Ni	0.1657944	0.1661781	0.1659229	0.1500166
Cu	Defined	0.1544422	0.1541869	0.1392247
Mo	Defined	0.0713607	0.0710747	-

C6. Reference Temperatures

Although absolute zero would be the ideal fundamental reference temperature, difficulties still exist for several elements in obtaining low temperature measurements and in view of this the adoption of absolute zero is still not ideal although required for those elements which are either liquid or gaseous at 293.15 K. However, room temperature represents a pivotal point for thermal expansion measurements with traditionally a switch from low temperature thermal expansion coefficient measurements to high temperature length change measurements. For thermal expansion a reference temperature of 293.15 K (20°C) was adopted by the International Committee for Weights and Measures in 1931 (Doiron 2007).

C7. Crystal Geometry – Volumes of the Unit Cell

Cubic: $V = a^3$

Tetragonal: $V = a^2 c$

Orthorhombic: $V = abc$

Hexagonal: $V = (\sqrt{3}/2)\, a^2 c$

Rhombohedral: $V = a^3 \sqrt{(1 - 3\cos^2\alpha + 2\cos^3\alpha)}$

Monoclinic: $V = abc \sin\beta$

Triclinic: $V = abc \sqrt{(1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma)}$

C8. Pearson Designations for the 14 Bravais Lattices

Bravais lattice	Pearson Symbol
Cubic – primitive	cP
Cubic – body-centered	cI
Cubic – all face-centered	cF
Tetragonal – primitive	tP
Tetragonal – body-centered	tI
Orthorhombic - primitive	oP
Orthorhombic – one-face-centered	oS
Orthorhombic – body-centered	oI
Orthorhombic – all face-centered	oF
Hexagonal – primitive	hP
Rhombohedral – rhombohedral	hR
Monoclinic – primitive	mP
Monoclinic – one face-centered	mS
Triclinic - primitive	aP

The number following the Pearson symbol is the number of atoms in the unit cell.

D. THE RHOMBOHEDRAL – HEXAGONAL CONVERSION EQUATIONS

Elements crystallizing in the rhombohedral (hR) structure are also given in terms of an equivalent hexagonal (hP) structure because this facilitates the representation of thermal expansion data.

Rhombohedral and hexagonal conversion equations

a_r and α represent the rhombohedral lattice spacing and inclusive angle while a_h and c_h represent the equivalent hexagonal lattice spacings

$a_r^2 = a_h^2 / 3 + c_h^2 / 9$; $\sin(\alpha / 2) = a_h / (2\, a_r)$

$a_h = 2\, a_r \sin(\alpha/2)$; $c_h = a_r \sqrt{(3 + 6 \cos \alpha)}$

E. REPRESENTATION OF THERMAL EXPANSION DATA

While high temperature thermal expansion data can usually be represented by simple linear or polynomial equations, low temperature data tends to behave in a more complex manner but can also be represented by a series of high order polynomials if sufficient high quality data is available. However, if the data is more limited then the approach suggested in Appendix A is adopted in which thermodynamic thermal expansion (α) and specific heat (C_p) data were related to a high degree of correlation by means of the equation:

$$\alpha = C_p (A + B T + C/ T) \quad (A)$$

Where A, B and C are constants.

When, instead of thermal expansion coefficients only limited length change values (L_T) were available below room temperature, then these were combined with values of absolute enthalpy ($H_T - H_0$) in the equation also suggested in Appendix A:

$$\ln (L_T) = (H_T - H_0) (D + E T + F/ T) + G \quad (B)$$

Where D, E, F and G are constants.

Differentiation of equation B lead to thermal expansion:

$$\alpha = D C_p + E [C_p T + (H_T - H_0)] + F [C_p / T - (H_T - H_0) / T^2] \quad (C)$$

F. GRAPHICAL DATA

Although a significant amount of data originally reported in the form of graphs was given as actual length change values by Touloukian et al. 1975, 1977 it is unfortunate that data subsequently continued to be reported in this form. It is considered that the accuracy of the graphs can be read to 0.5 mm of the original graphical scale and although the graphs can be expanded electronically to any size it is then reliant on the expertise in creating the graphs in the first place and this remains as a chief source of systematic errors. In order to smooth out estimates from the graphs, readings were fitted to straight lines or polynomials. The philosophy of reporting data only in graphical form is extraordinary because it diminishes the great effort in trying to obtain the best possible values experimentally.

G. ACKNOWLEDGEMENTS

The author is indebted to the following for supplying data that was originally given only in the form of graphs: U.Benedict (alpha thorium), R.M.Ibberson (ozone, beta monoclinic sulfur and iodine), T.Lundström (beta boron), J.A.C.Marples (alpha thorium and alpha americium) and V.Pecharsky (alpha and beta dysprosium) and also to G.K.White for supplying revised thermal expansion coefficients of rhodium, palladium and iridium at 283 K. The author is also indebted to CINDAS LLC for allowing the reproduction of equations given by Touloukian et al. 1975 for indium (p. 143), lanthanum (p. 173) and yttrium (p. 387) and as given by Touloukian et al. 1977 for arsenic (p. 7) where the page references are those given in the original publications. The author also wishes to thank J.Meija for supplying the values of the 2017 atomic weights ahead of publication.

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The Elements

1 HYDROGEN H

Although the physical properties of the isotopes hydrogen (H_2) and deuterium (D_2) are similar, because the mass of D_2 is twice that of H_2, evaluations of the crystallographic properties are considered separately. The mechanisms of the crystallographic transitions of both isotopes was reviewed by Silvera 1980.

PART 1A. HYDROGEN

Distinction is made between protium, pure $^1H_2$, and "hydrogen" which is considered to be natural hydrogen containing 0.015574 (5) at% deuterium for the best representative sample (Meija et al. 2016). Measurements are carried out on natural hydrogen.

Atomic weight: 1.00784 to 1.00811 (Meija 2017)
Select 2007 value 1.00794 (7) (Wieser and Berglund 2009).

Hydrogen has either spin quantum numbers J = 0 *para* hydrogen (*p*-H_2) or J=1 *ortho* hydrogen (*o*-H_2). The two common compositions available are normal hydrogen (*n*-H_2) consisting of 75% *o*-H_2 25% *p*-H_2 and equilibrium hydrogen (*e*-H_2) consisting of 99.8% *p*-H_2 0.2% *o*-H_2. The triple point of *e*-H_2 is a primary fixed point on ITS-90 at 13.8033 K (Preston-Thomas 1990) and the triple point of *n*-H_2 is a secondary fixed point at 13.952 (2) K (Bedford et al. 1996).

1.1 Crystallographic properties of hydrogen

Allotropy: Alpha: Hexagonal close-packed (hP4)
Beta: Face-centered cubic (cF8)

Keesom et al. 1930a, 1930 b, 1930c first identified the structure of the alpha phase while electron diffraction studies on thin films by Bostanjoglo 1965 and Curzon and Mascall 1965 suggested the existence of the beta phase which was confirmed by lattice parameter measurements on bulk samples by Mills and Schuch 1965.

The bulk liquid solidifies into the orientationally disordered alpha phase but for *o*-H_2 there is a transformation below 2.9 K (Schuch et al. 1968, Jarvis et al. 1969) into the orientationally ordered beta phase which Raich and James 1966 concluded was face-centered cubic corresponding to the space group Pa3. The structural transformation does not occur in *p*-H_2 with the critical concentration at 0 K being at 56% *o*-H_2 below which there is no cooperative ordering, although because of hysteresis in the transformation a value of 49% *o*-H_2 is obtained from the cubic – hexagonal transformation and 58% *o*-H_2 for the hexagonal – cubic transformation (Gates et al. 1979). From the graphical representation of the temperatures of transition by Schuch et al. 1968 and the experimental values given by Jarvis et al. 1969 the transition temperature for *n*-H_2 is selected as 1.6 K. Haase et al. 1979 could find no evidence of a transition below 1 K to a

glassy phase proposed by Sullivan et al. 1978 to explain abrupt changes in NMR absorption lines.

Lattice parameter thermal expansion has been determined for *e*-H_2 by Krupskii et al. 1983a (0-13.8 K) and for alpha phase *n*-H_2 by Krupskii et al. 1983b (0-13.5 K). In both cases the values were corrected to nm using the default ratio 0.100207697/1.00202. In the case of *e*-H_2 thermal expansion coefficients were extrapolated below 4 K by fixing the selected values at 4 K and 5 K to the Debye equation: $\alpha\ (K^{-1}) = 2.59 \times 10^{-7}\ T^3$ which applies to both axes. For *n*-H_2 the abnormal behavior at low temperatures is due to the presence of a rotational subsystem. It is uncertain how the thermal expansion coefficients continues to behave below 3 K but at some point there must be a sudden sharp decrease so that the value is zero at 0 K. Lattice parameter and thermal expansion coefficients for both phases were extrapolated to the triple points. In comparison with the lattice parameters values the H_2 bond length is 0.074144 nm (Huber and Herzberg 1979).

Dilatometric determination of the thermal expansion of *e*-H_2 by Aleksandovskii et al. 1989 (0.9-5 K) are considered to be far more sensitive than values derived from lattice parameters and therefore the relatively large difference of $10 \times 10^{-6}\ K^{-1}$ at 5 K is probably due to the difficulty in deriving thermal expansion coefficients from lattice parameter measurements at the lowest temperatures. Volumetric thermal expansion measurements of Krause and Swenson 1980 (0-13.8 K) are also systematically lower than the selected values with an average deviation of 4.5% low over the range 4 to 13.8 K. The volume thermal expansion coefficient determined by Udovidchenko et al. 1999 at the triple point is only 0.9% lower than the selected value.

Ishmaev et al. 1983 determined lattice parameter values for *e*-H_2 at 4.2 K leading to a molar volume 23.00 (2) $cm^3\ mol^{-1}$ which is similar to the value of 23.068 (16) $cm^3\ mol^{-1}$ determined by Kruspskii 1983a at the same temperature. However, from bulk determination of the molar volume Krause and Swenson 1980 (0-13.8 K) determined a much higher value of 23.234 (50) $cm^3\ mol^{-1}$ at 0 K and Driessen and Silvera 1984 obtained a similar value of 23.21 (5) $cm^3\ mol^{-1}$. Krause and Swenson also extrapolated to a molar volume of 23.48 (5) $cm^3\ mol^{-1}$ at the triple point compared to 23.316 (16) $cm^3\ mol^{-1}$ obtained from the lattice parameter measurements. However, based on a new determination of the density of liquid *e*-H_2 then Roder 1981 determined the molar volume of the solid at the triple point to be 42.91 mol L^{-1}, equivalent to $23.30_5\ cm^3\ mol^{-1}$, in excellent agreement with the lattice parameter value and appearing to resolve the discrepancy.

As shown in Table 1a measurements of the lattice parameters of alpha phase *n*-H_2 given to significant accuracy showed only poor agreement with the selected value when reduced to molar volumes:

Table 1a. Derived molar volume values for alpha *n*-H_2

References	Temperature K	Molar Volume $cm^3\ mol^{-1}$	Note
Mills and Schuch 1965	1.3	22.52 (9)	
Barrett et al. 1966	4.2	23.04 (8)	a
Bostanjoglo and Kleinschmidt 1967	2.8 – 4.5	22.91 (10)	
Selected (Krupskii et al. 1983b)	2 - 4	22.808 (16)	

Note for Table 1a

a. From lattice parameter values calculated by Donohue 1974

1.2 Properties of alpha *ortho* hydrogen

Silvera 1980 selected values for the molar volume at 0 K across the whole range of concentrations from J = 0 to J = 1 (or $C_1 = 0$ to $C_1 = 1$) by use of the volume equation: V_m ($cm^3\ mol^{-1}$) = 23.16 – 0.091 C_1 – 0.217 C_1^2. However, the selected value at $C_1 = 0$ is 23.067 $cm^3\ mol^{-1}$ so the molar volume equation should be modified to give the equation V_m ($cm^3\ mol^{-1}$) = 23.067 – 0.091 C_1 – 0.217 C_1^2 which leads to 22.76 $cm^3\ mol^{-1}$ for pure *o*-H_2 at $C_1 = 1$. Jarvis et al. 1967 determined that the molar volume difference between *p*-H_2 and *o*-H_2 at 4.2 K to be 1.3 (2) % so that the molar volume of *o*-H_2 would be 22.770 (46) $cm^3\ mol^{-1}$ in agreement with the extrapolated value. Selecting the directly determined molar volume value then the density for the *o*-H_2 alpha phase would be equal to 88.5 (2) kg m^{-3} at 4.2 K but because the *c*/*a* ratio for *e*-H_2 and *n*-H_2 showed a composition trend then it would be speculative to suggest a value for *o*-H_2 which would allow an estimate of the lattice parameters.

1.3 Beta hydrogen

From the measurements of Jarvis et al. 1969 the values as shown in Table 1b are selected as “equilibrium” alpha-beta transition tenperatures as an average of the heating and cooling values.

Table 1b. Hexagonal – cubic transition temperatures for hydrogen

% *o*-H_2	55	56	57	58	59	60	61	62	63
T K	< 0.4	< 0.4	< 0.4	< 0.4	0.68	0.70	0.83	0.91	0.99
% *o*-H_2	65	67	70	75	80	85	90	95	100
T K	1.08	1.23	1.39	1.65	1.89	2.16	2.42	2.64	2.90

For *n*-H_2 lattice parameter determinations by Mills and Schuch 1965 at 0.5312 (10) nm at 1.25-1.3 K show poor agreement with the measurements of Bostanjoglo and Kleinschmidt 1967 for thin films at 0.5338 (8) nm at 2.8-4.5 K. For a composition close to *n*-H_2, Jarvis et al. 1967 determined an alpha-beta molar volume change to be 0.15% on cooling and 0.08% on heating. Averaging to 0.115 (35)% and selecting 22.785 (16) $cm^3\ mol^{-1}$ for the molar volume of the alpha phase at the transition temperature at 1.6 K then

the beta phase molar volume is 22.759 (18) $cm^3\ mol^{-1}$, equivalent to a density value of 88.58 (7) kg m^{-3} and a lattice parameter of 0.5327 (1) nm. The use of this procedure for other compostions is limited by the general lack of lattice parameter data available for the alpha phase.

Table 1c. Crystallographic properties of alpha *e*-H_2

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 ε_0 *a*	100 ε_0 *c*	100 ε_0 avr
0	0	0	0	0	0	0
1.0	0.3	0.3	0.3	< 0.001	< 0.001	< 0.001
2.0	2	2	2	< 0.001	< 0.001	< 0.001
3.0	7	7	7	< 0.001	< 0.001	< 0.001
4.0	16	16	16	0.002	0.002	0.002
5.0	33	33	33	0.005	0.005	0.005
6.0	63	63	63	0.008	0.010	0.009
7.0	109	108	109	0.019	0.018	0.019
8.0	175	171	174	0.032	0.032	0.032
9.0	269	250	263	0.053	0.053	0.053
10.0	396	340	377	0.087	0.083	0.086
10.5	482	388	451	0.108	0.100	0.105
11.0	569	438	525	0.135	0.121	0.130
11.5	677	493	616	0.167	0.144	0.159
12.0	790	546	709	0.204	0.172	0.193
12.5	931	600	821	0.246	0.199	0.230
13.0	1082	662	942	0.296	0.231	0.274
13.5	1253	726	1077	0.354	0.265	0.324
13.8033	1367	766	1167	0.393	0.289	0.358

Table 1d. Crystallographic properties of alpha *e*-H_2

T K	*a* nm	*c* nm	*c*/*a*	Molar Volume $cm^3\ mol^{-1}$	Density kg m^{-3}
0	0.37837	0.61787	1.6330	23.067	87.40
1.0	0.37837	0.61788	1.6330	23.067	87.39
2.0	0.37837	0.61788	1.6330	23.067	87.39
3.0	0.37837	0.61788	1.6330	23.067	87.39
4.0	0.37838	0.61789	1.6330	23.068	87.39
5.0	0.37839	0.61790	1.6330	23.070	87.38
6.0	0.37841	0.61794	1.6330	23.074	87.37
7.0	0.37844	0.61799	1.6330	23.080	87.35
8.0	0.37849	0.61807	1.6330	23.089	87.31
9.0	0.37857	0.61820	1.6330	23.104	87.26
10.0	0.37870	0.61839	1.6329	23.126	87.17
10.5	0.37878	0.61850	1.6329	23.140	87.12
11.0	0.37888	0.61863	1.6328	23.157	87.05
11.5	0.37900	0.61877	1.6326	23.177	86.98
12.0	0.37914	0.61893	1.6324	23.200	86.89
12.5	0.37931	0.61911	1.6322	23.227	86.79
13.0	0.39750	0.61930	1.6319	23.258	86.68
13.5	0.37971	0.61952	1.6315	23.292	86.55
13.8033	0.37986	0.61966	1.6313	23.316	86.46

Table 1e. Crystallographic properties of alpha *n*-H_2

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_0 a$	100 $\varepsilon_0 c$	100 ε_0 avr
0	0	0	0	0	0	0
1.0	-	-	-	0.029	0.025	0.028
1.6	-	-	-	0.042	0.041	0.042
2.0	-	-	-	0.053	0.050	0.052
3.0	244	238	242	0.077	0.075	0.076
4.0	239	224	234	0.101	0.097	0.100
5.0	235	210	227	0.125	0.119	0.123
6.0	240	210	230	0.149	0.140	0.146
7.0	258	226	247	0.175	0.162	0.171
8.0	341	250	311	0.205	0.187	0.199
9.0	415	290	373	0.242	0.213	0.232
10.0	527	346	467	0.289	0.245	0.274
10.5	605	380	530	0.316	0.263	0.298
11.0	683	420	595	0.351	0.283	0.328
11.5	778	470	675	0.388	0.305	0.360
12.0	877	526	760	0.428	0.330	0.395
12.5	993	592	859	0.475	0.357	0.436
13.0	1113	676	967	0.529	0.390	0.483
13.5	1242	766	1083	0.587	0.426	0.533
13.952	1366	863	1198	0.645	0.461	0.584

Table 1f. Crystallographic properties of alpha *n*-H_2

T K	*a* nm	*c* nm	*c*/*a*	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
0	0.37654	0.61547	1.6345	22.756	88.59
1.0	0.37665	0.61563	1.6345	22.774	88.52
1.6	0.37670	0.61573	1.6345	22.785	88.48
2.0	0.37674	0.61579	1.6345	22.791	88.45
3.0	0.37683	0.61593	1.6345	22.808	88.39
4.0	0.37692	0.61607	1.6345	22.823	88.33
5.0	0.37701	0.61620	1.6344	22.839	88.27
6.0	0.37710	0.61634	1.6344	22.835	88.20
7.0	0.37720	0.61648	1.6343	22.873	88.14
8.0	0.37731	0.61663	1.6343	22.892	88.06
9.0	0.37745	0.61679	1.6341	22.914	87.98
10.0	0.37763	0.61698	1.6338	22.943	87.87
10.5	0.37774	0.61709	1.6337	22.960	87.80
11.0	0.37786	0.61721	1.6335	22.980	87.73
11.5	0.37800	0.61735	1.6332	23.002	87.64
12.0	0.37816	0.61751	1.6330	23.027	87.55
12.5	0.37833	0.61768	1.6326	23.055	87.44
13.0	0.37853	0.61788	1.6323	23.086	87.32
13.5	0.37875	0.61809	1.6319	23.121	87.19
13.952	0.37897	0.61831	1.6315	23.156	87.06

PART 1B. DEUTERIUM

Atomic mass of ^{2}H: 2.01410177811 (12) (Wang et al. 2017)

Deuterium has either spin quantum numbers J = 0 *ortho* deuterium (*o*-D_2) or J = 1 *para* deuterium (*p*-D_2). The two common compositions are normal deuterium (*n*-D_2) consisting of 66.7% *o*-D_2 33.3% *p*-D_2 and equilibrium deuterium (*e*-D_2) consisting of 98.5% *o*-D_2 1.5% *p*-D_2 The triple points of *n*-D_2 and *e*-D_2 are secondary fixed points on ITS-90 at 18.724 (1) K and 18.689 (1) K respectively (Bedford et al. 1996).

1.4 Crystallographic properties of deuterium

Allotropy: Alpha: Hexagonal close-packed (hP4)
Beta: Face-centered cubic (cF8)

The crystal structure of the alpha phase was first correctly identified by Kogan et al. 1964 while using electron diffraction of thin films Curzon and Mascall 1965 identified the beta phase. However, it was the bulk X-ray diffraction measurements of Schuch and Mills 1966 which correctly identified that both phases were present.

The bulk liquid solidifies into the orientationally disordered alpha phase but for *p*-D_2 there is a transformation below 3.9 K (Schuch et al. 1968, Ramm et al. 1970) into the orientationally ordered face-centered cubic beta phase of space group Pa3. This transformation does not occur in o-D_2 with the critical concentration at 0 K being at 51% to 54% *p*-D_2 below which there is no cooperative ordering (Ramm et al. 1970). Therefore, neither *n*-D_2 or *e*-D_2 transform to the cubic structure. For deuterium, Sokol et al. 1985 could find no evidence of a glass transition below 0.5 K proposed by Gaines and Sokol 1983 as an explanation for abrupt changes in the shape of NMR absorption lines.

Lattice parameter thermal expansion have been determined for *e*-D_2 by Krupskii et al. 1984 (0-18.5 K) and for *n*-D_2 by Shcherbakov 1991 (0-18.73 K). In both cases the values were corrected to nm using the default ratio 0.100207697/1.00202. In the case of *e*-D_2 thermal expansion coefficients were extrapolated below 5 K by fixing the tabulated values at 5 K and 6 K and then fitting to the Debye equations: α_a (K^{-1}) = 1.94 x 10^{-7} T^3 and α_c (K^{-1}) = 1.85 x 10^{-7} T^3. For *n*-D_2 the abnormal behavior at low temperatures is due to the presence of a rotational subsystem. It is uncertain how the thermal expansion coefficients continues to behave below 4 K but at some point there must be a sudden sharp decrease so that the value is zero at 0 K. Lattice parameter and thermal expansion coefficients of *e*-D_2 were extrapolated to the triple point while for *n*-D_2 the triple point values were determined by interpolation. In comparison with the lattice parameter values the D_2 bond length is 0.074152 nm (Huber and Herzberg 1979).

Dilatometric determination of the thermal expansion of *e*-D_2 by Soldatov et al. 1992 (1.5-5.6 K) are considered to be far more sensitive than values derived from lattice parameters and therefore agreement at 5 K to within a value of 3 x 10^{-6} K^{-1} is considered to be satisfactory. Neutron scattering measurements of Nielsen 1973 (5 K to triple point) show

poor agreement with selected values leading to average length change values which on the basis $100\Delta\varepsilon$ differ by 0.046 high at 12 K to 0.063 low at the triple point. For *n*-D_2 volume thermal expansion coefficients of Udovidchenko et al. 1984 (4.0-18.73 K) trend sharply from 84% low to 15% low between 4 and 11 K but then trend less sharply to 7% low at the triple point.

Neutron diffraction measurements of Sokol et al. 1985 (0.2-14.0 K) for 46% *p*-D_2 were unfortunately only shown graphically as molar volume values but do suggest that over the temperature range the *c*/*a* ratio remains constant at 1.6322 (2). Lattice parameter measurements have also been determined by Mucker et al. 1968 over the range 3% to 80% *p*-D_2 for various temperatures from 2.0 to 12.9 K. For an *e*-D_2 sample at 12.9 K the derived molar volume value is only 0.03 $cm^3\ mol^{-1}$ lower than the selected value while for a sample of *n*-D_2 at 10.2 K the difference is 0.04 $cm^3\ mol^{-1}$ lower.

Table 1g. Derived molar volume values for alpha *e*-D_2

References	Temperature K	Molar Volume $cm^3\ mol^{-1}$	Note
Nielsen 1973	5	19.94	
Yarnell et al. 1975	1.5 – 4	19.994 (13)	a
Driessen and Silvera 1984	0	19.95 (5)	
Ishmaev et al. 1985	4.2	19.934 (15)	
Selected (Krupskii et al. 1984)	2 - 4	19.934 (16)	

Notes for Table 1g

a. Calculated from equation

Table 1h. Derived molar volume values for alpha *n*-D_2

References	Temperature K	Molar Volume $cm^3\ mol^{-1}$	Note
Schuch and Mills 1966	1.4 – 1.5	19.80 (3)	
Bostanjoglo and Kleinschmidt 1967	2.8 – 4.5	19.90 (8)	
Yarnell et al. 1975	1.5 – 4	19.930 (13)	a
Selected (Shcherbakov 1991)	2 - 4	19.889 (12)	

Notes for Table 1h

a. Calculated from equation

1.5 The crystallographic properties of alpha *para* deuterium

Silvera 1980 selected for the molar volume at 0 K across the concentration range from J = 0 to J = 1 (or $C_1 = 0$ to $C_1 = 1$) as $V_m\ (cm^3\ mol^{-1}) = 19.95 - 0.16\ C_1 - 0.04\ C_1^2$. However, the selected value at $C_1 = 0$ is 19.934 $cm^3\ mol^{-1}$ so the equation should be modified to give: $V_m\ (cm^3\ mol^{-1}) = 19.934 - 0.16\ C_1 - 0.04\ C_1^2$. For *n*-$D_2$ ($C_1 = 0.333$) this modified equation leads to 19.87_6 $cm^3\ mol^{-1}$ which is only 0.00_6 $cm^3\ mol^{-1}$ higher than the selected value although the molar volume measurement determined at 0 K by Sokol et al. 1985 for

46% *p*-D_2 is 0.072 $cm^3\ mol^{-1}$ higher. For metastable hexagonal *p*-D_2 (C_1 = 1) the calculated value is $19.73_4\ cm^3\ mol^{-1}$. This value appears to be significantly lower than the value of $19.79_5\ cm^3\ mol^{-1}$ for C_1 = 1 calculated from the equation of Yarnell et al. 1975. However, for *e*-D_2 Yarnell et al. 1975 obtain a value of 19.994 $cm^3\ mol^{-1}$ which is significantly higher than the selected value. Assuming a systematic error then the molar volume values given by Yarnell et al. 1975 were corrected by the ratio 19.934 / 19.994 which leads to a molar volume at of $19.73_6\ cm^3\ mol^{-1}$ at C_1 = 1 in excellent agreement with the value obtained above. Therefore, selecting the molar volume calculated from the modified equation of Silvera 1980 then the equivalent density is 204.1 kg m^{-3} and assuming that the *c*/*a* ratio is ideal at 1.6330 then the derived lattice parameters would be *a* 0.3592 nm and *c* 0.5866 nm.

1.6 Beta deuterium

From the measurements of Ramm et al. 1970, values given in Table 1i are selected as "equilibrium" alpha-beta transition tenperatures as an average of the heating and cooling values.

Table 1i. Hexagonal – cubic transition temperatures for deuterium

% *p*-D_2	52	53	54	55	56	58	60	65
T K	< 0.4	< 0.4	(0.43)	0.75	0.92	1.14	1.31	1.64
% *p*-D_2	70	75	80	85	90	95	100	
T K	1.96	2.29	2.63	2.95	3.29	(3.60)	(3.96)	

Table 1j. Lattice parameter measurements for beta deuterium

References	% *p*-D_2	T K	*a* nm	Notes
Curzon and Mascall 1965	-	5	0.5069 (9)	a, b
Schuch and Mills 1966	-	0.95-1.4	0.5081 (6)	
Mucker et al. 1966	83	1.9	0.5083 (5)	c
Mucker et al. 1968	79	1.9	0.5074 (9)	
Bostanjoglu and Kleinschmidt 1967	-	2.8-4.5	0.5092 (7)	a, d
Yarnell et al. 1975	96	1.5	0.5076 (1)	
	Selected	1.5	0.5077 (6)	

Notes for Table 1j

a. Electron diffraction on thin films

b. Temperature above the beta range – not included in the average

c. Superceded by Mucker et al. 1968 – not included in the average

d. Not included in the average

The selected lattice parameter at 1.5 K leads to a molar volume of 19.70 (7) $cm^3\ mol^{-1}$ and to a density of 204.5 (7) kg m^{-3}.

Table 1k. Crystallographic properties of alpha *e*-D_2

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_0 a$	100 $\varepsilon_0 c$	100 ε_0 avr
0	0	0	0	0	0	0
1.0	0.2	0.2	0.2	< 0.001	< 0.001	< 0.001
2.0	1.5	1.5	1.5	< 0.001	< 0.001	< 0.001
3.0	5	5	5	< 0.001	< 0.001	< 0.001
4.0	12	12	12	0.001	0.001	0.001
5.0	23	23	23	0.003	0.003	0.003
6.0	43	40	42	0.006	0.006	0.006
7.0	76	70	74	0.011	0.014	0.012
8.0	123	114	120	0.022	0.022	0.022
9.0	193	178	188	0.039	0.036	0.038
10.0	289	264	281	0.061	0.059	0.061
11.0	396	353	382	0.097	0.090	0.095
12.0	526	454	502	0.142	0.129	0.137
13.0	674	552	633	0.203	0.180	0.195
13.5	758	606	707	0.239	0.209	0.229
14.0	854	672	793	0.277	0.241	0.265
14.5	947	726	873	0.325	0.275	0.308
15.0	1044	784	957	0.375	0.314	0.355
15.5	1151	848	1050	0.430	0.355	0.405
16.0	1273	914	1153	0.488	0.399	0.459
16.5	1402	986	1263	0.558	0.447	0.521
17.0	1527	1056	1370	0.630	0.498	0.586
17.5	1666	1138	1490	0.710	0.554	0.658
18.0	1824	1242	1630	0.799	0.615	0.738
18.5	1990	1370	1783	0.894	0.678	0.822
18.689	2060	1430	1850	0.932	0.703	0.855

Table 1l. Crystallographic properties of alpha *e*-D_2

T K	*a* nm	*c* nm	*c*/*a*	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.36040	0.58852	1.6330	19.934	202.1
1.0	0.36040	0.58852	1.6330	19.934	202.1
2.0	0.36040	0.58852	1.6330	19.934	202.1
3.0	0.36040	0.58853	1.6330	19.934	202.1
4.0	0.36040	0.58853	1.6330	19.934	202.1
5.0	0.36041	0.58854	1.6330	19.835	202.1
6.0	0.36042	0.58856	1.6330	19.937	202.0
7.0	0.36044	0.58860	1.6330	19.941	202.0
8.0	0.36048	0.58865	1.6330	19.946	201.9
9.0	0.36054	0.58873	1.6329	19.954	201.9
10.0	0.36062	0.58887	1.6329	19.970	201.7
11.0	0.36705	0.58905	1.6329	19.990	201.5
12.0	0.36092	0.58928	1.6328	20.016	201.3
13.0	0.36113	0.58958	1.6326	20.051	200.9
13.5	0.36126	0.58975	1.6325	20.071	200.7
14.0	0.36140	0.58994	1.6324	20.093	200.5
14.5	0.36157	0.59014	1.6322	20.118	200.2
15.0	0.36175	0.59037	1.6320	20.146	199.9
15.5	0.36195	0.59061	1.6318	20.177	199.6
16.0	0.36212	0.59087	1.6317	20.205	199.4
16.5	0.36241	0.59115	1.6312	20.247	199.0
17.0	0.36267	0.59145	1.6308	20.286	198.6
17.5	0.36296	0.59178	1.6304	20.330	198.1
18.0	0.36238	0.59214	1.6300	20.378	197.7
18.5	0.36362	0.59251	1.6295	20.429	197.2
18.689	0.36376	0.59266	1.6293	20.449	197.0

Table 1m. Crystallographic properties of alpha *n*-D_2

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avt} x 10^6 K^{-1}	100 $\varepsilon_0 a$	100 $\varepsilon_0 c$	100 ε_0 avr
0	0	0	0	0	0	0
1.0	-	-	-	0.014	0.013	0.014
2.0	-	-	-	0.022	0.024	0.023
3.0	-	-	-	0.033	0.032	0.033
4.0	83	81	82	0.042	0.041	0.041
5.0	84	80	83	0.047	0.048	0.047
6.0	98	88	95	0.058	0.056	0.058
7.0	127	110	121	0.069	0.066	0.068
8.0	173	148	165	0.083	0.078	0.082
9.0	238	204	227	0.103	0.095	0.100
10.0	325	277	309	0.131	0.119	0.127
11.0	433	361	409	0.167	0.151	0.162
12.0	561	454	525	0.217	0.192	0.209
13.0	707	552	655	0.281	0.242	0.268
13.5	785	604	725	0.317	0.270	0.301
14.0	874	659	802	0.358	0.304	0.340
14.5	967	716	883	0.403	0.338	0.381
15.0	1064	779	969	0.456	0.378	0.430
15.5	1167	847	1060	0.511	0.420	0.481
16.0	1280	919	1160	0.572	0.463	0.536
16.5	1405	990	1267	0.638	0.510	0.596
17.0	1531	1063	1375	0.714	0.563	0.664
17.5	1673	1147	1498	0.795	0.617	0.735
18.0	1826	1247	1633	0.881	0.677	0.813
18.5	1997	1359	1784	0.978	0.743	0.900
18.724	2078	1411	1856	1.024	0.773	0.940

Table 1n. Crystallographic properties of alpha *n*-D_2

T K	*a* nm	*c* nm	*c*/*a*	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.35999	0.58797	1.6333	19.870	202.7
1.0	0.36004	0.58805	1.6333	19.878	202.6
2.0	0.36007	0.58811	1.6333	19.883	202.6
3.0	0.36011	0.58816	1.6333	19.889	202.5
4.0	0.36014	0.58821	1.6333	19.894	202.5
5.0	0.36016	0.58825	1.6333	19.898	202.4
6.0	0.36020	0.58830	1.6333	19.904	202.4
7.0	0.36024	0.58836	1.6332	19.911	202.3
8.0	0.36029	0.58843	1.6332	19.918	202.2
9.0	0.36036	0.58853	1.6332	19.930	202.1
10.0	0.36046	0.58867	1.6331	19.945	202.0
11.0	0.36059	0.58886	1.6331	19.966	201.8
12.0	0.36077	0.58910	1.6329	19.994	201.5
13.0	0.36100	0.58939	1.6327	20.030	201.1
13.5	0.36113	0.58956	1.6325	20.050	200.9
14.0	0.36128	0.58976	1.6324	20.073	200.7
14.5	0.36144	0.58996	1.6323	20.098	200.4
15.0	0.36163	0.59019	1.6320	20.127	200.1
15.5	0.36183	0.59044	1.6318	20.158	199.8
16.0	0.36205	0.59069	1.6315	20.190	199.5
16.5	0.36229	0.59097	1.6312	20.227	199.1
17.0	0.36256	0.59128	1.6309	20.268	198.7
17.5	0.36283	0.59160	1.6304	20.311	198.3
18.0	0.36316	0.59195	1.6300	20.358	197.9
18.5	0.36351	0.59234	1.6295	20.411	197.4
18.724	0.36368	0.59252	1.6292	20.435	197.1

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2 HELIUM He

Natural helium contains only 1.343 (13) x 10^{-4} % of ^{3}He for the best representative sample (Meija et al. 2016) and therefore the atomic weight is only 1 x 10^{-6} less than the atomic mass of ^{4}He (Wang et al. 2017). Neither ^{3}He or ^{4}He can be obtained as a solid at ambient pressure and therefore all solid values are based on temperature and pressure parameters. The atomic mass difference leads to differences in physical properties and therefore the two isotopes are considered separately. In order to remove the confusion over the historical identification of phases they are identified as structural types hexagonal close-packed (hP2), face-centered cubic (cF4) and body-centered cubic (cI2) using the abreviations hcp, fcc and bcc respectively. Because the *c*/*a* ratio for the hcp structure is assumed to be constant at all temperatures and pressures at the ideal value of 1.6330 (even the measurements of Mao et al. 1988 at very high pressure at 300 K appear to confirm this) and because the possible effect of thermal vacancy effects was not considered then derived lattice parameters are given only as nominal values.

PART 2A. NATURAL HELIUM

Atomic weight: 4.002602 (2) (Meija 2017)

Lattice parameter measurements of Keesom and Taconis 1938 identified the hcp phase at 1.45 K and 37 bar. The fcc phase was first identified by Dugdale and Simon 1953 with the structure being established by Mills and Schuch 1961 with a lattice parameter measurement at 15.8 K and 1272 bar. Vignos and Fairbank 1961 discovered the narrow range of the bcc phase and Schuch and Mills 1962 identified the structure at 1.73 K and 29.4 bar.

2.1 Transition temperatures for ^{4}He

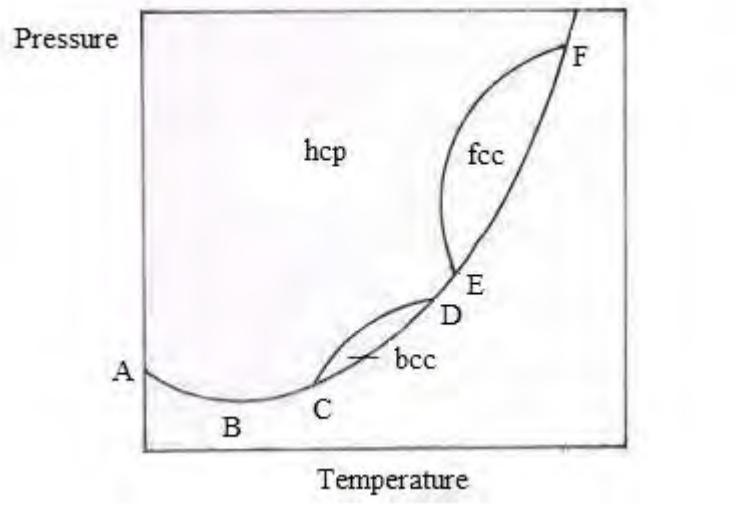


Fig 2a. ^{4}He Phase Diagram

A. Liquid-hcp transition at 0 K and 25.324 bar based on a difference of 8.15 x 10^{-3} bar between the 0 K pressure and the minimum pressure at 0.775 K (Hoffer et al. 1976)

B. Minimum on the liquid-hcp melting line at 0.775 K and 25.316 bar (Straty and Adams 1966b and Grilly 1973a)

C. Lower liquid-hcp-bcc triple point at 1.464 K and 26.362 bar (Grilly 1973a and Hoffer et al. 1976)

D. Upper liquid-hcp-bcc triple point at 1.772 K and 30.403 bar (Grilly 1973a and Hoffer et al. 1976)

E. Lower liquid-hcp-fcc triple point at 14.992 K (Franck 1980) and 1129 bar (Krause and Swenson 1976)

F. Upper liquid-hcp-fcc triple point at 285 K (Loubeyre et al. 1993) and 111.6 kbar (Vos et al. 1990)

2.2 Crystallographic properties of the ^{4}He hcp phase along the melting line: 0 K to 1.464 K [A to C]

Values are based on Grilly 1973a with additional data from Hoffer et al. 1976. In both cases all values are based on reference molar volumes for the solid and liquid respectively as determined by Grilly and Mills 1962 where the reference values used by Hoffer et al. 1976 were given by Gardner et al. 1973. Because the *c*/*a* ratio is assumed to be ideal value of 1.6330 at all temperatures and pressures then the interatomic distances *d*1 and *d*2 and the *a* axis values are all equal

Table 2a. Crystallographic properties of the hcp phase along the melting line

T K	Pressure bar	*a* nm	*c* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	25.324	0.3666	0.5987	20.982	190.8
0.1	25.324	0.3666	0.5987	20.982	190.8
0.2	25.324	0.3666	0.5987	20.982	190.8
0.3	25.324	0.3666	0.5987	20.982	190.8
0.4	25.323	0.3666	0.5987	20.982	190.8
0.5	25.322	0.3666	0.5987	20.982	190.8
0.6	25.320	0.3666	0.5987	20.982	190.8
0.7	25.318	0.3666	0.5987	20.983	190.8
0.775	25.316	0.3666	0.5987	20.983	190.8
0.8	25.316	0.3666	0.5987	20.983	190.8
0.9	25.322	0.3666	0.5987	20.983	190.8
1.0	25.346	0.3666	0.5987	20.983	190.8
1.1	25.405	0.3666	0.5986	20.979	190.8
1.2	25.523	0.3666	0.5986	20.972	190.9
1.3	25.721	0.3665	0.5985	20.959	191.0
1.4	26.049	0.3663	0.5982	20.937	191.2
1.464	26.362	0.3662	0.5980	20.916	191.4

2.3 Crystallographic properties of the ^{4}He hcp phase along the hcp – bcc transition line: 1.464 K to 1.772 K [C to D]

Values are based on Grilly 1973a which are closely confirmed by measurements of Hoffer et al. 1976.

Table 2b. Crystallographic properties of the hcp phase along the hcp - bcc transition line

T K	Pressure bar	*a* nm	*c* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1.464	26.362	0.3662	0.5980	20.916	191.4
1.50	27.289	0.3661	0.5978	20.888	191.6
1.55	27.310	0.3658	0.5974	20.847	192.0
1.60	27.925	0.3656	0.5970	20.803	192.4
1.65	28.588	0.3653	0.5965	20.757	192.8
1.70	29.298	0.3650	0.5960	20.707	193.3
1.75	30.055	0.3647	0.5955	20.654	193.8
1.772	30.403	0.3645	0.5953	20.630	194.0

2.4 Crystallographic properties of the ^{4}He bcc phase along the hcp – bcc transition line: 1.464 K to 1.772 K [C to D]

Values based on Grilly 1973a which are closely confirmed by measurements of Hoffer et al. 1976.

Table 2c. Crystallographic properties of the bcc phase along the hcp – bcc transition line

T K	Pressure bar	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1.464	26.362	0.4123	0.3571	21.102	189.6
1.50	27.289	0.4121	0.3569	21.075	189.9
1.55	27.310	0.4117	0.3566	21.016	190.5
1.60	27.925	0.4116	0.3565	20.995	190.6
1.65	28.588	0.4113	0.3562	20.953	191.0
1.70	29.298	0.4110	0.3559	20.907	191.4
1.75	30.055	0.4107	0.3557	20.859	191.9
1.772	30.403	0.4106	0.3556	20.838	192.1

$$d = \sqrt{3}a/2$$

2.5 Crystallographic properties of the ^{4}He bcc phase along the melting line: 1.464 K to 1.772 K [C to D]

Values based on Grilly 1973a which are closely confirmed by measurements of Hoffer et al. 1976. Actual lattice parameter measurements of Granfors et al. 1987 average to a lower value of 0.4101 nm at 1.73 K, compared to the value of 0.4110 nm derived from the molar volume determinations

Table 2d. Crystallographic properties of the bcc phase along the melting line

T K	Pressure bar	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1.464	26.362	0.4123	0.3571	21.102	189.6
1.50	26.564	0.4122	0.3570	21.089	189.9
1.55	26.912	0.4121	0.3569	21.067	190.5
1.60	27.361	0.4119	0.3567	21.039	190.6
1.65	27.932	0.4116	0.3565	21.004	191.0
1.70	28.697	0.4113	0.3562	20.954	191.4
1.75	29.774	0.4108	0.3558	20.881	191.9
1.772	30.403	0.4106	0.3556	20.838	192.1

$$d = \sqrt{3}a/2$$

2.6 Crystallographic properties of the ^{4}He hcp phase along the melting line: 1.772 K to 14.992 K [D to E]

The values at 1.772 K are those derived from Grilly 1973a. For the melting line 2 K to 4.5 K, Driessen et al. 1986 selected a combination of the measurements of Swenson 1953, Grilly 1973a and Krause and Swenson 1976 while for the range 4.5 to 14.992 K only the measurements of Krause and Swenson 1976 were selected. Molar volume values were calculated from the constants given by Driessen et al. 1986.

2 – 4.5 K: $P\ (bar) = 15.40793\ T^{1.580795} - 8.052367$ (2a)

4.5 – 14.992 K: $P\ (bar) = 17.452\ T^{1.54681} - 20.6$ (2b)

Table 2e. Crystallographic properties of the hcp phase along the melting line

T K	Pressure bar	*a* nm	*c* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1.772	30.403	0.3645	0.5953	20.630	194.0
2.0	38.038	0.3619	0.5909	20.180	198.3
2.5	57.533	0.3562	0.5817	19.246	208.0
3.0	79.441	0.3514	0.5738	18.475	216.6
3.5	103.58	0.3472	0.5670	17.823	224.6
4.0	129.82	0.3435	0.5609	17.260	231.9
4.5	158.15	0.3402	0.5555	16.764	238.8
5.0	189.79	0.3370	0.5504	16.303	245.5
6.0	258.33	0.3316	0.5415	15.528	257.8
7.0	333.44	0.3270	0.5340	14.894	268.7
8.0	414.67	0.3231	0.5276	14.360	278.7
9.0	501.65	0.3196	0.5219	13.901	287.9
10.0	594.09	0.3165	0.5168	13.499	296.5
11.0	691.77	0.3137	0.5122	13.144	304.5
12.0	794.35	0.3111	0.5081	12.825	312.1
13.0	901.77	0.3088	0.5042	12.538	319.2
14.0	1014	0.3066	0.5007	12.276	326.1
14.992	1129	0.3046	0.4975	12.038	332.5

2.7 Crystallographic properties of the ^{4}He fcc phase along the melting line: 14.992 K to 285 K [E to F]

The selected melting line is based on the measurements of Krause and Swenson 1976 (4-25 K), Mills et al. 1980 (14-97 K) and Vos et al. 1990 (200-460 K). The measurements of Krause and Swenson 1976 were used to 20 K while those of Mills et al. 1980 and Vos et al. 1990 were both extrapolated to 163 K in order to ensure a smooth curve:

14.992 – 20 K: $P\ (kbar) = 0.017452\ T^{1.54681} - 0.0206$ (2c)

20-163 K: $P\ (kbar) = 0.01691\ T^{1.555} - 0.008112$ (2d)

163-285 K: $P\ (kbar) = 0.016067\ T^{1.5650}$ (2e)

Above 100 K Driessen et al. 1986 relied mainly on the three data points of Loubeyre et al. 1982 whereas the later measurements of Voss et al. 1990 consisted of over 200 data points and were therefore selected in preference although the constants of Driessen et al. 1986 were used to calculate the molar volumes. No change in the molar volume at the lower transition temperature was detected by Franck 1980 while Vos et al. 1990 could not detect the upper transition temperature which could also be considered as proving that the molar volume change at this transition was also negligible. In the fcc phase region pressure values of Grilly and Mills 1959 (17.158-30.770 K) trended from 1 bar low to 10 bar high while solid molar volume values trend from 0.26% high to 0.65% low.

Table 2f. Crystallographic properties of the fcc phase along the melting line

T K	Pressure kbar	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
14.992	1.129	0.4308	0.3046	12.038	332.5
15	1.130	0.4308	0.3046	12.036	332.6
20	1.775	0.4190	0.2963	11.074	361.4
25	2.515	0.4100	0.2899	10.374	385.8
30	3.342	0.4026	0.2847	9.823	407.5
35	4.250	0.3961	0.2801	9.355	427.9
40	5.232	0.3903	0.2760	8.950	447.2
45	6.285	0.3851	0.2723	8.597	465.6
50	7.406	0.3803	0.2690	8.284	483.2
60	9.836	0.3721	0.2631	7.755	516.1
70	12.50	0.3650	0.2581	7.321	546.8
80	15.39	0.3588	0.2537	6.956	575.4
90	18.48	0.3534	0.2499	6.644	602.4
100	21.78	0.3485	0.2464	6.373	628.0
110	25.26	0.3441	0.2433	6.135	652.5
120	28.92	0.3401	0.2405	5.923	675.8
130	32.75	0.3364	0.2379	5.733	698.2
140	36.75	0.3330	0.2355	5.561	719.8
150	40.91	0.3299	0.2333	5.404	740.6
160	45.23	0.3269	0.2312	5.261	760.7
170	49.73	0.3242	0.2292	5.129	780.4
180	54.38	0.3216	0.2274	5.007	799.4
190	59.18	0.3191	0.2257	4.893	818.0
200	64.13	0.3168	0.2240	4.787	836.1
210	69.22	0.3146	0.2225	4.688	853.7
220	74.44	0.3125	0.2210	4.596	870.0
230	79.81	0.3105	0.2196	4.509	887.8
240	85.30	0.3086	0.2182	4.426	904.2
250	90.93	0.3068	0.2170	4.349	920.3
260	96.69	0.3051	0.2157	4.276	936.1
270	102.5	0.3034	0.2146	4.206	951.6
280	108.6	0.3018	0.2134	4.140	966.6
285	111.6	0.3010	0.2129	4.108	974.3

$$d = a/\sqrt{2}$$

2.8 Crystallographic properties of the ^{4}He hcp - fcc phases along the hcp – fcc transition line: 14.992 K to 285 K [E to F]

The behavior of the transition line is only well established up to 9 kbar. Franck 1980 suggested a slope of 550 bar K^{-1} above 15.8 K and up to 3.9 kbar while Franck and Daniels 1981 measured 622 bar K^{-1} over the equally narrow range 4 to 9 kbar. Lattice parameter measurements of Mills and Schuch 1974 defined the boundary line up to 4.5 kbar. Dugdale and Simon 1953 suggested a molar volume change at the lower transition point of 4×10^{-4} $cm^3\ mol^{-1}$ whereas Franck 1980 could not detect a volume change at this temperature but did determine a constant value of 3.3×10^{-4} $cm^3\ mol^{-1}$ above 15.8 K. Lattice parameter measurements by Loubeyre et al. 1993 in the region of 250 K

constrained the general shape of the transition curve confirming that it was a loop and showed it to be consistent with the selected upper transition temperature. This was further confirmed by high pressure lattice parameter measurements of Mao et al. 1988 at 300 K and Loubeyre et al. 1993 at 304 K which were all consistent with the original hcp phase. These measurements as well as the smooth melting curve obtained by Vos et al. 1990 rule out a possible high temperature transition of the fcc phase to a bcc phase as proposed in particular by Besson et al. 1984.

PART 2B. HELIUM 3

Atomic mass of ^{3}He: 3.01602932265 (22) (Wang et al. 2017)

Mills and Grilly 1958 reported that a solid-solid transition intersected the melting curve at 3.15 K and 138 bar. Lattice parameter measurements by Schuch et al. 1958 at 1.9 K and 98 bar identified the lower pressure phase to be body-centered cubic (bcc) and measurements at 3.3 K and 179 bar identified the higher pressure phase to be hexagonal close packed (hcp). Mills and Grilly 1958 had therefore identified the liquid – bcc – hcp triple point. Schuch and Mills 1961 identified a face-centered cubic (fcc) phase at 18.76 K and 1712 bar while Franck 1961 first identified the liquid – hcp – fcc triple point.

2.9 Transition temperatures for ^{3}He

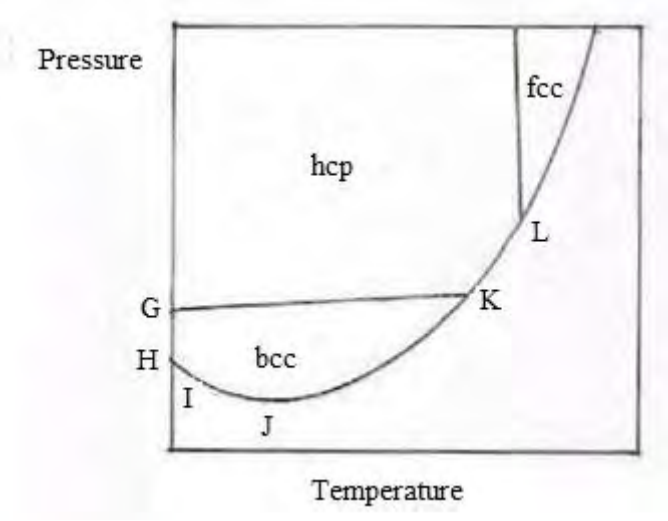


Fig.2b. ^{3}He phase diagram

G. bcc - hcp transition at 0 K and 106.4 bar obtained by extrapolating the transition curve of Straty and Adams 1966a

H. Liquid – bcc melting line at 0 K and 34.4674 bar as the temperature independent term on the Provisional Low Temperature Scale PLTS-2000 (Rusby et al. 2002)

I. Néel transition temperature at 0.902 mK and 34.3934 bar as a fixed point on PLTS-2000 (Rusby et al. 2002)

J. Minimum on the liquid-bcc melting line at 0.31524 K and 29.3113 bar as a fixed point on PLTS-2000 (Rusby et al. 2002)

K. Liquid-bcc-hcp triple point at 3.138 K and 137.23 bar (Straty and Adams 1966a)

L. Liquid-hcp-fcc triple point at 17.65 K and 1560 bar (Ryschkewitsch et al. 1982)

2.10 Crystallographic properties of the ^{3}He bcc phase along the melting line: 0 K to 3.138 K [H to K]

The melting line is based on the Provisional Low Temperature Scale PLTS-2000 (Rusby et al. 2002) to 0.9 K, on the measurements of Grilly 1971, 1973b over the range 1.0 to 1.6 K and those of Grilly and Mills 1959 from 1.6 to 3.1 K. All values at the triple point 3.138 K are those determined by Straty and Adams 1966a. The melting line determined by Grilly and Mills 1959 extrapolates to a pressure at the triple point only 0.06 bar lower than the selected value. Although the melting line determined by Grilly 1971, 1973b is 0.13 bar higher than the selected PLTS-2000 value at 0.02 K the molar volume values of Grilly 1971, 1973b are selected to 1.8 K because they are closely confirmed by corrected values of Scribner et al. 1969. The molar volume at 0 K was estimated by extrapolating values from 0.02 to 0.20 K. Above 1.8 K and up to 3.1 K the molar volume values of Grilly and Mills 1959 were accepted.

Table 2g. Crystallographic properties of the bcc phase along the melting line

T K	Pressure bar	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	34.467	0.4316	0.3738	24.206	124.6
0.02	33.640	0.4322	0.3743	24.312	124.1
0.04	32.924	0.4328	0.3748	24.407	123.6
0.06	32.302	0.4333	0.3752	24.492	123.1
0.08	31.762	0.4337	0.3756	24.567	122.8
0.10	31.295	0.4341	0.3760	24.634	122.4
0.12	30.893	0.4345	0.3762	24.692	122.1
0.14	30.548	0.4347	0.3765	24.742	121.9
0.16	30.255	0.4350	0.3767	24.787	121.7
0.18	30.009	0.4352	0.3769	24.823	121.5
0.20	29.805	0.4354	0.3771	24.857	121.3
0.25	29.461	0.4357	0.3774	24.913	121.1
0.30	29.319	0.4359	0.3775	24.937	120.9
0.31524	29.311	0.4359	0.3775	24.939	120.9
0.35	29.350	0.4359	0.3775	24.934	121.0
0.40	29.533	0.4357	0.3773	24.907	121.1
0.45	29.852	0.4354	0.3771	24.859	121.3
0.50	30.296	0.4350	0.3768	24.792	121.7
0.60	31.519	0.4340	0.3759	24.618	122.5
0.70	33.192	0.4347	0.3747	24.397	123.6
0.80	35.120	0.4313	0.3735	24.152	124.9
0.90	37.414	0.4297	0.3721	23.886	126.3
1.00	40.10	0.4279	0.3706	23.599	127.8

Table 2h. Crystallographic properties of the bcc phase along the melting line

T K	Pressure bar	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1.10	42.94	0.4262	0.3691	23.316	129.4
1.20	46.04	0.4245	0.3676	23.030	131.0
1.30	49.28	0.4228	0.3661	22.756	132.5
1.40	52.75	0.4211	0.3647	22.487	134.1
1.50	56.46	0.4195	0.3633	22.223	135.7
1.60	60.33	0.4178	0.3619	21.967	137.3
1.70	64.33	0.4163	0.3605	21.721	138.9
1.80	68.51	0.4148	0.3592	21.486	140.4
1.90	72.86	0.4133	0.3579	21.256	141.9
2.00	77.36	0.4118	0.3567	21.031	143.4
2.10	82.01	0.4104	0.3554	20.813	144.9
2.20	86.81	0.4090	0.3542	20.603	146.4
2.30	91.73	0.4077	0.3530	20.400	147.8
2.40	96.79	0.4064	0.3519	20.204	149.3
2.50	101.96	0.4051	0.3508	20.015	150.7
2.60	107.20	0.4039	0.3497	19.833	152.1
2.70	112.62	0.4027	0.3487	19.658	153.4
2.80	118.09	0.4015	0.3477	19.489	154.8
2.90	123.65	0.4004	0.3467	19.327	156.1
3.00	129.28	0.3993	0.3458	19.171	157.3
3.10	134.99	0.3983	0.3449	19.020	158.6
3.138	137.23	0.3977	0.3444	18.945	159.2

$$d = \sqrt{3}a/2$$

2.11 Crystallographic properties of the ^{3}He hcp phase along the hcp – bcc transition line: 0 K to 3.138 K [G to K]

Selected values are based on Straty and Adams 1966a (1-3.138 K). The transition pressure was extrapolated to 106.4 bar at 0 K while molar volume values from 1.0 to 1.6 K were fitted to: $V_m\ (cm^3\ mol^{-1}) = 19.7983 - 0.05274\ T^2$ and extrapolated below 1 K. Transition pressures given by Grilly and Mills 1959 (1.846-3.148 K) average 1.2% high except at the triple point where the difference is only 0.1% high.

Table 2i. Crystallographic properties of the hcp phase along the hcp – bcc transition line

T K	Pressure bar	*a* nm	*c* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	106.4	0.3596	0.5872	19.798	152.3
0.2	106.5	0.3596	0.5872	19.796	152.4
0.4	106.5	0.3595	0.5871	19.790	152.4
0.6	106.6	0.3595	0.5870	19.779	152.5
0.8	106.7	0.3594	0.5869	19.765	152.6
1.0	106.8	0.3593	0.5867	19.745	152.7
1.2	107.1	0.3591	0.5864	19.723	152.9
1.4	107.6	0.3590	0.5862	19.695	153.1
1.6	108.5	0.3588	0.5859	19.663	153.4
1.8	109.8	0.3585	0.5854	19.617	153.7
2.0	111.9	0.3581	0.5848	19.553	154.2
2.2	114.7	0.3576	0.5839	19.467	154.9
2.4	118.1	0.3569	0.5828	19.355	155.8
2.6	122.4	0.3560	0.5814	19.220	156.9
2.8	127.4	0.3552	0.5800	19.078	158.1
3.0	133.0	0.3542	0.5785	18.928	159.3
3.138	137.23	0.3536	0.5774	18.826	160.2

2.12 Crystallographic properties of the ^{3}He bcc phase along the hcp – bcc transition line: 0 K to 3.138 K [G to K]

Selected values are based on Straty and Adams 1966a (1-3.138 K) with the modifications as given above. The hcp – bcc molar volume differences from 1.4 to 2.0 K were fitted to: $\Delta V_m\ (cm^3\ mol^{-1}) = 0.0785 + 0.01\ T$ and based on the selected molar volumes of the hcp phase allows extrapolation for the bcc phase below the experimental limit of 1.4 K.

Table 2j. Crystallographic properties of the bcc phase along the hcp – bcc transition line

T K	Pressure bar	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	106.4	0.4042	0.3500	19.877	151.7
0.2	106.5	0.4042	0.3500	19.877	151.7
0.4	106.5	0.4041	0.3500	19.872	151.8
0.6	106.6	0.4041	0.3499	19.864	151.8
0.8	106.7	0.4040	0.3499	19.851	151.9
1.0	106.8	0.4039	0.3498	19.834	152.1
1.2	107.1	0.4037	0.3496	19.813	152.2
1.4	107.6	0.4035	0.3495	19.787	152.4
1.6	108.5	0.4033	0.3493	19.738	152.6
1.8	109.8	0.4030	0.3490	19.714	153.0
2.0	111.9	0.4026	0.3487	19.651	153.5
2.2	114.7	0.4021	0.3482	19.572	154.1
2.4	118.1	0.4014	0.3476	19.473	154.9

Table 2k. Crystallographic properties of the bcc phase along the hcp – bcc transition line (Continued)

T K	Pressure bar	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
2.6	122.4	0.4005	0.3469	19.347	155.9
2.8	127.4	0.3995	0.3460	19.205	157.0
3.0	133.0	0.3985	0.3451	19.053	158.3
3.138	137.23	0.3977	0.3444	18.945	159.2

$$d = \sqrt{3}a/2$$

2.13 Crystallographic properties of the ^{3}He hcp phase along the melting line: 3.138 K to 17.65 K [K to L]

The values at the lower triple point 3.138 K are those of Straty and Adams 1966a while at 3.5 K and above values are based on the equation of state constants given by Driessen 1982, except at the upper transition temperature at 17.65 K where values were adjusted to the selected transition pressure of 1560 bar instead of the value of 1557 bar derived from the selected values of Driessen 1982 which are based on the measurements of Grilly and Mills 1959 (3.252 – 30.184 K) and the T = 0 pressure – volume values of Stewart 1963.

Table 2l. Crystallographic properties of the hcp phase along the melting line

T K	Pressure bar	*a* nm	*c* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
3.138	137.23	0.3536	0.5774	18.826	160.2
3.5	156.6	0.3506	0.5726	18.362	164.3
4.0	186.0	0.3470	0.5666	17.789	169.5
4.5	218.0	0.3436	0.5611	17.271	174.6
5.0	251.2	0.3405	0.5561	16.818	179.2
6.0	323.4	0.3351	0.5473	16.030	188.1
7.0	401.9	0.3305	0.5397	15.376	196.2
8.0	486.6	0.3265	0.5331	14.816	203.6
9.0	576.4	0.3229	0.5273	14.334	210.4
10.0	672.2	0.3197	0.5220	13.908	216.9
11.0	766.1	0.3169	0.5175	13.556	222.5
12.0	878.4	0.3141	0.5128	13.190	228.7
13.0	988.0	0.3116	0.5089	12.885	234.1
14.0	1105	0.3093	0.5051	12.600	239.4
15.0	1223	0.3072	0.5017	12.345	244.3
16.0	1346	0.3052	0.4985	12.111	249.0
17.0	1472	0.3034	0.4955	11.894	253.6
17.65	1560	0.3022	0.4935	11.755	256.6

2.14 Crystallographic properties of the ^{3}He fcc phase along the melting line: 17.65 - 110 K [L to Experimental Limit]

All values are calculated from the equation of state constants given by Driessen 1982 which are partially based on the measurements of Grilly and Mills 1959 (3.252 – 30.184 K) but are extended to a molar volume of 6.00 cm^3 mol^{-1} at 119.20 K. Dugdale and Franck 1964 determined the hcp-fcc molar volume difference to be only 1.4 $x10^{-4}$ cm^3 mol^{-1} at the triple point.

Table 2m. Crystallographic properties of the fcc phase along the melting line

T K	Pressure kbar	*a* nm	*d* nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
17.65	1.560	0.4274	0.3022	11.755	256.6
18	1.604	0.4266	0.3017	11.690	258.0
19	1.739	0.4243	0.3000	11.500	262.3
20	1.878	0.4221	0.2985	11.322	266.4
25	2.625	0.4126	0.2918	10.576	285.2
30	3.457	0.4051	0.2864	10.006	301.4
35	4.356	0.3986	0.2819	9.535	316.3
40	5.327	0.3929	0.2778	9.131	330.3
45	6.372	0.3877	0.2742	8.776	343.7
50	7.467	0.3831	0.2709	8.466	356.3
60	9.841	0.3749	0.2651	7.931	380.3
70	12.429	0.3677	0.2600	7.485	402.9
80	15.214	0.3614	0.2555	7.105	424.5
90	18.161	0.3557	0.2515	6.776	445.1
100	21.330	0.3504	0.2478	6.480	465.5
110	24.653	0.3456	0.2444	6.216	485.2

$$d = a/\sqrt{2}$$

2.15 Crystallographic properties of the ^{3}He hcp - fcc phases along the hcp – fcc transition line: 17.65 K to 110 K [L to Experimental Limit]

There appears to be little data available with regards to this transition but Ryschkewitsch et al. 1982 determined a slope of 617 (22) bar K^{-1} in the narrow range 2.5 to 6.3 kbar so that from the triple point to this pressure the boundary can be represented by the equation: P (kbar) = 1.560 + 0.617 (T – 17.65). Within this narrow limit there is no evidence that the transition involves the same type of boundary loop as found for ^{4}He.

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3 LITHIUM Li

PART 3A. NATURAL LITHIUM AND LITHIUM 7

Atomic Weight of Natural Lithium: 6.938 to 6.997 (Meija 2017)
Select 2007 value 6.941 (2) (Wieser and Berglund 2009)

Atomic mass of ^{7}Li: 7.016003437 (5) (Wang et al. 2017)

Allotropy: Alpha: Hexagonal close-packed (hP2)
Beta: Body-centered cubic (cI2)

The transition is martensitic. Alcock et al. 1994 selected M_S = 70 (5) K for the direct transformation beta to alpha; A_S = 95 (5) K for the start of the reverse transformation and 165 (10) K for the end of the reverse transformation and an "equilibrium" transition temperature of 125 K. The beta phase is easily retained to the lowest temperatures. Alcock et al. 1994 selected a melting point of 453.65 (5) K.

3.1 Beta Phase: Body-centered cubic (hP2): 125 K to 453.65 K.

Beta Phase – Low Temperature

Precision measurement of the lattice parameters of both ^{6}Li and ^{7}Li by Covington and Montomery 1957 showed by interpolation that the lattice parameters of natural lithium and ^{7}Li agree to within 1 x 10^{-5} nm and therefore are assumed to be the same.

Thermal expansion coefficients of Pearson 1954 (80-300 K) were selected to represent the low temperature data and were fitted to Equation A using the specific heat values selected by Alcock et al. 1994:

$$\alpha\ (K^{-1}) = C_p\ (1.56379 \times 10^{-6} + 9.74577 \times 10^{-10}\ T + 1.13799 \times 10^{-5} / T) \qquad (3a)$$

Because of a marked scatter in experimental values below 80 K the above equation was extrapolated to give metastable values in the region below this temperature. The selected value of the thermal expansion coefficient at 293.15 K shows excellent agreement with the values of 47 x 10^{-6} K^{-1} calculated from a fit to the lattice parameters of Owen and Williams 1954 and 46 (1) x 10^{-6} K^{-1} determined by Lynch and Edwards 1970

On the basis 100Δε length change values derived from the smooth lattice parameter measurements of Owen and Williams 1954 (79-294 K) show an average bias of 0.006 low while a single data point of Lonsdale and Hume-Rothery 1945 at 90 K agrees to within 0.002. Thermal expansion coefficients determined by Simon and Bergmann 1930 (95-270 K) when converted to length change values show an average bias of only 0.004 low. Dilatometric measurements of Laquer 1952 (0-300 K) initially averaged 0.022 high below 80 K but above 120 K agreed closely with the selected values. However, the values of Snyder et al. 1964 (0-275 K) show poor agreement being on average 0.11 high

below 80 K and then trend to agree with selected values. Volume ratios of Anderson and Swenson 1983 (4-350 K) when corrected to length change values average 0.038 low below 82 K. Deviations between the low temperature selected values and other published values (Δa nm) are shown in Table 3a:

Table 3a. A comparison of lattice parameter values for beta lithium

References	T K	*a* nm	Δa nm
Pearson 1954	4	0.3472_5	– 0.0008
Barrett 1956	78	0.3491	+ 0.0009
Kogan and Khotkevic 1962	20	0.3480	– 0.0001
	78	0.3483	+ 0.0001
Beg and Nielson 1976	110	0.3490	+ 0.0005
	150	0.3497	+ 0.0008
McCarthy et al. 1980	4.2	0.3480	– 0.0001
	78	0.3482	– 0.0001
Chernyshov et al. 1983	60	0.3475	– 0.0007
Berliner and Werner 1986b	20	0.34769	– 0.0004
Smith 1987	78	0.3483	+ 0.0001
Berliner et al. 1989	20	0.347851	– 0.0002

Table 3b. Lattice parameter of beta lithium at 293.15 K

References	Original Temperature K	*a* nm	Notes
Perlitz and Aruja 1940	293	0.35092	
Lonsdale and Hume-Rothery 1945	293	0.35096	
Pearson 1954	293	0.35089	
Owen and Williams 1954	293	0.35098	
Covington and Montgomery 1957	293	0.35095	a
Keller et al. 1958	298	0.35094	
Vogel and Kempter 1959	298	0.35089	
Nadler and Kempter 1959	298	0.35094	
Feder 1970	293	0.35093	
Beg and Nielson 1976	293	0.35107	b
	Selected	0.35093 (3)	

Notes for Table 3b

a. Based on an interpolation assuming 7.4% ^{6}Li and 92.6% ^{7}Li

b. Not included in the average

At 293.15 K: Density: nat Li 533.4 (2) kg m^{-3} Density: ^{7}Li 539.1 (1) kg m^{-3}
Molar volume: 13.013 (3) cm^{3} mol^{-1}.

Beta Phase – High Temperature

The lattice parameter measurements of Feder 1970 (310-450 K) were selected. These values were only shown graphically with actual data points as length change values being

given by Touloukian et al. 1975 which were fitted to the following equation to represent the thermal expansion from 293.15 K to the melting point:

$$\varepsilon_T = -5.25783 \times 10^{-5}\, T + 4.05070 \times 10^{-7}\, T^2 - 7.54158 \times 10^{-10}\, T^3 + 5.56475 \times 10^{-13}\, T^4 - 4.50774 \times 10^{-3} \quad (3b)$$

3.2 Alpha Phase: Hexagonal close-packed (hP2): 0 K to 125 K.

Using X-ray diffraction Barrett 1956 initially identified the structure as being hexagonal close-packed and this was confirmed by Chernyshov et al. 1983. However, neutron diffraction measurements of Berliner and Werner 1986a, 1986b, Smith 1987 and Berliner et al. 1989 all suggested that the structure was in fact rhombohedral, the same as alpha-samarium, the so called *9R* structure. The same structure was found for the alpha phase of sodium. However, Schwarz et al. 1992, using diffuse-neutron-scattering, found for sodium that the low temperature phase consisted of a mixture of both the hexagonal close-packed and the *9R* structures contaminated with the high temperature body-centered cubic phase. Because the presence of the *9R* structure did not appear to be due to stacking faults, Sankaran et al. 1992 suggested that the hexagonal close-packed structure was the stable phase but that the transition from the body-centered cubic phase initially required the production of an intermediate rhombohedral distortion which, because of the sluggish nature of the transition, would be retained. Based on these suggestions the structure for both alpha lithium and alpha sodium are assumed to ideally be hexagonal close-packed.

In order to obtain a set of reference values for the alpha phase the molar volume difference from the beta phase is determined and assumed to be constant between 0 and 125 K. The *c*/*a* ratio for the hexagonal structure is then also assumed to be constant at the ideal value of 1.6330 so that the *a*-axis lattice parameter is equal to both of the interatomic distances *d*1 and *d*2. Vaks et al. 1989 determined the initial slope of the pressure transition curve at $dT/dP = +0.015$ K MPa^{-1} at a temperature between M_s and A_s. If the actual temperature is therefore assumed to be about 80 K and the enthalpy of transition of 54 J/mol determined by Alcock et al. 1994 at the actual equilibrium temperature is retained then from the Clausius-Clapeyron equation the molar volume difference $V_\alpha - V_\beta = -0.010$ cm^3 mol^{-1} which is selected at all temperatures up to the equilibrium transition at 125 K. This molar volume difference can be compared with other determinations where the molar volume values for the *9R* structure have been reduced by 4.5. In comparison with the values given in Table 3d, a combination of the lattice parameter values at 20 K for the *9R* structure as determined by Berliner and Werner 1986a, 1986b and Berliner et al. 1989, when reduced to an equivalent hexagonal cell, agrees with the selected value to within 0.0001 nm along the *a*-axis and to 0.0004 nm low along the *c*-axis. The similar measurements of Smith 1987 at 78 K agree within the selected values for both axes to within 0.0001 nm. This would appear to give some credibility to the procedure used.

Table 3c. Molar volume differences between the alpha and beta phases

Authors	V_α $cm^3\ mol^{-1}$	V_β $cm^3\ mol^{-1}$	$V_\alpha - V_\beta$ $cm^3\ mol^{-1}$	Notes
Barrett 1956	12.81_1	12.85_4	– 0.043	a
Basinski and Verdini 1959	-	-	– 0.009	
Chernyshov et al. 1983	12.63_5	12.59_2	+ 0.043	a
Berliner and Werner 1986b	12.65_6	12.64_9	+ 0.007	b
Smith 1987	12.72_3	12.71_9	+ 0.004	b
Berliner et al. 1989	12.67_4	12.68_6	– 0.012	b
Vaks et al. 1989	-	-	– 0.010	

Notes for Table 3c

a. V_α for hexagonal close-packed structure.

b. V_α for *9R* structure reduced.

3.3 Bulk properties of lithium

Dilatometric measurements of Feder 1970 (310-450 K) were only shown graphically with actual data points given as length change values by Touloukian et al. 1975. From a combination with the lattice parameter measurements Feder estimated a net defect concentration of $\Delta N/N_0 = 4.41 \times 10^{-4}$ at the melting point, an enthalpy of thermal vacancy formation $H_V = 0.34$ (4) eV and an entropy of thermal vacancy formation $S_V/k = 0.9$ (8). However, these values are incompatible and can only be reconciled if $S_V/k = 0.97$ which is used to calculate the values in Table 3g.

Table 3d. Crystallographic properties of alpha lithium

T K	100 ε_T	*a* nm	*c* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$ nat Li	Density $kg\ m^{-3}$ ^7Li
0	- 0.835	0.31003	0.50628	12.690	547.0	552.9
5	- 0.835	0.31003	0.50628	12.690	547.0	552.9
10	- 0.835	0.31003	0.50628	12.690	547.0	552.9
15	- 0.835	0.31003	0.50628	12.690	547.0	552.9
20	- 0.835	0.31003	0.50628	12.690	547.0	552.9
25	- 0.835	0.31003	0.50628	12.690	547.0	552.9
30	- 0.834	0.31004	0.50629	12.690	546.9	552.9
40	- 0.830	0.31005	0.50630	12.692	546.9	552.8
50	- 0.825	0.31007	0.50633	12.694	546.8	552.7
60	- 0.815	0.31009	0.50638	12.697	546.7	552.6
70	- 0.798	0.31013	0.50644	12.702	546.5	552.3
80	- 0.788	0.31018	0.50652	12.708	546.2	552.1
90	-0.769	0.31024	0.50661	12.715	545.9	551.8
100	-0.746	0.31031	0.50673	12.724	545.5	551.4
110	- 0.723	0.31038	0.50685	12.733	545.1	551.0
120	- 0.697	0.31046	0.50699	12.743	544.7	550.6
125	- 0.684	0.31051	0.50705	12.748	544.5	550.4

Table 3e. Low temperature crystallographic properties of beta lithium

T K	$\alpha \times 10^6$ K^{-1}	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density kg m^{-3} nat Li	Density kg m^{-3} ^{7}Li
0	0	- 0.810	0.34809	0.30145	12.700	546.6	552.5
5	0.06	- 0.810	0.34809	0.30145	12.700	564.6	552.5
10	0.17	- 0.810	0.34809	0.30145	12.700	546.6	552.5
15	0.41	- 0.810	0.34809	0.30145	12.700	546.6	552.5
20	0.84	- 0.809	0.34809	0.30145	12.700	546.5	552.5
25	1.47	- 0.809	0.34809	0.30146	12.700	546.5	552.4
30	2.34	- 0.808	0.34809	0.30146	12.700	546.5	552.4
40	4.64	- 0.804	0.34811	0.30147	12.702	546.5	552.4
50	7.54	- 0.799	0.34813	0.30149	12.704	546.4	552.3
60	10.72	- 0.789	0.34816	0.30151	12.707	546.2	552.1
70	14.01	- 0.772	0.34820	0.30155	12.712	545.9	551.9
80	17.25	- 0.762	0.34826	0.30160	12.718	545.8	551.7
90	20.31	- 0.743	0.34832	0.30166	12.725	545.5	551.3
100	23.05	- 0.721	0.34840	0.30172	12.734	545.1	551.0
110	25.33	- 0.697	0.34848	0.30179	12.743	544.7	550.6
120	27.62	- 0.671	0.34857	0.30187	12.753	544.3	550.2
125	28.59	- 0.657	0.34862	0.30192	12.758	544.0	549.9
130	29.56	- 0.643	0.34867	0.30196	12.764	543.8	549.7
140	31.30	- 0.612	0.34875	0.30205	12.775	543.3	549.2
150	32.88	- 0.581	0.34889	0.30215	12.788	542.8	548.6
160	34.31	- 0.547	0.34901	0.30225	12.801	542.2	548.1
170	35.64	- 0.512	0.34913	0.30236	12.814	541.7	547.5
180	36.87	- 0.476	0.34926	0.30247	12.828	541.1	546.9
190	38.01	- 0.439	0.34939	0.30258	12.843	540.5	546.3
200	39.07	- 0.401	0.34952	0.30270	12.857	539.9	545.7
210	40.06	- 0.361	0.34966	0.30282	12.873	539.2	545.0
220	41.00	- 0.321	0.34980	0.30294	12.888	538.6	544.4
230	41.87	- 0.279	0.34995	0.30306	12.904	537.9	543.7
240	42.70	- 0.237	0.35010	0.30319	12.921	537.2	543.0
250	43.50	- 0.194	0.35025	0.30332	12.937	536.5	542.3
260	44.25	- 0.150	0.35040	0.30346	12.954	535.8	541.6
270	44.97	- 0.106	0.35056	0.30359	12.972	535.1	540.9
280	45.67	- 0.061	0.35072	0.30373	12.990	534.4	540.1
290	46.35	- 0.015	0.35088	0.30387	13.007	533.6	539.4
293.15	46.56	0	0.35093	0.30391	13.013	533.4	539.1

$$d = \sqrt{3}a/2$$

Table 3f. High temperature crystallographic properties of beta lithium

T K	$\alpha \times 10^6$ K^{-1}	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density kg m^{-3} nat Li	Density kg m^{-3} ^7Li
293.15	46.56	0	0.35093	0.30391	13.013	533.4	539.1
300	46.93	0.032	0.35104	0.30401	13.026	532.9	538.6
310	47.42	0.079	0.35121	0.30416	13.044	532.1	537.9
320	47.87	0.127	0.35138	0.30430	13.063	531.4	537.1
330	48.29	0.175	0.35154	0.30445	13.082	530.6	536.3
340	48.71	0.224	0.35171	0.30459	13.101	529.8	535.5
350	49.12	0.273	0.35189	0.30474	13.120	529.0	534.8
360	49.55	0.322	0.35206	0.30489	13.139	528.3	534.0
370	50.00	0.372	0.35224	0.30505	13.159	527.5	533.2
380	50.50	0.423	0.35241	0.30520	13.179	526.7	532.4
390	51.05	0.474	035259	0.30535	13.199	525.9	531.6
400	51.67	0.525	0.35277	0.30551	13.219	525.1	530.7
410	52.37	0.577	0.35296	0.30567	13.240	524.2	529.9
420	53.16	0.631	0.35314	0.30583	13.261	523.4	529.1
430	54.06	0.684	0.35333	0.30599	13.282	522.6	528.2
440	55.07	0.739	0.35352	0.30616	13.300	521.7	527.4
450	56.22	0.796	0.35342	0.30633	13.326	520.9	526.5
453.65	56.68	0.816	0.35379	0.30640	13.334	520.5	526.2

$$d = \sqrt{3}a/2$$

Table 3g. Bulk properties of lithium

$3\ (\varepsilon_T L - \varepsilon_T a) = \exp(0.97 - 3945.5 / T)$ $\quad \alpha_L - \alpha_a = (1315.2 / T^2) \exp(0.97 - 3945.5 / T)$

T K	$\alpha \times 10^6$ K^{-1}	100 ε_T	Molar Volume $cm^3\ mol^{-1}$	Density kg m^{-3} nat Li	Density kg m^{-3} ^7Li
320	47.87	0.127	13.063	531.4	537.1
330	48.50	0.176	13.082	530.6	536.3
340	48.98	0.224	13.101	529.8	535.5
350	49.48	0.274	13.120	529.0	534.7
360	50.01	0.324	13.140	528.2	533.9
370	50.60	0.374	13.160	527.4	533.1
380	51.24	0.425	13.180	526.6	532.7
390	51.97	0.477	13.200	525.8	531.5
400	52.80	0.530	13.221	525.0	530.7
410	53.73	0.583	13.242	524.2	529.8
420	54.79	0.638	13.264	523.3	529.0
430	56.00	0.694	12.286	522.4	528.1
440	57.36	0.751	13.308	521.6	527.2
450	58.89	0.809	13.332	520.6	526.3
453.65	59.49	0.831	13.340	520.3	525.9

This Table is assumed to be identical to Table 3f below 320 K.

PART 3B. LITHIUM 6

Atomic mass of ^{6}Li: 6.0151228874 (15) (Wang et al. 2017)

Covington and Montgomery 1957 determined the lattice parameter to be 0.35109 (9) nm at 293 K and this value is selected leading to a derived density 461.6 (4) kg m^{-3} and derived molar volume 13.031 (10) cm^3 mol^{-1}. Crystallographic properties are summarized in Table 3g. Other determinations of the lattice parameter are scarce and appear to consist of three relatively low accuracy measurements by Kogan and Khotkovic 1962 at 20, 78 and 300 K. In spite of this, Mel'nikova et al. 1987 and Mel'nikova and Mozgovoi 1988 estimated thermal expansion values over the whole temperature range. Magomedov 2009 used a theoretical approach to calculate thermal expansion coefficients for both ^{6}Li and ^{7}Li and showed the results graphically.

Table 3h. Crystallographic properties of isotope ^{6}Li

T K	*a* nm	*d* nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
293.15	0.35109	0.30405	13.031	461.6

$$d = \sqrt{3}a/2$$

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4 BERYLLIUM Be

Atomic weight: 9.0121831 (5) (Meija 2017)

Allotropy: Alpha phase: Hexagonal close–packed (hP2)
Beta phase: Body-centred cubic (cI2)

Arblaster 2016 selected values of 1543 (5) K for the alpha-beta transition temperature and 1560 (5) K for the melting point.

4.1 Alpha Phase: Hexagonal close-packed (hP2): 0 K to 1543 K.

Anisotropic dilatometric measurements on single crystals by Erfling 1939 (57-293 K) were selected because on the basis $100\Delta\varepsilon$ the average derived length change values agree to within 0.001 with values obtained from the dilatometric measurements of Swenson 1991 (4-300 K). In combination with enthalpy values selected by Arblaster 2016 the selected values were fitted to Equation B:

$$\ln (L_a) = (H_T - H_0) (8.55478 \times 10^{-7} - 2.82387 \times 10^{-10} T + 4.64307 \times 10^{-7} / T) - 1.44481 \times 10^{-3} \quad (4a)$$

$$\ln (L_c) = (H_T - H_0) (5.76771 \times 10^{-7} + 1.22738 \times 10^{-11} T - 1.69264 \times 10^{-5} / T) - 2.75226 \times 10^{-4} \quad (4b)$$

These equations were extrapolated to 0 K. On the basis $100\Delta\varepsilon$ anisotropic dilatometric measurements of Meyerhoff and Smith 1962 (77-273 K) trend from 0.023 high along the *a* axis and 0.012 high along the *c* axis at the lowest temperatures to then converge with the selected values. Lattice parameter values of Finkel and Papirov 1968 (79-299 K) were only shown graphically with derived length change values being given by Touloukian et al. 1975. For the 99.9% purer sample these trend along the *a* axis from initially 0.023 low at 80 K but for the *c* axis, although initially just lower, they show a maximum deviation of 0.012 high in the region of 180-190 K.

In the high temperature region there is a major problem in that while the *a* axis expansion appears to be unaffected by sample quality, the *c* axis is highly affected and there is a major increase in the thermal expansion coefficient. This effect was demonstrated by Amonenko et al. 1962a, 1962b but unfortunately their measurements for pure beryllium were only shown in the form of graphs. However, it was possible to read lattice parameter values for the *c* axis from the graphs which were then converted to length change values and combined with the selected thermal expansion coefficient at 293.15 K. For the *a* axis the equations given by Touloukian et al. 1975 were accepted but adjusted to the selected thermal expansion coefficient at 293.15 K and combined to give a single equation:

$$\varepsilon_T a = 1.84081 \times 10^{-6} T + 2.16586 \times 10^{-8} T^2 - 1.05521 \times 10^{-11} T^3 + 2.09582 \times 10^{-15} T^4 - 2.15055 \times 10^{-3} \quad (4c)$$

$$\varepsilon_T c = 8.92377 \times 10^{-6} T - 6.05952 \times 10^{-10} T^2 + 1.31731 \times 10^{-12} T^3 - 3.18721 \times 10^{-16} T^4 - 2.59476 \times 10^{-3} \quad (4d)$$

In consideration of high temperature lattice parameter measurements then on the basis $100\Delta\varepsilon$ those of Owen and Richards 1936 (293-823 K) on metal said to be of commercial purity 99.8% showed a bias of only 0.007 high along the *a* axis but showed a mark trend of 0.21 high along the *c* axis. The measurements of Kossolapow and Trapeznikow 1936 (293-727 K) scatter 0.022 high to 0.027 low along the *a* axis but show a trend to 0.17 high along the *c* axis.Those of Gordon 1949 (297-1286 K) on metal said to be only 97% pure shows scatter along the *a* axis but averaged 0.016 high, while along the *c* axis there is also a scatter but generally a trend upwards averaging 0.29 high above 1000 K. The measurements of Martin and Moore 1959 (75-77 K at low temperature and 290-1520 K at high temperature) on metal of commercial purity 99.4% was shown only graphically with actual data points being given by Touloukian et al. 1975. Along the *a* axis there is a trend reaching a maximum of 0.11 low in the range 1100 to 1200 K while along the *c* axis the trend is up to 0.86 high at the highest temperature on heating and 0.46 high on cooling.

Table 4a. Lattice parameters of alpha beryllium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Notes
Neuburger 1932a, 1932b, 1935	293	0.22727	0.36017	a
Neuburger 1933	RT	0.22726	0.36017	a
Owen et al. 1935	291	0.22860	0.35856	
Owen and Pickup 1935	291	0.22858	0.35846	
Owen and Richards 1936	293	0.22861	0.35847	
Kossolapow and Trapesnikow 1936	291	0.22856	0.35810	b
Gordon 1949	297-299.7	0.22859	0.35843	
Kaufman et al. 1950	298	0.22854	0.35829	
Schwarzenberger 1959	295	0.22867	0.35834	
Martin and Moore 1959	290	0.22871	0.35837	c
Amonenko et al. 1962b	293	0.22851	0.35849	
Mackay and Hill 1963	293.7	0.22859	0.35845	
Dupony et al. 1964	RT	0.22861	0.35839	
	Selected	0.22860 (6)	0.35842 (7)	

Notes for Table 4a

a. Not included in the average

b. *c* axis value not included in the average

c. Values given by Touloukian et al. 1975

At 293.15 K: Density 1845.2 (1.0) kg m^{-3} Molar volume 4.884 (3) cm^3 mol^{-1}.

4.2 Beta Phase: Body-centered cubic (cI2): 1543 K to 1560 K.

Amonenko et al. 1961 determined the lattice parameter to be 0.25517 nm at 1528 K and a second value of 0.25544 nm at 1553 K was estimated from a graphical representation. These values were fitted to the equations:

$$a \text{ (nm)} = 1.08224 \times 10^{-5} T + 0.238632 \quad (4e)$$

$$\varepsilon_T = 4.27530 \times 10^{-5} T - 5.73063 \times 10^{-2} \quad (4f)$$

The derived thermal expansion coefficient is 42×10^{-6} K^{-1}. The molar volume difference between the alpha and beta phases is 0.189 (8) cm^3 mol^{-1} by assuming that all lattice parameters at the transition temperature have an accuracy of 0.0001 nm. Abey 1984 determined the slope of the pressure curve to be – 0.043 (7) K Mpa^{-1} which when combined with an enthalpy of transition of 6855 (500) as selected by Arblaster 2016 leads to a volume difference of 0.191 (34) cm^3 mol^{-1} using the Clausius-Clapeyron equation, in excellent agreement with the crystallographic value. Martin and Moore 1959 determined lattice parameters to be 0.2545 nm and 0.2550 nm in the beta region.

Table 4b. Crystallographic properties of alpha beryllium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 ε_T *a*	100 ε_T *c*	100 ε_T avr
0	0	0	0	- 0.144	- 0.098	- 0.129
10	0.002	< 0.001	0.001	- 0.144	- 0.098	- 0.129
20	0.008	< 0.001	0.005	- 0.144	- 0.098	- 0.129
30	0.021	0.004	0.016	- 0.144	- 0.098	- 0.129
40	0.051	0.016	0.040	- 0.144	- 0.098	- 0.129
50	0.11	0.042	0.088	- 0.144	- 0.097	- 0.129
60	0.22	0.092	0.17	- 0.144	- 0.097	- 0.129
70	0.38	0.18	0.31	- 0.144	- 0.097	- 0.128
80	0.63	0.31	0.52	- 0.143	- 0.097	- 0.128
90	0.94	0.49	0.79	- 0.142	- 0.097	- 0.127
100	1.39	0.75	1.17	- 0.141	- 0.096	- 0.126
110	1.95	1.08	1.66	- 0.140	- 0.095	- 0.125
120	2.57	1.48	2.21	- 0.137	- 0.094	- 0.123
130	3.24	1.91	2.80	- 0.135	- 0.092	- 0.120
140	3.92	2.36	3.40	- 0.131	- 0.090	- 0.117
150	4.61	2.84	4.02	- 0.127	- 0.087	- 0.114
160	5.30	3.32	4.64	- 0.122	- 0.084	- 0.109
170	5.97	3.80	5.24	- 0.116	- 0.081	- 0.104
180	6.62	4.28	5.84	- 0.110	- 0.077	- 0.099
190	7.25	4.76	6.42	- 0.103	- 0.072	- 0.093
200	7.87	5.23	6.99	- 0.095	- 0.067	- 0.086
210	8.47	5.71	7.55	- 0.087	- 0.062	- 0.079
220	9.05	6.17	8.09	- 0.079	- 0.056	- 0.071
230	9.58	6.61	8.59	- 0.069	- 0.049	- 0.063
240	10.08	7.03	9.07	- 0.059	- 0.043	- 0.054
250	10.54	7.44	9.51	- 0.049	- 0.035	- 0.045
260	10.96	7.81	9.91	- 0.038	- 0.028	- 0.035
270	11.34	8.17	10.28	- 0.027	- 0.020	- 0.025
280	11.67	8.49	10.61	- 0.016	- 0.011	- 0.014
290	11.95	8.79	10.90	- 0.004	- 0.003	- 0.003
293.15	12.03	8.88	10.98	0	0	0
300	12.21	8.88	11.10	0.008	0.006	0.008
400	14.62	8.98	12.74	0.143	0.095	0.127
500	16.58	9.13	14.10	0.300	0.186	0.262
600	18.16	9.32	15.21	0.474	0.278	0.409
700	19.40	9.54	16.11	0.663	0.373	0.567
800	20.35	9.78	16.83	0.864	0.470	0.733
900	21.07	10.05	17.40	1.073	0.570	0.905
1000	21.61	10.32	17.85	1.289	0.672	1.084
1100	22.01	10.59	18.20	1.510	0.777	1.266
1200	22.33	10.86	18.51	1.736	0.886	1.452
1300	22.63	11.12	18.79	1.965	0.997	1.642
1400	22.94	11.35	19.08	2.197	1.110	1.835
1500	23.32	11.55	19.40	2.434	1.226	2.031
1543	23.51	11.63	19.55	2.537	1.276	2.117

Table 4c. Crystallographic properties of alpha beryllium

T K	*a* nm	*c* nm	*c*/*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.22827	0.35807	1.5686	0.22231	4.865	1852.3
10	0.22827	0.35807	1.5686	0.22231	4.865	1852.3
20	0.22827	0.35807	1.5686	0.22231	4.865	1852.3
30	0.22827	0.35807	1.5686	0.22231	4.865	1852.3
40	0.22827	0.35807	1.5686	0.22231	4.865	1852.3
50	0.22827	0.35807	1.5686	0.22231	4.865	1852.3
60	0.22827	0.35807	1.5686	0.22231	4.865	1852.3
70	0.22827	0.35807	1.5686	0.22231	4.865	1852.3
80	0.22827	0.35807	1.5686	0.22231	4.866	1852.3
90	0.22827	0.35807	1.5686	0.22231	4.866	1852.2
100	0.22828	0.35808	1.5686	0.22232	4.866	1852.2
110	0.22828	0.35808	1.5686	0.22232	4.866	1852.1
120	0.22829	0.35808	1.5686	0.22232	4.866	1852.0
130	0.22829	0.35809	1.5686	0.22233	4.867	1851.8
140	0.22830	0.35810	1.5685	0.22233	4.867	1851.7
150	0.22831	0.35811	1.5685	0.22234	4.868	1851.5
160	0.22832	0.35812	1.5685	0.22235	4.868	1851.2
170	0.22833	0.35813	1.5684	0.22236	4.869	1850.9
180	0.22835	0.35814	1.5684	0.22237	4.870	1850.6
190	0.22836	0.35816	1.5684	0.22238	4.871	1850.3
200	0.22838	0.35818	1.5683	0.22239	4.872	1849.9
210	0.22840	0.35820	1.5683	0.22241	4.873	1849.5
220	0.22842	0.35822	1.5682	0.22242	4.874	1849.1
230	0.22844	0.35824	1.5682	0.22244	4.875	1848.6
240	0.22846	0.35827	1.5682	0.22246	4.876	1848.1
250	0.22849	0.35829	1.5681	0.22248	4.878	1847.6
260	0.22851	0.35832	1.5681	0.22250	4.879	1847.1
270	0.22854	0.35835	1.5680	0.22252	4.881	1846.5
280	0.22856	0.35838	1.5679	0.22254	4.882	1845.9
290	0.22859	0.35841	1.5679	0.22256	4.884	1845.3
293.15	0.22860	0.35842	1.5679	0.22257	4.884	1845.2
300	0.22862	0.35844	1.5679	0.22258	4.885	1844.7
400	0.22893	0.35876	1.5671	0.22282	4.903	1838.1
500	0.22928	0.35909	1.5661	0.22307	4.923	1830.8
600	0.22968	0.35942	1.5648	0.22334	4.944	1822.8
700	0.23012	0.35976	1.5634	0.22362	4.968	1814.1
800	0.23057	0.36010	1.5618	0.22392	4.992	1805.3
900	0.23105	0.36046	1.5601	0.22423	5.018	1796.0
1000	0.23155	0.36083	1.5583	0.22455	5.045	1786.4
1100	0.23205	0.36121	1.5566	0.22487	5.072	1776.9
1200	0.23257	0.36159	1.5548	0.22520	5.100	1767.1
1300	0.23309	0.36199	1.5530	0.22554	5.129	1757.3
1400	0.23362	0.36240	1.5512	0.22589	5.158	1747.3
1500	0.23416	0.36281	1.5494	0.22624	5.188	1737.3
1543	0.23440	0.36300	1.5486	0.22640	5.201	1732.8

$$d1 = (a^2/3 + c^2/4)^{½} \quad d2 = a$$

Table 4d. Crystallographic properties of beta beryllium

T K	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1543	0.866	0.25533	0.22112	5.012	1798.1
1560	0.939	0.25551	0.22128	5.023	1794.3

$$d = \sqrt{3}a/2$$

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5 BORON B

Atomic Weight: 10.806 to 10.821 (Meija 2017)
Select 2007 value 10.811 (7) (Wieser and Berglund 2009)

5.1 Allotropy

The possible existence of a large number of boron allotropes was considered by both Donohue 1974 and Amberger and Stumpf 1981 but in reality there appears only two ambient pressure allotropes, α - rhombohedral (hR12) and β - rhombohedral (hR107), and two high pressure allotropes below 89 GPa, β - tetragonal (tP190), which Vlasse et al. 1978, 1979a, 1979b established as being a true allotrope, and γ -orthorhombic (oP28) which was characterized by Oganov et al. 2009. Ma et al. 2003 established that the β - tetragonal allotrope was a high temperature phase and the temperature – pressure phase diagram of Oganov et al. 2009 suggested that it is the stable phase between 10 GPa and 30 GPa above 2000 K.. A further proposed room temperature allotrope, α - tetragonal, had Z=50 but Longuet-Higgins and Roberts 1955 pointed out that $B_{48}B_2$ does not have a stable electronic configuration and could not exist and Ploog 1974 suggested from the method of production that the phase observed was more likely to have had Z=52 and the actual composition was either $B_{48}B_2C_2$ or $B_{48}B_2N_2$. However, a pure boron tetragonal phase with Z=52, which was designated as t-B_{52}, was obtained by both Ekimov and Zibrov 2011 and by Kurakevych and Solozhenko 2013 using high temperature and high pressure techniques. However, because of a large variation in reported experimental values for this phase its existence remains uncertain although on theoretical grounds Uemura et al. 2016 have suggested that it is a true allotrope. Solozhenko and Kurakevych 2013 even suggested that it is this phase t-B_{52} and not β-tetragonal which is the true high temperature high pressure phase. However, because both the β-tetragonal and the γ-orthorhombic phases have been fully characterized as metastable states at room temperature and pressure then it is these high pressure allotropes which are discussed in Part B while Part A concentrates on the ambient pressure allotropes.

Cooling below the melting point, selected as 2360 K as average of the determinations of Holcombe et al. 1973 and Krishnan et al. 1991, leads to the β - rhombohedral structure which can be retained to the lowest temperatures and which led to the suggestion that it was the thermodynamically stable allotrope at all temperatures. This appeared to be confirmed by *ab initio* calculations by Van Setten et al. 2007, Widom and Mikhalkovic 2008 and Ogitsu et al. 2009 and also appeared to be suggested by a new assessment of the thermodynamic properties of both allotropes by Cerqueira 2011. However, similar theoretical calculations by Masago et al. 2006 and Shang et al. 2007 favored the α - rhombohedral allotrope as being the most stable in the room temperature region. Experimentally, Parakhonskiy et al. 2011b established an alpha – beta phase boundary in the range 4 GPa to 8 GPa and by extrapolation to ambient pressure suggested that the alpha allotrope was the thermodynamically stable phase below 933 (50) K, in excellent agreement with a value of 970 K predicted by Masago et al. 2006. However, Solozhenko and Kurakevych 2013 questioned the validity of these measurements suggesting that the α – rhombohedral boron phase is only a thermodynamically stable phase above a pressure

of about 2 GPa. Because similar conclusion was reached by White et al. 2015 then no thermodynamic limits are given for these two phases.

PART 5A. AMBIENT PRESSURE ALLOTROPES OF BORON

5.2 Alpha Rhombohedral Boron

Structure: Rhombohedral (hR12)

Based on the direct density value of 2460 kg m^{-3} determined by McCarty et al. 1958 then Z=12 but Werheit and Kuhlmann 2012 from the infra red - phonon spectra has suggested that the true structure is $B_{12}B_2$ so that Z=14 which would lead to a calculated density of 2877 kg m^{-3}. Because this value differs considerably from the currently measured value, then until this difference has been resolved density values are calculated on the assumption that Z=12 for this rhombohedral structure. Measurements of the thermal expansion coefficients by Tsagareishvili et al. 1986 (300-1270 K) were unfortunately shown in the form of a small graph which suggested only that expansion varied erratically with temperature and meaningful values could not be estimated from the graph.

Table 5a. Lattice parameters of α - rhombohedral boron at 293.15 K

Values given only in either hexagonal or rhombohedral cell parameters were automatically converted to the other cell.

References	Original Temperature K	a_h nm	c_h nm	a_r nm	α°
Decker and Kasper 1959	RT	0.4908	1.2568	0.5058	58.06
Morosin et al. 1986	RT	0.4927	1.2564	0.5063	58.23
Will and Kiefer 2001	RT	0.49179	1.25805	0.50643	58.096
Parakhonskiy et al. 2011b	293	0.49065	1.25658	0.50566	58.046
	Selected	0.49065	1.25658	0.50566	58.046

At 293.15 K: Density 2467 (2) kg m^{-3} Molar volume 4.382 (2) cm^3 mol^{-1}.

The measurements of Morosin et al. 1986 were also given by Switendick and Morosin 1991. The hexagonal c axis measurements of Will and Kiefer 2001 is distinctly different from the other measurements in spite of the claimed accuracy. Therefore, the precision measurements of Parakhonskiy et al. 2011b were chosen based on the use of ultra pure starting materials and the fact that the accuracy of the values and the temperature of measurement were reported. However, based on possible systematic errors due to the differences the accuracy of the values for the hexagonal cell were considered to be equal to ± 0.0001 nm. Bond distances given by both Donohue 1974 and Amberger and Stumpf 1981 were based on Decker and Kasper 1959 but because their lattice parameters values are very close to those obtained by Parakhonskiy et al. 2011b then at the level of accuracy given the reported bond distances are still valid.

5.3 Beta Rhombohedral Boron

Structure: Rhombohedral (hR107)

Lattice parameter measurements of Lundström et al. 1998 (10-1273 K) were only shown graphically with actual data points given by Lundström 2001. As summarized by Werheit and Franz 1986, a significant number of physical property measurements showed discontinuities in the range 150 to 180 K and it was found that an apparent marked scatter in the low temperature lattice parameter values of Lundström et al. 1998 could be completely resolved if a transition temperature of 163 K was assumed. The transition appears to be first order with a volume contraction on heating of 0.0018 $cm^3\ mol^{-1}$. In order to correlate the low temperature data, lattice parameter values 10 to 150 K were reduced to length change values and fitted to Equation B using the enthalpy values selected in Part 5.3. These were considered to be representative to 62.9 K for the *a* axis and 77.3 K for the *c* axis because above these temperatures and up to 293.15 K the length change values were considered as varying linearly with temperature:

a axis

$$0 - 62.9\ K: \quad \ln (L_a) = (H_T - H_0)\,(-3.65050 \times 10^{-6} + 8.47604 \times 10^{-9}\,T + 4.12772 \times 10^{-4}/T) - 2.83282 \times 10^{-4} \qquad (5a)$$

$$62.9 - 163\ K: \quad \ln (L_a) = 4.87149 \times 10^{-7}\,T - 3.01082 \times 10^{-4} \qquad (5b)$$

$$163 - 293.15\ K: \quad \ln (L_a) = 2.92897 \times 10^{-6}\,T - 8.58621 \times 10^{-4} \qquad (5c)$$

c axis

$$0 - 77.3\ K: \quad \ln (L_c) = (H_T - H_0)\,(-6.40036 \times 10^{-6} + 1.31179 \times 10^{-8}\,T + 8.75607 \times 10^{-4}/T) - 5.05102 \times 10^{-4} \qquad (5d)$$

$$77.3 - 163\ K: \quad \ln (L_c) = 1.66875 \times 10^{-6}\,T - 5.81805 \times 10^{-4} \qquad (5e)$$

$$163 - 293.15\ K: \quad \ln (L_c) = 3.01369 \times 10^{-6}\,T - 8.83458 \times 10^{-4} \qquad (5f)$$

Above room temperature lattice parameter measurements of Lundström et al. 1998 show considerable scatter and only the measurements at 873, 973 and 1073 K showed any correlation with the low temperature data. After conversion to length change values these three values were fitted to the following equations which are assumed to be representative of crystallographic properties to 1300 K for comparison with actual experimental values:

$$\varepsilon_T\, a = 2.13744 \times 10^{-7}\,T + 4.63112 \times 10^{-9}\,T^2 - 4.60643 \times 10^{-4} \qquad (5g)$$

$$\varepsilon_T\, c = -1.60137 \times 10^{-6}\,T + 7.87150 \times 10^{-9}\,T^2 - 2.07011 \times 10^{-4} \qquad (5h)$$

Thermal expansion coefficients of Tsagareishvili et al. 1986 (300-1470 K) were unfortunately shown in the form of a small graph which suggested only that the

expansion varied erratically with temperature. Mean length change values given by Holcombe et al. 1973 (173-1273 K) were also only shown graphically. Tsagareishvili et al. 1980 developed a semi-theoretical expansion equation based on specific heat and enthalpy values selected by McDonald and Stull 1962. Compared with selected values calculated values are estimated to vary from 1.0 x 10^{-6} K^{-1} high at 300 K to 1.6 x 10^{-6} K^{-1} low at 1100 K. Gabunia et al. 2009 determined the thermal expansion for various isotopic compositions but again only showed the results graphically. Direct density measurements of Paradis et al. 2005 (2010-2360 K) are not compatible with an extrapolation of the crystallographic properties.

The number of atoms in the unit cell should be determined by a complete description of the structure but for this allotrope it is usually determined on specific samples by comparing lattice parameters with direct determinations of density. Measurements on natural samples and highly enriched ^{10}B and ^{11}B samples by Slack et al. 1988 established Z = 320.1 (4) for the hexagonal cell which is accepted. The extremely large number of bond lengths were reviewed by Amberger and Stumpf 1981 with additional values given by Slack et al. 1988.

Table 5b. Lattice parameters of β - rhombohedral boron at 293.15 K

Values given only in either hexagonal or rhombohedral cell parameters were automatically converted to the other cell. All values were given only at room temperature except for the measurements of Slack et al. 1988 (295 K) and Lundström et al. 1998 (298 K) which were both corrected to 293.15 K.

References	a_h nm	c_h nm	a_r nm	α°	Notes
Sands and Hoard 1957	1.095	2.373	1.012	65.47	
Kolakowski 1962	1.096	2.378	1.014	65.41	
Hughes et al. 1963	1.0944	2.381	1.0145	65.28	
Jaumann and Werheit 1969	1.096	2.389	1.017	65.20	
Hoard et al. 1970	1.0944	2.381	1.0145	65.28	
Geist et al. 1970	1.096	2.389	1.017	65.20	
Andersson and Lundström 1970	1.09259	2.38107	1.01384	65.209	
Holcombe et al. 1973	1.0927	2.371	1.0112	65.40	
Callmer 1977	1.09251	2.3814	1.01390	65.199	
Slack et al. 1988	1.0930	2.3816	1.0141	65.22	a
Lundström et al. 1998	1.09328	2.38245	1.01444	65.212	
Gabunia et al. 2004	1.09401	2.38112	1.01436	65.267	b
Selected	1.09328	2.38245	1.01444	65.212	

Notes for Table 5h

a. Average of three samples

b. Values for sample closest to natural boron – 81% ^{11}B of 97.2% sample purity

The selected values are based entirely on the measurements of Lundström et al. 1998 because the sample purity at 99.995% far exceeded that available in other experiments. The suggested accuracy of the hexagonal lattice parameters at ± 0.0001 nm takes into

account the general accuracy in the measurements of Lundström et al. 1998 in the room temperature region. The reported accuracies of the density and molar volume take into account the reported experimental density accuracies given by Slack et al. 1988:

At 293.15 K: Density 2330.1 (2.0) kg m^{-3} Molar volume 4.6396 (50) cm^3 mol^{-1}.

In Table 5e density and molar volumes in the low temperature region are given to five significant figures to account for the very small changes in this region. Lattice parameter measurements on samples containing from 98.45% ^{10}B to 98.51% ^{11}B by Slack et al. 1988 show virtually no compositional variation within experimental limits while measurements on samples containing from 87% ^{10}B to 99.8% ^{11}B by Gabunia et al. 2004 showed only a very peculiar trend. Later measurements of Gabunia et al. 2009 for the compositional range 0.2 to 97.2% ^{10}B did show a distinct trend but the results were given only for the *a* axis of the rhombohedral structure. At present therefore, it would appear that satisfactory lattice parameter values for pure ^{10}B and ^{11}B are not yet available.

5.3 Selected specific heat and enthalpy values for β – rhombohedral boron in the low temperature region

Specific heat values of Bogdanov et al. 1970 were converted from C_v to C_p values but because experimental values given for C_v below 50 K were abnormally high they were rejected and instead values of C_p derived from C_V values in the range 50 K to 90 K were fitted to the equation: C_p (J mol^{-1} K^{-1}) = 8.8690 x 10^{-7} T^3 + 2.4894 x 10^{-11} T^5 which was used to calculate all values at 90 K and below. Values of C_v and therefore C_p above 280 K were estimated. Specific heat values determined on 99.5% pure material by Cerqueira 2011 (0.4-391 K) are on average systematically 0.10 J mol^{-1} K^{-1} higher between 100 and 200 K but agree to within 0.05 J mol^{-1} K^{-1} between 200 and 298.15 K. Low temperature specific heat values of Johnston et al. 1951 (13-305 K) were not considered because the actual structure of the crystalline phase used was unknown. Units of C_p are J mol^{-1} K^{-1} and $H_T - H_0$ values in J $mol^{-1:}$

Table 5c. Specific heat and enthalpy values for β – rhombohedral boron

T K	5	10	15	20	25	30	35	40	45
C_p	0.00011	0.00089	0.0030	0.0072	0.014	0.025	0.039	0.059	0.085
$H_T - H_0$	0.00014	0.0022	0.0113	0.0357	0.0876	0.183	0.340	0.585	0.944
T K	50	60	70	80	90	100	110	120	130
C_p	0.119	0.211	0.346	0.536	0.794	1.046	1.390	1.829	2.261
$H_T - H_0$	1.451	3.067	5.812	10.17	16.75	25.88	37.98	54.08	74.50
T K	140	150	160	170	180	190	200	210	220
C_p	2.722	3.221	3.737	4.283	4.863	5.510	5.843	6.517	7.217
$H_T - H_0$	99.39	129.1	163.9	203.9	249.7	301.6	358.3	420.1	488.8
T K	230	240	250	260	270	280	290	293.15	298.15
C_p	7.863	8.447	9.006	9.554	10.055	10.528	10.958	11.087	11.282
$H_T - H_0$	564.2	645.4	733.1	825.9	924.0	1026.9	1134.4	1169.1	1225.0

5.4 Lattice parameters of β – rhombohedral boron

Unpublished lattice parameter values of Lundström et al. 1998 reproduced by permission of Lundström 2001.

T K	a_h Å	c_h Å		T K	a_h Å	c_h Å
10	10.9299 (2)	23.8117 (8)		275	10.9321 (2)	23.8225 (8)
25	10.9294 (2)	23.8130 (8)		298	10.9330 (2)	23.8252 (8)
50	10.9301 (2)	23.8139 (8)		298	10.933 (5)	23.825 (2)
75	10.9297 (2)	23.8125 (8)		373	10.927 (4)	23.830 (11)
100	10.9291 (2)	23.8120 (8)		523	10.945 (3)	23.850 (14)
100	10.9288 (2)	23.8158 (8)		573	10.938 (1)	23.876 (4)
125	10.9303 (2)	23.8153 (8)		723	10.942 (3)	23.904 (12)
150	10.9302 (2)	23.8170 (8)		873	10.970 (2)	23.928 (6)
175	10.9291 (2)	23.8156 (8)		973	10.978 (2)	23.968 (5)
200	10.9296 (2)	23.8182 (8)		1073	10.987 (2)	23.988 (8)
225	10.9308 (2)	23.8202 (8)		1176	10.988 (2)	24.004 (7)
250	10.9315 (2)	23.8201 (8)		1273	10.998 (2)	24.020 (18)

Table 5d. Crystallographic properties of β – rhombohedral boron

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 ε_T *a*	100 ε_T *c*	100 ε_T avr
0	0	0	0	- 0.028	- 0.051	- 0.036
10	0.025	0.053	0.034	- 0.028	- 0.051	- 0.036
20	0.087	0.19	0.12	- 0.028	- 0.050	- 0.036
30	0.18	0.40	0.25	- 0.028	- 0.050	- 0.035
40	0.27	0.63	0.39	- 0.028	- 0.050	- 0.035
50	0.37	0.91	0.55	- 0.028	- 0.049	- 0.035
60	0.46	1.19	0.71	- 0.027	- 0.048	- 0.034
70	0.49	1.47	0.81	- 0.027	- 0.046	- 0.033
80	0.49	1.67	0.88	- 0.026	- 0.045	- 0.032
90	0.49	1.67	0.88	- 0.026	- 0.043	- 0.032
100	0.49	1.67	0.88	- 0.025	- 0.041	- 0.031
110	0.49	1.67	0.88	- 0.025	- 0.040	- 0.030
120	0.49	1.67	0.88	- 0.024	- 0.038	- 0.029
130	0.49	1.67	0.88	- 0.024	- 0.036	- 0.028
140	0.49	1.67	0.88	- 0.024	- 0.035	- 0.027
150	0.49	1.67	0.88	- 0.023	- 0.033	- 0.026
160	0.49	1.67	0.88	- 0.023	- 0.032	- 0.025
163	0.49	1.67	0.88	- 0.022	- 0.031	- 0.025
163	2.93	3.01	2.96	- 0.038	- 0.039	- 0.038
170	2.93	3.01	2.96	- 0.036	- 0.037	- 0.036
180	2.93	3.01	2.96	- 0.033	- 0.034	- 0.033
190	2.93	3.01	2.96	- 0.030	- 0.031	- 0.031
200	2.93	3.01	2.96	- 0.027	- 0.028	- 0.028
210	2.93	3.01	2.96	- 0.024	- 0.025	- 0.025
220	2.93	3.01	2.96	- 0.021	- 0.022	- 0.022
230	2.93	3.01	2.96	- 0.019	- 0.019	- 0.019
240	2.93	3.01	2.96	- 0.016	- 0.016	- 0.016
250	2.93	3.01	2.96	- 0.013	- 0.013	- 0.013
260	2.93	3.01	2.96	- 0.010	- 0.010	- 0.010
270	2.93	3.01	2.96	- 0.007	- 0.007	- 0.007
280	2.93	3.01	2.96	- 0.004	- 0.004	- 0.004
290	2.93	3.01	2.96	- 0.001	- 0.001	- 0.001
293.15	2.93	3.01	2.96	0	0	0
300	2.99	3.12	3.04	0.002	0.002	0.002
400	3.92	4.69	4.18	0.037	0.041	0.038
500	4.84	6.26	5.32	0.080	0.096	0.086
600	5.76	7.83	6.45	0.133	0.167	0.145
700	6.68	9.39	7.59	0.196	0.253	0.215
800	7.10	11.0	8.72	0.267	0.355	0.297
900	8.52	12.5	9.85	0.348	0.473	0.390
1000	9.43	14.1	11.0	0.438	0.606	0.494
1100	10.3	15.6	12.1	0.538	0.756	0.610
1200	11.3	17.1	13.2	0.646	0.921	0.738
1300	12.2	18.7	14.3	0.764	1.101	0.877

Table 5e. Crystallographic properties of β – rhombohedral boron

T K	a_h nm	c_h nm	a_r nm	α°	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	1.09297	2.38125	1.01402	65.222	4.6347	2332.6
10	1.09297	2.38125	1.01402	65.222	4.6347	2332.6
20	1.09297	2.38125	1.01402	65.222	4.6347	2332.6
30	1.09297	2.38126	1.01402	65.222	5.4637	2332.6
40	1.09298	2.38127	1.01403	65.221	4.6347	2332.6
50	1.09298	2.38129	1.01403	65.221	4.6348	2332.6
60	1.09298	2.38132	1.01404	65.221	4.6349	2332.5
70	1.09299	2.38134	1.01405	65.221	4.6350	2332.5
80	1.09299	2.38139	1.01406	65.220	4.6351	2332.4
90	1.09300	2.38143	1.01408	65.220	4.6352	2332.3
100	1.09301	2.38147	1.01409	65.219	4.6354	2332.3
110	1.09301	2.38151	1.01410	65.218	4.6355	2332.2
120	1.09302	2.38155	1.01411	65.218	4.6356	2332.2
130	1.09302	2.38159	1.01412	65.217	4.6357	2332.1
140	1.09303	2.38162	1.01414	65.217	4.6359	2332.0
150	1.09303	2.38166	1.01415	65.216	4.6360	2332.0
160	1.09304	2.38170	1.01416	65.216	4.6361	2331.9
163	1.09304	2.38172	1.01416	65.216	4.6361	2331.9
163	1.09286	2.38152	1.01405	65.212	4.6343	2332.8
170	1.09289	2.38157	1.01407	65.212	4.6346	2332.7
180	1.09292	2.38164	1.01410	65.212	4.6350	2332.5
190	1.09295	2.38171	1.01413	65.212	4.6354	2332.3
200	1.09298	2.38179	1.01416	65.212	4.6358	2332.1
210	1.09301	2.38186	1.01419	65.212	4.6362	2331.9
220	1.09305	2.38193	1.01422	65.212	4.6366	2331.7
230	1.09308	2.38200	1.01425	65.212	4.6370	2331.4
240	1.09311	2.82207	1.01428	65.212	4.6375	2331.2
250	1.09314	2.38214	1.01431	65.212	4.6379	2331.0
260	1.09317	2.38222	1.01434	65.212	4.6383	2330.8
270	1.09321	2.38229	1.01437	65.212	4.6387	2330.6
280	1.09324	2.38236	1.01440	65.212	4.6391	2330.4
290	1.09327	2.38243	1.01443	65.212	4.6395	2330.2
293.15	1.09328	2.38245	1.01444	65.212	4.6396	2330.1
300	1.0933	2.3825	1.0145	65.21	4.640	2330
400	1.0937	2.3834	1.0148	65.21	4.645	2327
500	1.0942	2.3847	1.0154	65.20	4.652	2324
600	1.0947	2.3864	1.0160	65.20	4.660	2320
700	1.0954	2.3885	1.0168	65.19	4.670	2315
800	1.0962	2.3909	1.0177	65.17	4.681	2310
900	1.0971	2.3937	1.0188	65.16	4.694	2303
1000	1.0981	2.3969	1.0199	65.14	4.709	2296
1100	1.0992	2.4005	1.0213	65.11	4.725	2288
1200	1.1003	2.4044	1.0227	65.09	4.743	2279
1300	1.1016	2.4087	1.0243	65.06	4.763	2270

PART 5B. HIGH PRESSURE ALLOTROPES OF BORON

Values are given at room temperature and ambient pressure.

5.5 Beta Tetragonal Boron

Structure: Tetragonal (tP190)

Vlasse et al. 1978, 1979a, 1979b established that this was a true allotrope with Z = 190 based on a unit cell of 4 x (B_{21} . $2B_{12}$. $B_{2.5}$) while Ma et al. 2003 established that it was a high temperature, high pressure phase.

Table 5f. Room temperature lattice parameters of β – tetragonal boron

References	*a* nm	*c* nm
Talley et al. 1960	1.012	1.414
Sullenger et al. 1969	1.0062	1.4211
Amberger and Ploog 1971	1.012	1.414
Vlasse et al. 1978, 1979a, 1979b	1.014	1.417
Selected	1.014 (1)	1.417 (1)

Taking purity into account the measurements of Vlasse et al. 1978, 1979a, 1979b were accepted.

Room temperature: Density 2341 (5) kg m^{-3} Molar volume 4.618 (10) cm^3 mol^{-1}.

5.6 Gamma Orthorhombic Boron

Structure: Orthorhombic (oP28)

This high pressure phase exists between 19 and 89 GPa at room temperature and from the temperature - pressure phase diagram of Oganov et al. 2009 appears to be obtainable directly from the liquid above a pressure of about 30 GPa.

Table 5g. Room temperature lattice parameters of γ - orthorhombic boron

References	*a* nm	*b* nm	*c* nm
Zarechnaya et al. 2008	0.50563	0.56126	0.69710
Oganov et al. 2009	0.50544	0.56199	0.69873
Parakhonskiy et al. 2011a	0.50576	0.56245	0.69884
Selected	0.50576	0.56245	0.69884

The differences between the three sets of measurements is considered to be unsatisfactory. The earlier measurements of Zarechnaya et al. 2008 and Organov et al. 2009 were considered to be preliminary and the later measurements of Parakhonskiy et al. 2011a were selected but with the accuracies assigned to the selected values expanded to ± 0.0001 nm.

Room temperarure: Density 2529 (2) kg m^{-3} Molar volume 4.276(1) cm^3 mol^{-1}.

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6 CARBON C

Atomic weight: 12.0096 to 12.0116 (Meija 2017)
Select 2007 value 12.0107 (8) (Wieser and Berglund 2009).

Donohue 1974 reviewed the reported allotropes of carbon and in addition there are the more recent discoveries of the fullerenes and graphene. The well characterized allotropes are considered here which consist of hexagonal graphite, cubic diamond, and the fullerenes C_{60} and C_{70}. Limited structural data is also given for the fullerenes C_{76} and C_{84}.

PART 6A. GRAPHITE

Structure: Hexagonal (hP4): 0 K to 3979 K.

The summation of the partial pressures of C_1 to C_5 as selected by Gurvich et al. 1991 leads to a sublimation temperature of 3979 K, while Savvatimskiy 2005 selected a triple point of 4800 (100) K at 100 bar pressure. Whittaker 1978 proposed that graphite transforms to various carbyne structures between 2600 K and a triple point given by Whittaker et al. 1975 as 3780 (30) K at a pressure of 0.19 (2) atm in direct contradiction to the overwhelming evidence reviewed by Savvatimskiy 2005 suggesting that melting can only obtained at high pressures. It was conjectured that although the graphite structure had been directly observed at 3300 K (Kellett and Richards 1964) this was due to the fact that on heating the transformation to carbynes is very sluggish whereas on cooling the reverse reaction is rapid. However, until the crystal structures of the carbyne forms has been directly observed at high temperatures then their possible existence at these temperatures is considered to be speculative.

6.1 Low temperature

Selected thermal expansion coefficients are based on a compromise between the measurements of Bailey and Yates 1970 (30-270 K) and Hamamda and Popov 1990 (4-30 K). However, this combination does indicate that the *a*-axis thermal expansion values as given by Bailey and Yates 1970 were given in the wrong units of 10^{-5} K^{-1} instead of the correct units of 10^{-6} K^{-1}. The selected values were extrapolated to 293.15 K. On the basis $100\Delta\varepsilon$ length changes derived from the low temperature *a*-axis lattice parameter measurements of Kellett and Richards 1964 (77-328 K) scatter 0.007 low to 0.007 high while values derived from the interplanar spacings of Baskin and Meyer 1955 (4.2-297 K) are 0.041 high at 4.2 K and 0.028 high at 78 K. Lattice parameter measurements of Lowell 1963 (6-297 K) scatter 0.002 low to 0.017 high along the *a*-axis and 0.017 high to 0.040 high along the *c*-axis.

6.2 High temperature

The quality of the graphite used in experiments is defined by the p value where $p = 0$ for high purity single crystals up to $p = 1.0$ for heat treated hemicellulose material which exhibits no directional orientation.

Along the a-axis, length change values derived from the lattice parameter measurements of Nelson and Riley 1945 (287.8-1073 K) $p = 0.05$ and the high temperature region values of Kellett and Richards 1964 (291-3327 K) $p = 0.2$ were selected but essentially these are almost too coarse to derive thermal expansion values which do not exceed a maximum of $1.5 \times 10^{-6}\ K^{-1}$ over the whole temperature range. However, selected values at 723, 973 and 1073 K from the measurements of Nelson and Riley 1945 and 623, 923, 1073, 1373, 1488 and 1585 K from the measurements of Kellet and Richards 1964 were fitted to a curve which was then further refined to arrive at equation 6a. Above 1500 K the measurements of Kellet and Richards 1964 can be considered as being close to a linear relationship but in order to match up to equation 6a were fitted to the quadratic equation 6b with a cross-over point at 1430 K:

$$293.15 - 1430\ K: \varepsilon_T a = -1.86092 \times 10^{-6} T - 6.41118 \times 10^{-11} T^2 + 3.69023 \times 10^{-12} T^3 - 3.10248 \times 10^{-15} T^4 + 8.05910 \times 10^{-19} T^5 + 4.79240 \times 10^{-4} \quad (6a)$$

$$1430 - 3000\ K: \quad \varepsilon_T a = 1.18750 \times 10^{-6} T - 1.14954 \times 10^{-11} T^2 - 1.35087 \times 10^{-3} \quad (6b)$$

For the c-axis, distinction is made between the length changes derived from the accurate lattice parameter measurements of Nelson and Riley 1945 (287.8-1073 K) for $p = 0.05$ on Ceylon graphite and the interplanar spacings measurements of Kellett et al. 1964 on spectroscopic graphite (295-2785 K) $p = 0.2$ and pyrolytic graphite (295-2545 K) $p = 0.1$ which show marked scatter. The values of Nelson and Riley 1945 were fitted to equation 6c and the values obtained at 1073 K were used as fixed points to derive the high temperature equation 6d in which no values of Kellett et al. 1964 were rejected Values were extrapolated to 3000 K. On the basis $100\Delta\varepsilon$ equation 6c is accurate to ± 0.003 but equation 6d is only accurate to ± 0.18:

$$293.15 - 1073\ K: \varepsilon_T c = 2.76229 \times 10^{-5} T - 7.52920 \times 10^{-10} T^2 + 1.23568 \times 10^{-12} T^3 - 8.06407 \times 10^{-3} \quad (6c)$$

$$1073 - 3000\ K: \quad \varepsilon_T c = 2.67207 \times 10^{-5} T + 1.65631 \times 10^{-9} T^2 - 8.34431 \times 10^{-3} \quad (6d)$$

Interplanar measurements of Yang 1962 (1273-2873 K) were not related to room temperature values but can be made to agree with the selected curve if a value of 3.3566 Å at 293.15 K is adopted. The interplanar spacings values of Kellet and Richards 1971 (273-2873 K) for $p = 0.05$ should be superior to the earlier measurements of Kellet et al. 1964 but instead are not only incompatible with the measurements of Nelson and Riley 1945 but also lead to a room temperature c-axis thermal expansion coefficient of only $24.9 \times 10^{-6}\ K^{-1}$ which differs considerably from the selected value. Lattice parameter measurements of Matuyama 1955 determined the average thermal expansion between 1273 K and 2073 K to be $0.95 \times 10^{-6}\ K^{-1}$ along the a axis and $28.09 \times 10^{-6}\ K^{-1}$ along the c

axis. The latter is notably higher than the selected value but clearly indicates that further measurements are required. These two sets of measurements and other determinations of the interplanar spacings are compared with selected values in Table 6b. Morgan 1972 gave thermal expansion values in terms of complex Debye functions. However, for both axes the calculated equations differ from the selected values below room temperature while for the *c* axis there is an abnormal hump in the derived thermal expansion curve between 300 and 1000 K while above 1000 K there is a sudden sharp increase in the thermal expansion coefficient. In both cases this behavior is not consistent with actual experimental data.

Table 6a. Lattice parameters of graphite at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Notes
Trzebiatowski 1937	RT	0.24614	0.67095	
Nelson and Riley 1945	288.0	0.24613	0.67092	
Bacon 1950	288	0.24616	0.67089	
Baskin and Meyer 1955	297	0.24591	0.67073	a
Walker and Imperial 1957	291	-	0.67095	b
Matuyama 1958	293	-	0.67090	c
Lowell 1963	298	0.24614	0.67093	
Kellett and Richards 1964	291	0.24613	-	
Kellett and Richards 1971	293	-	0.67103	d
	Selected	0.24614 (2)	0.67094 (5)	

Notes for Table 6a

a. Not includes in the average

b. Calculated from interlayer spacing ($c = 2\ d$)

c. Calculated from lattice parameter equation

d. Calculated from interlayer spacing equation

At 293.15 K: Density 2266.2 (3) kg m^{-3} Molar volume 5.2999 (6) cm^3 mol^{-1}.

6.3 Deviations of experimental values from the selected values

Table 6b. Lattice parameter and interplanar spacing differences

References	Temperature Range K	Deviations 100Δε
Yang 1962	1273-2873	Scatter 0.11 low to 0.087 high
Walker et al. 1953	77, 300-1391	In the high temperature region trends from 0.020 high at 700 K to 0.093 low at 1391 K
Matyuma 1958	298-1073	Trends to 0.11 low at 1073 K
Steward at al 1960	273-2873	Trend 0.014 high at 973 K to 0.084 low at 2873 K
Kellett and Richards 1971	273-2873	For $p = 0.05$ trend from 0.12 low at 1423 K to 0.12 high at 2873 K

Table 6c. Low temperature crystallographic properties of graphite

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
0	0	0	0	0.0298	- 0.557	- 0.166
10	- 0.01	0.47	0.15	0.0298	- 0.557	- 0.166
15	- 0.04	0.83	0.25	0.0298	- 0.557	- 0.166
20	- 0.09	1.3	0.37	0.0298	- 0.556	- 0.165
25	- 0.15	2.1	0.60	0.0297	- 0.555	- 0.165
30	- 0.24	3.3	0.94	0.0296	- 0.554	- 0.165
40	- 0.38	4.6	1.28	0.0293	- 0.550	- 0.164
50	- 0.52	8.7	2.55	0.0289	- 0.534	- 0.159
60	- 0.66	11.3	3.33	0.0283	- 0.524	- 0.156
70	- 0.78	13.3	3.91	0.0275	- 0.512	- 0.152
80	- 0.89	14.9	4.37	0.0267	- 0.498	- 0.148
90	- 0.99	16.3	4.77	0.0258	- 0.482	- 0.144
100	- 1.07	17.6	5.15	0.0247	- 0.465	- 0.139
110	- 1.14	18.8	5.51	0.0236	- 0.447	- 0.133
120	- 1.19	19.8	5.81	0.0225	- 0.428	- 0.128
130	- 1.24	20.7	6.07	0.0213	- 0.408	- 0.122
140	- 1.28	21.5	6.31	0.0200	- 0.387	- 0.116
150	- 1.30	22.2	6.53	0.0187	- 0.365	- 0.109
160	- 1.32	22.9	6.75	0.0174	- 0.343	- 0.103
170	- 1.33	23.5	6.95	0.0161	- 0.319	- 0.096
180	- 1.34	24.1	7.14	0.0147	- 0.296	- 0.089
190	- 1.34	24.6	7.31	0.0134	- 0.271	- 0.082
200	- 1.33	25.0	7.45	0.0120	- 0.247	- 0.074
210	- 1.33	25.4	7.58	0.0107	- 0.222	- 0.067
220	- 1.32	25.8	7.72	0.0094	- 0.196	- 0.059
230	- 1.32	26.2	7.85	0.0081	- 0.170	- 0.051
240	- 1.31	26.5	7.96	0.0068	- 0.144	- 0.043
250	- 1.30	26.7	8.03	0.0055	- 0.117	- 0.035
260	- 1.28	27.0	8.15	0.0042	- 0.090	- 0.029
270	- 1.27	27.2	8.22	0.0029	- 0.063	- 0.019
280	- 1.25	27.3	8.27	0.0016	- 0.036	- 0.011
290	- 1.23	27.4	8.31	0.0004	- 0.009	- 0.003
293.15	- 1.23	27.5	8.35	0	0	0

Table 6d. Low temperature crystallographic properties of graphite

T K	*a* nm	*c* nm	*c*/*a*	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.24621	0.66720	2.7099	0.33360	5.274	2277.5
10	0.24621	0.66720	2.7099	0.33360	5.274	2277.5
15	0.24621	0.66721	2.7099	0.33360	5.274	2277.5
20	0.24621	0.66721	2.7099	0.33360	5.274	2277.5
25	0.24621	0.66721	2.7099	0.33361	5.274	2277.5
30	0.24621	0.66722	2.7099	0.33361	5.274	2277.5
40	0.24621	0.66725	2.7101	0.33363	5.274	2277.4
50	0.24621	0.66736	2.7105	0.33368	5.275	2277.1
60	0.24621	0.66742	2.7108	0.33371	5.275	2276.9
70	0.24621	0.66751	2.7112	0.33375	5.276	2276.6
80	0.24621	0.66760	2.7116	0.33380	5.276	2276.3
90	0.24620	0.66770	2.7120	0.33385	5.277	2276.0
100	0.24620	0.66782	2.7125	0.33391	5.278	2275.7
110	0.24620	0.66794	2.7130	0.33397	5.279	2275.3
120	0.24620	0.66807	2.7136	0.33403	5.280	2274.9
130	0.24619	0.66820	2.7142	0.33410	5.281	2274.5
140	0.24619	0.66834	2.7148	0.33417	5.282	2274.1
150	0.24619	0.66849	2.7154	0.33425	5.283	2273.7
160	0.24618	0.66864	2.7160	0.33432	5.284	2273.2
170	0.24618	0.66880	2.7167	0.33440	5.285	2272.7
180	0.24618	0.66896	2.7174	0.33448	5.286	2272.3
190	0.24617	0.66912	2.7181	0.33456	5.287	2271.8
200	0.24617	0.66928	2.7188	0.33464	5.288	2271.3
210	0.24617	0.66945	2.7195	0.33473	5.289	2270.7
220	0.24616	0.66962	2.7202	0.33481	5.291	2270.2
230	0.24616	0.66980	2.7210	0.33490	5.292	2269.7
240	0.24616	0.66998	2.7217	0.33499	5.293	2269.2
250	0.24615	0.67015	2.7225	0.33508	5.294	2268.6
260	0.24615	0.67033	2.7233	0.33517	5.296	2268.1
270	0.24615	0.67052	2.7240	0.33526	5.297	2267.5
280	0.24614	0.67070	2.7248	0.33535	5.298	2266.9
290	0.24614	0.67088	2.7256	0.33544	5.300	2266.4
293.15	0.24614	0.67094	2.7258	0.33547	5.300	2266.2

$d = c/2$

Table 6e. High temperature crystallographic properties of graphite

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
293.15	- 1.23	27.50	8.35	0	0	0
300	- 1.21	27.50	8.36	- 0.0008	0.019	0.006
400	- 0.83	27.53	8.62	- 0.0110	0.294	0.091
500	- 0.46	27.64	8.91	- 0.0175	0.571	0.179
600	- 0.11	27.82	9.20	- 0.0203	0.851	0.270
700	0.18	28.07	9.48	- 0.0199	1.133	0.364
800	0.42	28.39	9.74	- 0.0168	1.419	0.462
900	0.59	28.78	9.99	- 0.0117	1.709	0.562
1000	0.70	29.24	10.21	- 0.0052	2.004	0.678
1100	0.78	29.68	10.41	0.0022	2.305	0.770
1200	0.84	29.91	10.53	0.0103	2.611	0.877
1300	0.93	30.15	10.67	0.0190	2.919	0.986
1400	1.08	30.38	10.85	0.0290	3.231	1.096
1500	1.15	30.60	10.97	0.0405	3.546	1.209
1600	1.15	30.83	11.04	0.0520	3.865	1.323
1700	1.15	31.05	11.12	0.0635	4.187	1.438
1800	1.15	31.27	11.19	0.0749	4.512	1.557
1900	1.14	31.49	11.26	0.0864	4.840	1.671
2000	1.14	31.71	11.33	0.0978	5.172	1.789
2100	1.14	31.92	11.40	0.109	5.507	1.909
2200	1.14	32.13	11.47	0.121	5.846	2.029
2300	1.13	32.34	11.53	0.132	6.188	2.151
2400	1.13	32.54	11.60	0.143	6.533	2.273
2500	1.13	32.75	11.67	0.155	6.881	2.397
2600	1.13	32.95	11.74	0.166	7.233	2.521
2700	1.12	33.15	11.80	0.177	7.588	2.647
2800	1.12	33.35	11.86	0.188	7.946	2.774
2900	1.12	33.54	11.93	0.200	8.308	2.902
3000	1.12	33.73	11.99	0.211	8.672	3.031

Table 6f. High temperature crystallographic properties of graphite

T K	*a* nm	*c* nm	*c*/*a*	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
293.15	0.24614	0.67094	2.7258	0.33547	5.300	2266
300	0.24614	0.67107	2.7264	0.33553	5.301	2266
400	0.24611	0.67292	2.7342	0.33646	5.314	2260
500	0.24610	0.67477	2.7419	0.33739	5.328	2254
600	0.24609	0.67665	2.7496	0.33832	5.343	2248
700	0.24609	0.67854	2.7573	0.33927	5.358	2242
800	0.24610	0.68046	2.7650	0.34023	5.373	2235
900	0.24611	0.68240	2.7727	0.34120	5.389	2229
1000	0.24613	0.68439	2.7806	0.34219	5.406	2222
1100	0.24615	0.68641	2.7886	0.34320	5.422	2215
1200	0.24617	0.68846	2.7967	0.34423	5.439	2208
1300	0.24619	0.69053	2.8049	0.34526	5.457	2201
1400	0.24621	0.69262	2.8131	0.34631	5.474	2194
1500	0.24624	0.69473	2.8214	0.34737	5.492	2187
1600	0.24627	0.69687	2.8297	0.34844	5.510	2180
1700	0.24630	0.69903	2.8382	0.34952	5.529	2172
1800	0.24632	0.70121	2.8467	0.35061	5.547	2165
1900	0.24635	0.70342	2.8553	0.35171	5.566	2158
2000	0.24638	0.70564	2.8640	0.35282	5.585	2151
2100	0.24641	0.70789	2.8728	0.35395	5.604	2143
2200	0.24644	0.71016	2.8817	0.35508	5.623	2136
2300	0.24646	0.71245	2.8907	0.35623	5.643	2129
2400	0.24649	0.71477	2.8998	0.35738	5.662	2121
2500	0.24652	0.71711	2.9089	0.35855	5.682	2114
2600	0.24655	0.71947	2.9182	0.35973	5.702	2106
2700	0.24658	0.72185	2.9275	0.36092	5.722	2099
2800	0.24660	0.72425	2.9369	0.36213	5.743	2091
2900	0.24663	0.72668	2.9464	0.36334	5.763	2084
3000	0.24666	0.72913	2.9560	0.36456	5.784	2077

$$d = c/2$$

PART 6B. DIAMOND

Structure: Cubic (cF8)

Diamond is only metastable at atmospheric pressure and the conversion to graphite increases rapidly above 1300 K. However, at high pressures diamond remains stable up to a triple point at 4700 K and 125 kbar (Gurvich et at 1991). Evidence of melting above this pressure was obtained by Gold et al. 1984.

6.3 Low temperature

The high precision thermal expansion coefficient values of Stoupin and Shvyd'ko 2011 (10-295 K) were selected with equivalent length change values obtained by three point integration. However, below 50 K values were adjusted to correspond to an exact Debye function obtained in the region 50 to 70 K: $\alpha\ (K^{-1}) = 4.23 \times 10^{-14}\ T^{3}$.

Length change values have been derived from various sets of lattice parameter measurements but because the value of ε_T is so low the differences from selected value are obtained by converting to equivalent lattice parameter deviations and are compared with selected values in Table 6g. Agreement to within 5 x 10^{-6} nm is considered to be satisfactory because this is the assigned accuracy to the room temperature selected lattice parameter value. Measurements of Thewlis and Davey 1956 (139-1214 K) were only shown graphically with actual data points given by Touloukian et al. 1977. The measurements of Haruna et al. 1992 (4.2-320 K) were given in the form of a thermal expansion equation which was integrated to obtain length change values. The thermal expansion coefficient values of Novikova 1960 (28-754 K) was only shown graphically with actual data points given by Touloukian et al. 1977. These show considerable scatter and therefore comparison with selected values was obtained by using the equivalent length change values also derived by Touloukian et al. 1977. When smoothed, the thermal expansion coefficients of Novikova 1960 actually agree with the selected values to within ± 3 x 10^{-8} K^{-1} between 230 K and room temperature. Lattice parameter values of Straumanis and Aka 1951b (283-323 K) lead to a room temperature thermal expansion coefficient of 1.38 (12) x 10^{-6} K^{-1} which is notably higher than the selected value. X-ray diffraction measurements of Giles et al. 2005 (10-300 K) were only shown graphically,

Table 6g. A comparison between low temperature length change values and selected values for diamond

References	Temperature Range K	Deviations Δa nm
Thewlis and Davey 1956	139-1214	In the low temperature region scatter 8 x 10^{-6} nm low to 2 x 10^{-5} nm high
Novikova 1960	28-754	In the low temperature region maximum deviation is 6 x 10^{-6} nm low at 85 K
Haruna et al. 1992	4.2-320	Maximum deviation 2 x 10^{-6} nm high at 180 K
Saotome et al. 1998	4.2-300	Maximum deviation 2 x 10^{-6} nm low at 10 K
Sato et al. 2002	4.2-300	Maximum deviation 5 x 10^{-6} nm low at 105 K
Paszkowicz et al. 2010	4-295	The measurements show scatter and deviate by up to 2 x10^{-5} nm low at 50 K
Stoupin and Shvyd'ko 2010	6-300	Maximum deviation 7 x 10^{-7} nm low at 65 K

6.4 High temperature

Length change values derived from the lattice parameter measurements on gem quality samples by Thewlis and Davey 1956 (139-1214 K) and Skinner 1957 (290-944 K) were combined with dilatometric measurements on thick films by Pickrell et al. 1994 (90-1090 K) and fitted to equation 6e which, on the basis ± 100ε, has an accuracy of ± 0.004. The measurements of Thewlis and Davey 1956 were only shown graphically with actual data points given by Touloukian et al. 1977. Lattice parameter values of Wright 1965 (1073-1960 K) were unpublished but were given in graphical form by Orlov 1978. Because these were isolated they were normalized by connecting to values of ε and α* selected from equation 6e at 1150 K (the median of the experimental overlap region 1080 to 1220 K). This resulted in reducing the experimental values of Wright 1965 by 0.00008 nm

which were then fitted to the equation: a (nm) = 5.54734 x 10^{-6} T – 3.49947 x 10^{-3}. The temperature dependent coefficient was taken as being α* at an extrapolation of the data to 2000 K and combined with the values of ε and α* at 1160 K to obtain equation 6f to represent the expansion from 1160 K to 2000 K:

$$293.15 – 1160\ K: \varepsilon_T = – 1.36222 \times 10^{-6} T + 4.51451 \times 10^{-9} T^2 – 1.02648 \times 10^{-12} T^3 + 3.72307 \times 10^{-5} \quad (6e)$$

$$1160 – 2000\ K: \quad \varepsilon_T = 4.40911 \times 10^{-6} T + 2.34557 \times 10^{-10} T^2 – 2.50071 \times 10^{-3} \quad (6f)$$

Deviations of other high temperature measurements from equations 69e and 69f are given in Table 6j for dilatometric measurements, and Table 6k for lattice parameter measurements. The lattice parameter measurements of Mauer and Bolz 1955 and Thewlis and Davey 1956, and the dilatometric measurements Novikova 1960, were given by Touloukian et al. 1975.

Table 6h. Lattice parameter of commercial quality diamond at 293.15 K

References	Original Temperature K	*a* nm	Note
Ehrenburg 1926	291	0.35671	
Renninger 1937	293	0.356688	
Trzebiatowski 1937	293	0.356696	
Lonsdale 1944	291	0.356711	
Riley 1944	291	0.356704	
Lonsdale 1947	291	0.356709	
Straumanis and Aka 1951a	293	0.356703	
Straumanis and Aka 1951b	293	0.356707	
Swanson and Fuyat 1953	299	0.356669	
Thewlis and Davey 1956	293	0.356714	
Skinner 1957	298	0.356698	
Kaiser and Bond 1959	RT	0.356745	
Vogel and Kempter 1959, 1961	298	0.356732	
Perdok 1960	298	0.356676	a
Straumanis and James 1960	298	0.356706	a
Beu 1960	298	0.356721	a
Kempter 1960	298	0.356737	a
Tournarie 1960	298	0.356725	a
Wilkens 1960	298	0.356714	a
Sokhur and Vitol 1969	RT	0.356686	
Paszkowicz et al. 2010	295	0.356726	
	Average	0.35671 (2)	

Notes for Table 6h

a. Measurement as part of the I.U.Cr. Precision Lattice Parameter Project (Parrish 1960)

Table 6i. Lattice parameter of high quality diamond at 293.15 K

References	Original Temperature K	*a* nm
Tu 1932	291	0.356701
Straumanis and Aka 1950	293	0.356706
Straumanis and Aka 1951b	293	0.356704
Thewlis and Davey 1956	293	0.356705
Skinner 1957	298	0.356707
Kaiser et al. 1959	RT	0.356706
Kaiser and Bond 1959	RT	0.356703
Delf 1963	298	0.356710
Mykolajewycz et al. 1965	298	0.356709
Hom et al. 1975	298	0.356704
Holloway et al. 1991	298	0.356712
Yamanaka et al. 1994	299	0.356711
Sato et al. 2002	300	0.356711
Stoupin and Shvyd'ko 2010, 2011	298	0.356710
	Selected	0.356707 (5)

At 293.15 K: Density 3515.4 (2) kg m^{-3} Molar volume 3.41661 (5) cm^3 mol^{-1}.

Table 6j. A comparison between high temperature dilatometric values and selected values for diamond

References	Temperature Range K	Deviations 100Δε
Krishnan 1944	298-923	Trends to average 0.009 high at 573 K and above
Krishnan 1946	378-870	Trends to 0.017 high
Berman and Thewlis 1955	300-1100	Maximum deviation 0.010 high at 700 K
Novikova 1960	28-754	In high temperature region trends to 0.004 high at 677 K and above

Table 6k. A comparison between high temperature length change values derived from lattice parameter values and selected values for diamond

References	Temperature Range K	Deviations 100Δε
Mauer and Bolz 1955	273-1663	Scatters 0.015 low to 0.019 high
Thewlis and Davey 1956	119-1198	For industrial quality in high temperature region maximum deviation reaches 0.015 high at 856 K
Skinner 1957	295-1002	For commercial diamond dust trends to 0.015 low
Sokhor and Vitol 1969	273-973	For synthetic diamond trends to 0.027 high and for natural diamond trends to 0.020 high

6.6 A Comparison with previous evaluations for diamond

Touloukian et al. 1977 did not include the measurements of Wright 1965. Although extended to 1650 K the extrapolation appears to be based on experimental values available up to 1000 K. On the basis $100\Delta\varepsilon$ the deviation from the present assessment reaches a maximum of 0.012 low at 1300 K. The evaluation of Reeber and Wang 1996 in the high temperature region appears to be based on the same sources as the present evaluation and therefore differences are down to different interpretations of the input values. However, the agreement is satisfactory with a maximum difference of only 0.006 low at 1300 K before converging towards the selected values. Reeber and Wang 1996 extend the evaluation to 3000 K but the present evaluation is restricted to 2000 K which is close to the experimental limit.

6.5 ^{13}C Diamond

Atomic mass: 13.00335483521 (23) (Wang et al. 2017)

Structure: Cubic (cF8)

Lattice parameter measurements by Holloway et al. 1991 and Yamanaka et al. 1994 on sample containing 1% to 98.5% ^{13}C were extrapolated to pure ^{13}C and corrected to 293.15 K using the thermal expansion coefficients selected for natural diamond.

Table 6l. Lattice parameter of ^{13}C diamond at 293.15 K

References	Original Temperature K	*a* nm
Holloway et al. 1991	298	0.356658
Yamanaka et al. 1994	299	0.356657
	Selected	0.356658 (10)

At 293.15 K: Density 3807.5 (3) kg m^{-3} Molar volume 3.4152 (3) cm^3 mol^{-1}.

$$d1 = \sqrt{3}a/4 = 0.154437 \text{ nm} \quad d2 = a/\sqrt{2} = 0.252195 \text{ nm}$$

Table 6m. Crystallographic properties of diamond

T K	α x 10^6 K^{-1}	100 ε	*a* nm	*d1* nm	*d2* nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
0	0	- 0.00816	0.356678	0.154446	0.252209	3.4158	3516.2
10	< 0.0001	- 0.00816	0.356678	0.154446	0.252209	3.4158	3516.2
20	0.0003	- 0.00816	0.356678	0.154446	0.252209	3.4158	3516.2
30	0.0011	- 0.00816	0.356678	0.154446	0.252209	3.4158	3516.2
40	0.0027	- 0.00816	0.356678	0.154446	0.252209	3.4158	3516.2
50	0.0053	- 0.00815	0.356678	0.154446	0.252209	2.4158	3516.2
60	0.0091	- 0.00815	0.356678	0.154446	0.252209	3.4158	3516.2
70	0.0145	- 0.00814	0.356678	0.154446	0.252209	3.4158	3516.2
80	0.0218	- 0.00812	0.356678	0.154446	0.252209	3.4158	3516.2
90	0.0312	- 0.00807	0.356678	0.154446	0.252210	3.4158	3516.2
100	0.0432	- 0.00805	0.356678	0.154446	0.252210	3.4158	3516.2
110	0.0580	- 0.00800	0.356678	0.154446	0.252210	3.4158	3516.2
120	0.0761	- 0.00794	0.356679	0.154446	0.252210	3.4158	3516.2
130	0.0977	- 0.00785	0.356679	0.154447	0.252210	3.4158	3516.2
140	0.123	- 0.00774	0.356679	0.154447	0.252210	3.4158	3516.2
150	0.153	- 0.00760	0.356680	0.154447	0.252211	3.4158	3516.2
160	0.188	- 0.00743	0.356680	0.154447	0.252211	3.4159	3516.2
170	0.227	- 0.00723	0.356681	0.154447	0.252212	3.4159	3516.1
180	0.271	- 0.00698	0.356682	0.154448	0.252212	3.4159	3516.1
190	0.320	- 0.00668	0.356683	0.154448	0.252213	3.4159	3516.1
200	0.374	- 0.00634	0.356684	0.154449	0.252214	3.4160	3516.1
210	0.431	- 0.00593	0.356686	0.154450	0.252215	3.4160	3516.0
220	0.493	- 0.00547	0.356687	0.154450	0.252216	3.4161	3516.0
230	0.558	- 0.00495	0.356689	0.154451	0.252217	3.4161	3515.9
240	0.626	- 0.00435	0.356691	0.154452	0.252219	3.4162	3515.8
250	0.697	- 0.00369	0.356694	0.154453	0.252221	3.4162	3515.8
260	0.769	- 0.00296	0.356696	0.154454	0.252222	3.4163	3515.7
270	0.843	- 0.00215	0.356699	0.154455	0.252225	3.4164	3515.6
280	0.918	- 0.00127	0.356702	0.154457	0.252227	3.4165	3515.5
290	0.995	- 0.00032	0.356706	0.154458	0.252229	3.4166	3515.4
293.15	1.020	0	0.356707	0.154459	0.252230	3.4166	3515.4
300	1.07	0.0007	0.35671	0.15446	0.25223	3.4167	3515.3
400	1.76	0.0149	0.35676	0.15448	0.25227	3.4181	3513.8
500	2.38	0.0356	0.35683	0.15451	0.25232	3.4202	3511.6
600	2.94	0.0623	0.35693	0.15455	0.25239	3.4230	3508.8
700	3.45	0.0940	0.35704	0.15460	0.25247	3.4263	3505.5
800	3.89	0.131	0.35717	0.15466	0.25256	3.4301	3501.6
900	4.26	0.172	0.35732	0.15472	0.25266	3.4343	3497.3
1000	4.58	0.216	0.35748	0.15479	0.25278	3.4388	3492.7
1100	4.87	0.263	0.35765	0.15487	0.25289	3.4437	3487.7
1200	4.96	0.313	0.35782	0.15494	0.25302	3.4488	3482.6
1300	5.01	0.363	0.35800	0.15502	0.25315	3.4539	3477.4
1400	5.05	0.403	0.35815	0.15508	0.25325	3.4581	3473.2
1500	5.09	0.464	0.35836	0.15518	0.25340	3.4644	3466.9
1600	5.13	0.515	0.35855	0.15525	0.25353	3.4697	3461.6
1700	5.18	0.567	0.35873	0.15533	0.25366	3.4751	3456.2
1800	5.22	0.620	0.35892	0.15542	0.25379	3.4805	3450.8
1900	5.27	0.672	0.35911	0.15550	0.25393	3.5860	3445.4
2000	5.31	0.726	0.35930	0.15558	0.25406	3.4915	3440.0

Interatomic distance calculations for Table 6m: $d1 = \sqrt{3}a/4 \quad d2 = a/\sqrt{2}$

PART 6C. FULLERENE C_{60}

Allotropy: Alpha phase: Cubic (cP240)
Beta phase: Face-centered cubic (cF240)

A value of 260 K is selected for the alpha-beta transformation temperature while a nominal value of 1498 K at one atmosphere pressure is selected for the sublimation point by extrapolating the Clausius-Clapeyron equation selected by Gigli 1999.

6.7 Alpha Phase of C_{60}: Cubic (cP240): 0 K to 260 K.

The structure is cubic conforming to space group Pa3 and undergoes an orientational glass transition in the region of 90 K. Neutron diffraction lattice parameter measurements of David et al. 1992 (5-320 K) were selected. The results were only shown graphically but could generally be read to 0.0001 nm. Powder X-ray measurements of Aksenova et al. 1999 (30-290 K) showed an average bias of only 0.0001 nm low but the measurements of David et al. 1992 were preferred because they agreed with the selected lattice parameter at 293.15 K. A value for the orientational glass transition of 90 K was selected to be consistent with this data although a more likely value is 86 K determined by David et al. 1993 (5-320 K) which agrees with a value of 84.6 K obtained by Miyazaki et al. 1999 on high purity single crystals. A slight anomaly observed in the measurements of Aksenova et al. 1999 at 155 K was not observed by either David et al. 1992 or in the dilatometric measurements of Gugenberger et al. 1992 and was therefore, not included. Values estimated from the measurements of David et al. 1992 were smoothed by fitting to polynomials from which approximate values of the derived thermal expansion coefficients were calculated. These are quoted to the nearest 1×10^{-7} K^{-1} in Table 6k but the most likely accuracies are probably of the order of 10 to 20 %. Thermal expansion values at 10 K and 20 K were estimated:

$$30 - 90\ K: \quad \varepsilon_T = -4.22046 \times 10^{-6} T + 3.79612 \times 10^{-7} T^2 - 3.64887 \times 10^{-9} T^3 + 1.40771 \times 10^{-11} T^4 - 8.14383 \times 10^{-3} \qquad (6g)$$

$$90 - 260\ K: \quad \varepsilon_T = -5.82775 \times 10^{-5} T + 6.44512 \times 10^{-7} T^2 - 2.66348 \times 10^{-9} T^3 + 4.36232 \times 10^{-12} T^4 - 5.50566 \times 10^{-3} \qquad (6h)$$

It is uncertain if the lattice parameter measurements of David et al. 1993, which were also only shown graphically, were simply a re-interpretation of the measurements of David et al. 1992 or new measurements because they did show definate differences reaching 0.00018 nm higher at 100 K while the reported value at 170 K differs from the selected value. The dilatometric measurements of Gugenberger et al. 1992 (5-300 K) were shown only in the form of small graphs but generally appeared to confirm the selected values.

6.8 Beta Phase of C_{60}: Face-centered cubic (cF240): 260 K to 1498 K.

An alpha-beta transition temperature of 260 K is selected to be consistent with the lattice parameter measurements of David et al. 1992, 1993. This is within the experimental accuracy of the most likely value of 261 (1) K as an average of the measurements of De Bruijn et al. 1993 (261.4 K), Lebedev et al. 1996, 1997 (260.7 K) and Miyazaki et al. 1999 (262.1 K). Lattice parameter measurements of David et al. 1992 (260-320 K in the beta region) and Vogel 1996 (300-900 K) were combined. Both sets of measurements were only shown graphically but the latter measurements varied linearly with temperature and could be represented by an average thermal expansion coefficient of 15.23 x 10^{-6} K^{-1}. Over the range 260 K to 900 K the thermal expansion is then given by:

$$a \text{ (nm)} = 2.15670 \times 10^{-5} T + 1.40946 \quad (6i)$$

$$\varepsilon_T = 1.52333 \times 10^{-5} T - 4.46564 \times 10^{-3} \quad (6j)$$

Table 6n. Lattice parameter of beta fullerene C_{60} at 293.15 K

Referencess	Original Temperature K	*a* nm	Note
David et al. 1992	293	1.4158	a
Vogel 1996	RT	1.4155	
Aksenova et al. 1999	290	1.4162	
	Selected	1.4158 (4)	

Note. a. Estimated from graph

At 293.15 K: Density 1687 (1) kg m^{-3} Molar volume 427.25 (36) cm^3 mol^{-1}.

David et al. 1992 determined the lattice expansion at the transition temperature at 260 K to be 0.0049 nm (0.35%) which is equivalent to a molar volume increase of 4.38 cm^3 mol^{-1} (1.04%). From lattice parameter measurements, Heiney et al. 1992 obtained a difference of 0.0044 (4) nm (0.31%) while Gugenberger et al. 1992 determined 0.325 (25) % from dilatometric measurements. Heiney et al. 1992 also determined the thermal expansion coefficient in the room temperature region to be 21 x 10^{-6} K^{-1} which is much higher than the selected value. The lattice parameter measurements of Mathews et al. 1993 (298-773 K) did not show a linear trend with temperature but did give an average thermal expansion coefficient of 15 x 10^{-6} K^{-1}. Aksenova et al. 1999 suggested a very large change in the thermal expansion coefficient over a narrow region increasing from 15.2 x 10^{-6} K^{-1} at 260 K to 19.2 x 10^{-6} K^{-1} at 290 K. It is noted that the lattice parameter reported by David et al. 1993 at 270 K did not agree with the selected value.

Table 6o. Crystallographic properties of alpha fullerene C_{60}

T K	α x 10^6 K^{-1}	100 ε_T	*a* nm	*d* nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
0	0	- 0.820	1.4042	0.9929	416.82	1729
10	1.8	- 0.818	1.4042	0.9929	416.84	1729
20	6.5	- 0.809	1.4043	0.9930	416.96	1728
30	10.3	- 0.802	1.4044	0.9931	417.05	1728
40	12.3	- 0.790	1.4046	0.9932	417.20	1727
50	13.5	- 0.777	1.4048	0.9933	417.36	1727
60	14.2	- 0.764	1.4050	0.9935	417.53	1726
70	14.7	- 0.749	1.4052	0.9936	417.71	1725
75	15.0	- 0.742	1.4053	0.9937	417.81	1725
80	15.4	- 0.734	1.4054	0.9938	417.90	1724
85	15.9	- 0.727	1.4055	0.9938	418.00	1724
90	16.6	- 0.719	1.4056	0.9939	418.11	1724
95	7.1	- 0.715	1.4057	0.9939	418.14	1723
100	8.2	- 0.712	1.4057	0.9940	418.19	1723
105	9.2	- 0.707	1.4058	0.9940	418.25	1723
110	10.1	- 0.702	1.4058	0.9941	418.31	1723
120	11.6	- 0.692	1.4060	0.9942	418.44	1722
130	12.7	- 0.680	1.4062	0.9943	418.60	1722
140	13.5	- 0.666	1.4063	0.9944	418.76	1721
150	14.3	- 0.653	1.4065	0.9946	418.94	1720
160	15.0	- 0.638	1.4067	0.9947	419.12	1719
170	15.8	- 0.623	1.4070	0.9949	419.31	1719
180	16.7	- 0.607	1.4072	0.9950	419.52	1718
190	18.0	- 0.590	1.4074	0.9952	419.73	1717
200	19.6	- 0.571	1.4077	0.9954	419.97	1716
210	21.8	- 0.550	1.4080	0.9956	420.23	1715
220	24.5	- 0.527	1.4083	0.9958	420.52	1714
230	27.9	- 0.501	1.4087	0.9961	420.85	1712
240	32.2	- 0.472	1.4091	0.9964	421.23	1711
250	37.4	- 0.437	1.4096	0.9967	421.67	1709
260	43.6	- 0.397	1.4102	0.9971	422.17	1707

$$d = a/\sqrt{2}$$

Table 6p. Crystallographic properties of beta fullerene C_{60}

T K	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
260	- 0.050	1.4150	1.0006	426.55	1689
270	- 0.035	1.4153	1.0008	426.80	1688
280	- 0.020	1.4155	1.0009	426.99	1688
290	- 0.005	1.4157	1.0011	427.19	1687
293.15	0	1.4158	1.0011	427.25	1687
300	0.010	1.4159	1.0012	427.38	1686
350	0.087	1.4170	1.0020	428.36	1682
400	0.163	1.4181	1.0027	429.34	1678
450	0.239	1.4192	1.0035	430.32	1675
500	0.315	1.4202	1.0043	431.30	1671
550	0.391	1.4213	1.0050	432.28	1667
600	0.467	1.4224	1.0058	433.27	1663
650	0.544	1.4235	1.0066	434.25	1659
700	0.620	1.4246	1.0073	435.24	1656
750	0.696	1.4256	1.0081	436.23	1652
800	0.772	1.4267	1.0088	437.22	1648
850	0.848	1.4278	1.0096	438.21	1644
900	0.924	1.4289	1.0104	439.21	1641

$$d = a/\sqrt{2}$$

PART 6D. FULLERENE C_{70}

Allotropy: Alpha phase: Monoclinic (mS210)
Beta phase: Rhombohedral (hR70)
Gamma phase: Face-centered cubic (cF280)

An alpha-beta transformation temperature of 276 K is selected to be consistent with the crystallographic measurements of Isakina et al. 2001 while Diky and Kabo 2000 select 340 K for the beta-gamma transition. A nominal value of 1562 K at one atmosphere pressure is selected for the sublimation point by extrapolating the Clausius-Clapeyron equation selected by Gigli 1999.

6.10 Alpha Phase of C_{70}: Monoclinic (mS210): 0 K to 276 K.

Lattice parameter measurements of Isakina et al. 2001 (20-305 K) were generally accepted and extrapolated to the transition temperature. Over the range 20 to 276 K the *a* and c axes values could be represented by the equations:

$$a\ (\text{nm}) = 4.25848 \times 10^{-8}\,T + 1.72737 \times 10^{-8}\,T^{2} - 4.19951 \times 10^{-12}\,T^{3} + 1.00448 \qquad (6k)$$

$$c\ (\text{nm}) = -2.39253 \times 10^{-6}\,T + 9.21442 \times 10^{-8}\,T^{2} - 7.97239 \times 10^{-11}\,T^{3} + 2.77797 \qquad (6l)$$

The derived thermal expansion coefficients for the *c* axis indicated that they had been completely miscalculated by Isakina et al. 2001. The *b* axis thermal expansion coefficients behaves in a more complex manner and therefore, the values derived by

Isakina et al. 2001 were accepted except that the values at 70 K, 220 K and 265 K were adjusted in order to give a smooth continuity. Vaughan et al. 1993 determined lattice parameters values at 15 K which agree satisfactorily with those of Isakina et al. 2001 at 20 K except that the *a* and *b* axes were transposed.

Above 180 K the angle β thermal expansion is given by:

$$\beta \text{ (rads)} = -9.09026 \times 10^{-6} T + 2.08957 \quad (6m)$$

The principal thermal expansion coefficients are α_1 , α_2 and α_3 where $\alpha_2 = \alpha_b$ and α_1 and α_3 are given by: $\alpha_1 - \alpha_3 = -\Delta / \sin\beta \cos(2\varphi - \beta)$; $\alpha_1 + \alpha_3 = \alpha_a + \alpha_c + \Delta / \tan\beta$; where $\tan(2\varphi - \beta) = (\alpha_a - \alpha_c) / \Delta$ and $\alpha_{avr} = (\alpha_1 + \alpha_2 + \alpha_3)/3$ where Δ is the angle β thermal expansion coefficient = -9.09×10^{-6} rads K^{-1} and the φ is the angle between the *x* axis of the principal tensor ellipsoid and the crystallographic *a* axis. Because the abrupt change at 180 K from Δ = 0 to Δ = -9.09×10^{-6} rads K^{-1} is considered to be unnatural behavior then values of $\alpha_b = \alpha_2$ and α_{avr} at 190 K and 200 K were adjusted to give a smooth continuity.

6.11 Beta Phase of C_{70}: Rhombohedral (hR70): 276 K to 340 K.

Lattice parameter measurements of Isakina et al. 2001 (20-305 K) gave room temperature values in the text for the equivalent hexagonal cell as well as graphical representations which were completely different to the tabulated values. However, lattice parameter values determined by Vaughan et al. 1993 for the hexagonal cell at 300 K agree closely with the tabulated values which were therefore accepted and were converted to length change values and fitted to the following equations which were extrapolated to the upper transition temperature:

$$\varepsilon_T a = 5.28040 \times 10^{-3} T - 2.00286 \times 10^{-5} T^2 + 2.53551 \times 10^{-8} T^3 - 0.465509 \quad (6n)$$

$$\varepsilon_T c = -3.35886 \times 10^{-3} T + 1.36954 \times 10^{-5} T^2 - 1.85965 \times 10^{-8} T^3 + 0.276200 \quad (6o)$$

The molar volume change at the transition temperature at 260 K is an expansion of 7.61 $cm^3 mol^{-1}$ (1.6 %).

6.12 Gamma Phase of C_{70}: Face-centered cubic (cF280): 340 K to 1562 K.

Although face-centered cubic is the true structure the effect of impurities and different preparation techniques can lead to the formation of either a hexagonal close-packed structure or a mixture of both phases. Lattice parameters determined at the metastable temperature 293 K show relatively poor agreement varying between 1.489 nm (Valsakumar et al. 1993) and 1.508 nm (Misof et al. 1993). The lattice parameter measurements of McGhie et al. 1994 at 366 K and 381 K show a high degree of correlation with the value determined by Vaughan et al. 1991 at 440 K. Because the temperature range covered by these three values is too narrow to obtain a satisfactory thermal expansion value then the value of 25×10^{-6} K^{-1} determined by Mathews et al. 1993 as an average over the range 298 to 773 K is adopted. Although this appears to have

been determined on the hexagonal close-packed structure it is assumed that it could also be adopted for the face-centered cubic structure on the grounds that they are both close packed structures. In combination with the lattice parameter values of McGhie et al. 1994 and Mathews et al. 1991 then this leads to the equations:

a (nm) = 3.71030 x 10^{-5} T + 1.48412 (6p)

ε_T = 2.48719 x 10^{-5} T – 2.69480 x 10^{-3} (6q)

The extrapolated value at 293.15 K, 1.4950 (5) nm, is in agreement with values of 1.496 nm determined by Fleming et al. 1991 and Fisher and Heiney 1993 and 1.4943 nm determined by Christides et al. 1993. At the beta-gamma transition there is an estimated molar volume increase of 4.44 cm^3 mol^{-1} (0.89%) but this value must be considered to be tentative.

Table 6q. Crystallographic properties of alpha fullerene C_{70}

T K	α_a x 10^6 K^{-1}	α_b x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_1 x 10^6 K^{-1}	α_2 x 10^6 K^{-1}	α_3 x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	φ°
0	0	0	0	0	0	0	0	-
20	0.7	2.0	0.4	0	2.0	0	1.1	-
30	1.1	3.1	1.1	0	3.1	0	1.7	-
40	1.4	4.3	1.7	0	4.3	0	2.5	-
50	1.7	5.2	2.2	0	5.2	0	3.1	-
60	2.1	6.5	2.8	0	6.5	0	3.8	-
70	2.4	7.5	3.4	0	7.5	0	4.4	-
80	2.7	8.5	3.9	0	8.5	0	5.0	-
90	3.0	10.4	4.4	0	10.4	0	6.0	-
100	3.4	11.6	4.9	0	11.6	0	6.6	-
110	3.7	11.6	5.4	0	11.6	0	6.9	-
120	4.0	12.2	5.9	0	12.2	0	7.4	-
130	4.3	12.6	6.3	0	12.6	0	7.7	-
140	4.6	13.1	6.7	0	13.1	0	8.2	-
150	4.9	12.6	7.1	0	12.6	0	8.2	-
160	5.2	11.2	7.5	0	11.2	0	8.0	-
170	5.5	9.5	7.9	0	9.5	0	7.6	-
180	5.8	7.4	8.3	0	7.4	0	7.2	-
190	6.1	2.3	8.6	15.4	2.3	4.5	7.4	67.5
200	6.4	2.3	9.0	15.7	2.3	4.8	7.6	67.6
210	6.7	2.7	9.3	16.0	2.7	5.2	8.0	67.6
220	7.0	3.3	9.6	16.3	3.3	5.4	8.3	67.7
230	7.3	5.3	9.8	16.6	5.3	5.7	9.2	67.6
240	7.6	12.6	10.1	16.8	12.6	6.0	11.8	67.5
245	7.7	36.2	10.2	17.0	36.2	6.1	19.8	67.5
250	7.8	48.2	10.3	17.1	48.2	6.3	23.8	67.4
255	8.0	92.5	10.4	17.2	92.5	6.4	38.7	67.3
260	8.1	156	10.6	17.3	156	6.5	59.8	67.2
265	8.3	209	10.7	17.4	209	6.6	77.8	67.2
270	8.4	261	10.8	17.6	261	6.8	95.0	67.1
275	8.5	316	10.9	17.7	316	6.9	114	66.9
276	8.6	327	10.9	17.7	327	6.9	117	66.9

Table 6r. Crystallographic properties of alpha fullerene C_{70}

T K	100 ε_T avr	*a* nm	*b* nm	*c* nm	β°	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	- 0.842	1.0045	0.9936	2.7779	119.63	483.76	1738
20	- 0.842	1.0045	0.9936	2.7779	119.63	483.76	1738
30	- 0.839	1.0045	0.9936	2.7780	119.63	483.79	1738
40	- 0.836	1.0045	0.9937	2.7781	119.63	483.84	1738
50	- 0.835	1.0045	0.9937	2.7781	119.63	483.86	1737
60	- 0.830	1.0045	0.9938	2.7782	119.63	483.93	1737
70	- 0.826	1.0046	0.9938	2.7783	119.63	483.99	1737
80	- 0.822	1.0046	0.9939	2.7783	119.63	484.04	1737
90	- 0.818	1.0046	0.9940	2.7784	119.63	484.11	1736
100	- 0.813	1.0046	0.9941	2.7785	119.63	484.17	1736
110	- 0.804	1.0047	0.9942	2.7787	119.63	484.31	1736
120	- 0.796	1.0047	0.9944	2.7788	119.63	484.42	1735
130	- 0.787	1.0048	0.9945	2.7790	119.63	484.55	1735
140	- 0.782	1.0048	0.9946	2.7792	119.63	484.64	1735
150	- 0.769	1.0049	0.9948	2.7794	119.63	484.82	1734
160	- 0.764	1.0049	0.9949	2.7796	119.63	484.90	1734
170	- 0.754	1.0050	0.9950	2.7799	119.63	485.05	1733
180	- 0.750	1.0050	0.9950	2.7802	119.63	485.10	1733
190	- 0.741	1.0051	0.9950	2.7804	119.62	485.23	1733
200	- 0.735	1.0051	0.9951	2.7806	119.62	485.32	1732
210	- 0.733	1.0052	0.9950	2.7808	119.62	485.35	1732
220	- 0.724	1.0053	0.9950	2.7810	119.61	485.48	1732
230	- 0.720	1.0053	0.9950	2.7813	119.61	485.53	1732
240	- 0.707	1.0054	0.9951	2.7816	119.60	485.73	1731
245	- 0.696	1.0055	0.9952	2.7817	119.59	485.90	1730
250	- 0.687	1.0055	0.9954	2.7819	119.59	486.03	1730
255	- 0.679	1.0055	0.9956	2.7820	119.59	486.14	1729
260	- 0.640	1.0056	0.9966	2.7822	119.59	486.71	1727
265	- 0.609	1.0056	0.9974	2.7823	119.58	487.17	1726
270	- 0.577	1.0057	0.9982	2.7825	119.58	487.65	1724
275	- 0.526	1.0057	0.9997	2.7826	119.58	488.40	1721
276	- 0.516	1.0057	1.0000	2.7826	119.58	488.54	1721

$\varepsilon_{avr} = [(V_{m\,(T)} / V_{m\,(293.15)})^{⅓} - 1]$ where V_m = molar volume

Table 6s. Crystallographic properties of beta fullerene C_{70}

T K	$\alpha_{ah} \times 10^6$ K^{-1}	$\alpha_{ch} \times 10^6$ K^{-1}	$\alpha_{avr} \times 10^6$ K^{-1}	100 ε_T *a*	100 ε_T *c*	100 ε_T avr
276	19.0	- 48.8	- 3.6	- 0.075	0.143	- 0.002
280	27.9	- 63.3	- 2.5	- 0.064	0.121	- 0.003
290	60.9	- 107	4.8	- 0.021	0.036	- 0.004
293.15	74.4	- 124	8.0	0	0	0
300	109	- 163	18.4	0.062	- 0.098	0.009
310	172	- 230	38.2	0.202	- 0.293	0.037
320	250	- 308	64.0	0.413	- 0.560	0.089
330	343	- 399	95.4	0.709	- 0.909	0.170
340	449	- 502	132	1.108	- 1.354	0.287

Table 6t. Crystallographic properties of beta fullerene C_{70}

T K	a_h nm	c_h nm	a_r nm	α°	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
276	1.0111	2.7917	1.0985	54.802	496.15	1695
280	1.0112	2.7911	1.0984	54.815	496.14	1695
290	1.0116	2.7887	1.0978	54.869	496.15	1695
293.15	1.0119	2.7877	1.0976	54.894	496.18	1694
300	1.0125	2.7850	1.0970	54.963	496.31	1694
310	1.0139	2.7796	1.0959	55.106	496.73	1693
320	1.0160	2.7721	1.0945	55.310	497.48	1690
330	1.0190	2.7624	1.0927	55.588	498.67	1686
340	1.0231	2.7500	1.0905	55.950	500.37	1680

Table 6u. Crystallographic properties of gamma fullerene C_{70}

T K	$100\ \varepsilon_T$	a nm	d nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
340	0.576	1.4967	1.0584	504.81	1665
350	0.601	1.4971	1.0586	505.18	1664
400	0.726	1.4990	1.0599	507.06	1658
450	0.850	1.5008	1.0612	508.95	1652
500	0.975	1.5027	1.0625	510.84	1646
550	1.100	1.5045	1.0639	512.73	1640
600	1.224	1.5064	1.0652	514.63	1634
650	1.349	1.5082	1.0665	516.53	1628
700	1.474	1.5101	1.0678	518.44	1622
750	1.598	1.5119	1.0691	520.36	1616

$$d = a/\sqrt{2}$$

$$\varepsilon_{avr} = [(V_{m\,(T)} / V_{m\,(293.15)})^{\frac{1}{3}} - 1] \text{ where } V_m = \text{molar volume}$$

PART 6E. OTHER FULLERENES

6.13 FULLERENE C_{76}

Nakoa et al. 1998 (10-550 K) identified the structure to be both face-centered cubic (cF304) and hexagonal close-packed (hP152) with both structures showing transitions at 140 (10) K and 420 (10) K. In both cases the lattice thermal expansion was shown graphically. At 300 K the face-centered cubic structure has a lattice parameter of 1.5421 (11) nm, a density of 1653 (4) $kg\ m^{-3}$ and a molar volume of 552.1 (1.2) $cm^3\ mol^{-1}$ and the hexagonal structure lattice parameters of *a* 1.0931 (7) nm *c* 1.7716 (29) nm, a density of 1654 (4) $kg\ m^{-3}$ and a molar volume 552.0 (1.2) $cm^3\ mol^{-1}$.

6.14 FULLERENE C_{84}

Margadonna et al. 1998 (5-295 K) identified the structure to be face-centered cubic (cF336). The results were shown graphically. At 293 K the lattice parameter was estimated to be 1.5920 (4) nm, the density 1661 (1) kg m^{-3} and the molar volume 607.5 (0.5) cm^3 mol^{-1}.

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7 NITROGEN N

Natural nitrogen contains 0.3663 (4**)** % of ^{15}N for the best representative sample (Meija et al. 2016) and measurements are made on this basis although ^{15}N has been separated and crystallographic properties determined.

PART 7A. NATURAL NITROGEN

Atomic Weight: 14.00643 to 14.00728 (Meija 2017)
Select 2007 value 14.0067 (2) (Wieser and Berglund 2009)

Allotropy: Alpha: Cubic (cP8)
Beta: Hexagonal close-packed (hP4)

The alpha-beta transition temperature and triple point are secondary fixed points on ITS-90 at 35.614 (6) K and 63.151 (1) K respectively (Bedford et al. 1996). For both the alpha and beta phases the lattice parameter measurements of Krupskii et al. 1975 were selected after correction to nm using the default ratio 0.100207697/1.00202. Although given to five significant figures the lattice parameter values are considered at best to be accurate to 0.0001 nm (0.02%).

7.1 Alpha nitrogen: Cubic (cP8): 0 K to 35.614 K.

From single crystal diffraction measurements Jordan et al. 1964 concluded that the structure type was $P2_13$ but later diffraction measurements by Schuch and Mills 1970 and Krupskii et al. 1975 suggested that the structure conformed to space group Pa3 and this was accepted for both natural nitrogen and $^{15}N_2$.

Corrected lattice parameter measurements of Krupskii et al. 1975 (8-35.5 K) from 8 K to 28 K were fitted to Equation B using the enthalpy values tabulated in Part 7.2. This equation was extrapolated to 0 K:

$$\ln (a, \text{nm}) = (H_T - H_0)(6.45381 \times 10^{-6} + 1.20940 \times 10^{-7} T + 7.45446 \times 10^{-5}/T) - 0.571120 \quad (7a)$$

Above 28 K length change values relative to 0 K were represented by:

$$\varepsilon_0 = 2.39122 \times 10^{-3} T - 8.72944 \times 10^{-5} T^2 + 1.23188 \times 10^{-6} T^3 - 2.13278 \times 10^{-2} \quad (7b)$$

Direct thermal expansion coefficient measurements of Tolkachev et al. 1978 (2.2-21.0 K) are considerably lower than those derived from Equations 7a and 7b being initially four times lower and then converging towards the selected values but only showing agreement at 18 K and above. Similar measurements of Heberlein et al. 1970 (4.2 – 40 K) were only shown graphically but appear to be considerably lower than even the measurements of Tolkachev et al. 1978.

Table 7a. A comparison of lattice parameter measurements of alpha nitrogen at 20 K

References	*a* nm	Notes
Vegard 1929a	0.566	
Vegard 1929b	0.567	
De Smedt et al. 1929	0.5668	
Ruhemann 1932	0.568	
Bolz et al. 1959	0.5662	a
Kogan and Omarov 1963	0.5660	
Hörl and Marton 1961	0.5661	b
Tolkachev and Manzhelli 1965	0.5659	c
Schuch and Mills 1970	0.5649	
	0.5656	d
Selected (Krupskii et al. 1975)	0.5658_4	

Notes for Table 7a

a. Extrapolated from 4.2 K

b. Electron diffraction measurement

c. From direct density measurement 1025.3 kg m^{-3} at 20.4 K

d. From molar volume value 27.24 cm^3 mol^{-1}

Calculation of interatomic distances in alpha nitrogen

Positional parameter $x = r_e / [2 \sqrt{3}\, a\, (T)]$ where r_e is the bond length 0.109768071 (12) nm (Bendtsen 2001).

$d1 = a\,(0.5 - 2\,x + 4\,x^2)^{½}$ $d2 = a\,(0.5 - 2\,x + 8\,x^2)^{½}$

7.2 Selected values of the specific heat and enthalpy of alpha nitrogen

Values are based on the measurements of Bagatskii et al. 1968 (2.6-14.5 K) and Giauque and Clayton 1933 (15.8-61.4 K). Units for C_p are J mol^{-1} K^{-1} and for $H_T - H_0$ in J mol^{-1}

Table 7b. Specific heat and enthalpy values for alpha nitrogen

T K	1	2	3	4	5	6	7	8	9
C_p	0.0037	0.0293	0.0987	0.243	0.481	0.862	1.54	2.36	3.46
$H_T - H_0$	0.00092	0.0146	0.0752	0.238	0.588	1.23$_5$	2.42	4.35	7.24
T K	10	11	12	13	14	15	16	17	18
C_p	4.77	6.15	7.87	9.32	10.67	12.05	13.47	15.02	16.32
$H_T - H_0$	11.35	16.78	23.81	32.42	42.42	53.77	66.53	80.77	96.58
T K	19	20	21	22	23	24	25	26	27
C_p	18.23	19.83	21.32	22.76	24.17	25.56	26.99	28.41	29.76
$H_T - H_0$	114.0	133.1	153.6	175.7	199.2	224.0	250.3	278.0	307.1
T K	28	29	30	31	32	33	34	35	35.614
C_p	31.17	32.63	34.15	35.72	37.34	39.03	40.76	42.55	43.68
$H_T - H_0$	337.6	369.5	402.8	437.8	474.3	512.5	552.4	594.0	620.5

7.3 Beta nitrogen: Hexagonal close-packed (hP4): 35.614 K to 63.151 K.

Corrected lattice parameter measurements of Krupskii et al. 1975 (36.7-63 K) were fitted to the equations:

$$a \text{ (nm)} = 6.97471 \times 10^{-4} T - 1.14952 \times 10^{-5} T^2 + 9.44963 \times 10^{-8} T^3 + 0.3895795 \quad (7c)$$

$$c \text{ (nm)} = 1.17530 \times 10^{-3} T - 1.49472 \times 10^{-5} T^2 + 1.10130 \times 10^{-7} T^3 + 0.6310809 \quad (7d)$$

The molar volume increase at the alpha-beta transition of 0.20 cm^3 mol^{-1} (0.73%) is notably lower than the value of 0.311 (25) cm^3 mol^{-1} calculated by Brookeman and Scott 1973 from the Clausius-Clapeyron equation.

Table 7c. A comparison of lattice parameter measurements of beta nitrogen at 45 K

References	Original Temperature K	*a* nm at 45 K	*c* nm at 45 K
Ruhemann 1932	39	0.4056	0.6631
Vegard 1932	43-48	0.4047	0.6683
Schuch and Mills 1970	46	0.4048	0.6599
Selected (Krupskii et al. 1975)	45	0.4063$_0$	0.6637$_4$

The agreement is unsatisfactory and an average would be meaningless.

Table 7d. Crystallographic properties of alpha nitrogen

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_0$	*a* nm	*x*	*d*1 nm	*d*2 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	0	0.56489	0.05609	0.35745	0.36302	27.139	1032.2
2	1.02	0.0001	0.56489	0.05609	0.35745	0.36302	27.139	1032.2
4	5.13	0.0006	0.56490	0.05609	0.35745	0.36302	27.139	1032.2
5	8.88	0.0013	0.56490	0.05609	0.35745	0.36302	27.139	1032.2
6	14.5	0.0024	0.56491	0.05609	0.35746	0.36303	27.140	1032.2
8	35.0	0.0073	0.56493	0.05609	0.35748	0.36305	27.142	1032.0
10	65.0	0.0244	0.56499	0.05608	0.35751	0.36309	27.153	1031.7
12	102	0.0336	0.56508	0.05608	0.35758	0.36315	27.166	1031.2
14	133	0.0572	0.56522	0.05606	0.35767	0.36324	27.185	1030.5
15	148	0.0712	0.56529	0.05605	0.35773	0.36330	27.197	1030.0
16	164	0.0868	0.56538	0.05605	0.35779	0.36336	27.209	1029.5
18	183	0.123	0.56559	0.05603	0.35794	0.36350	27.239	1028.4
20	198	0.168	0.56584	0.05600	0.35811	0.36368	27.276	1027.1
22	279	0.220	0.56613	0.05597	0.35832	0.36388	27.318	1025.5
24	317	0.279	0.56647	0.05594	0.35855	0.36411	27.367	1023.6
25	337	0.312	0.56666	0.05592	0.35868	0.36424	27.394	1022.6
26	357	0.347	0.56685	0.05590	0.35882	0.36438	27.422	1021.6
28	398	0.423	0.56728	0.05586	0.35912	0.36467	27.484	1019.2
30	477	0.510	0.56778	0.05581	0.35947	0.36501	27.556	1016.6
32	585	0.617	0.56838	0.05575	0.35989	0.36543	27.644	1013.4
34	722	0.748	0.56912	0.05568	0.36041	0.36594	27.752	1009.4
35	801	0.825	0.56955	0.05564	0.36071	0.36624	27.816	1007.1
35.614	853	0.876	0.56984	0.05561	0.36092	0.36644	27.858	1005.6

Table 7e. Crystallographic properties of beta nitrogen

T K	$\alpha_a \times 10^6$ K^{-1}	$\alpha_c \times 10^6$ K^{-1}	$\alpha_{avr} \times 10^6$ K^{-1}	$100\ \varepsilon_0$ avr
35.614	589	803	660	1.120
36	586	799	657	1.146
38	574	782	645	1.278
40	571	769	637	1.408
42	572	759	634	1.536
44	578	753	637	1.665
45	583	752	640	1.730
46	590	752	644	1.796
48	607	754	656	1.928
50	630	760	673	2.063
52	658	770	695	2.203
54	692	785	723	2.348
55	710	793	738	2.423
56	731	803	755	2.499
58	775	825	792	2.658
60	825	850	834	2.825
62	881	880	880	3.001
63	910	897	906	3.093
63.151	915	899	910	3.107

Table 7f. Crystallographic properties of beta nitrogen

T K	*a* nm	*c* nm	*c*/*a*	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
35.614	0.40411	0.65895	1.6306	28.061	998.3
36	0.40420	0.65916	1.6308	28.082	997.5
38	0.40467	0.66020	1.6315	28.192	993.7
40	0.40513	0.66123	1.6321	28.301	989.8
42	0.40560	0.66224	1.6327	28.409	986.1
44	0.40606	0.66324	1.6333	28.517	952.3
45	0.40654	0.66374	1.6336	28.572	980.5
46	0.40702	0.66424	1.6339	28.627	978.6
48	0.40727	0.66524	1.6344	28.739	974.8
50	0.40753	0.66624	1.6348	28.853	970.9
52	0.40805	0.66726	1.6352	28.972	966.9
54	0.70860	0.66830	1.6356	29.096	962.8
55	0.40889	0.66883	1.6357	29.159	960.7
56	0.40918	0.66936	1.6359	29.225	958.5
58	0.40980	0.67045	1.6360	29.361	954.1
60	0.41046	0.67158	1.6362	29.504	949.5
62	0.41116	0.67274	1.6362	29.656	944.6
63	0.41152	0.67334	1.6362	29.735	942.1
63.151	0.41158	0.67343	1.6362	29.748	941.7

PART 7B. NITROGEN 15

Atomic mass ^{15}N: 15.0001088989 (6) (Wang et al. 2017)

Allotropy: Alpha: Cubic (cP8)
Beta: Hexagonal close-packed (hP4)

Clusius et al. 1959 determined the alpha-beta transition temperature to be 36.68 K and the triple point to be 63.19 K. For both the alpha and beta phases the lattice parameter measurements of Krupskii et al. 1980 were selected after correction to nm using the ratio 0.100207697/1.00202. Although given to five significant figures the lattice parameter values are considered at best to be accurate to 0.0001 nm.

7.4 Alpha nitrogen (^{15}N): Cubic (cP8): 0 K to 35.68 K.

Corrected lattice parameter measurements of Krupskii et al. 1980 (6-35.6 K), up to 20 K, were fitted to Equation B using the enthalpy values tabulated in Part 7.5. This equation was extrapolated to 0 K:

$$\ln (a, \text{nm}) = (H_T - H_0)(-1.13740 \times 10^{-5} + 5.88306 \times 10^{-7}\, T + 2.38610 \times 10^{-4}/T) - 0.572204 \quad (7e)$$

Above 20 K length change values relative to 0 K were represented by:

$\varepsilon_0 = -\ 7.50675 \times 10^{-4}\, T + 5.60558 \times 10^{-5}\, T^2 - 1.53542 \times 10^{-6}\, T^3 + 1.85964 \times 10^{-8}\, T^4 - 3.58504 \times 10^{-3}$ (7f)

Calculation of interatomic distances in alpha nitrogen (^{15}N)

Positional parameter $x = r_e / [2\sqrt{3}\, a\,(T)]$ where r_e is the bond length 0.109767730 (33) nm (Bendtsen 2001).

$d1 = a\,(0.5 - 2x + 4x^2)^{1/2}$ $\quad d2 = a\,(0.5 - 2x + 8x^2)^{1/2}$

7.5 Selected values of the specific heat and enthalpy of alpha nitrogen (^{15}N)

Measurements of Clausius et al. 1959 (10-63 K) were selected. Extrapolated specific heat values below 10 K were estimated by relating directly to the selected values for natural nitrogen as $C_p\,(^{15}N_2) = 4.94\ C_p\,(^{nat}N_2) / 4.77$. Units for C_p are J mol^{-1} K^{-1} and for $H_T - H_0$ in J mol^{-1}

Table 7g. Specific heat and enthalpy values for alpha nitrogen (^{15}N)

T K	1	2	3	4	5	6	7	8	9
C_p	0.0038	0.0303	0.102	0.25	0.50	0.89	1.59	2.45	3.58
$H_T - H_0$	0.00095	0.0151	0.077	0.25	0.61	1.28	2.51	4.51	7.50
T K	10	11	12	13	14	15	16	17	18
C_p	4.94	6.36	7.80	9.31	10.96	12.80	14.29	15.56	16.99
$H_T - H_0$	11.76	17.41	24.48	33.02	43.14	55.05	68.61	83.53	99.80
T K	19	20	21	22	23	24	25	26	27
C_p	18.41	19.87	21.16	22.43	23.81	25.23	26.64	28.07	29.55
$H_T - H_0$	117.5	136.7	157.2	179.0	202.1	226.6	252.5	279.9	308.7
T K	28	29	30	31	32	33	34	35	35.68
C_p	31.04	37.07	33.90	35.40	36.91	38.42	39.95	41.49	42.55
$H_T - H_0$	339.0	370.7	403.9	438.6	474.7	512.4	551.6	592.3	620.9

7.6 Beta nitrogen (^{15}N): Hexagonal close-packed (hP4): 35.614 K to 63.151 K.

Corrected lattice parameter measurements of Krupskii et al. 1980 (35.9-63 K) were fitted to the equations:

a (nm) $= 6.61141 \times 10^{-3}\, T - 1.86674 \times 10^{-4}\, T^2 + 2.38147 \times 10^{-6}\, T^3 - 1.10246 \times 10^{-8}\, T^4 + 0.3151493$ (7g)

c (nm) $= -1.17035 \times 10^{-2}\, T + 3.46343 \times 10^{-4}\, T^2 - 4.39168 \times 10^{-6}\, T^3 + 2.09198 \times 10^{-8}\, T^4 + 0.8015346$ (7h)

The molar volume increase at the alpha beta transition is 0.27 cm^3 mol^{-1} (0.97%)

Table 7h. Crystallographic properties of alpha nitrogen (^{15}N)

T K	α x 10^6 K^{-1}	100 ε_0	*a* nm	*x*	*d*1 nm	*d*2 nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
0	0	0	0.56428	0.05616	0.35702	0.35702	27.051	1109.0
2	2.41	0.0002	0.56428	0.05616	0.35702	0.35702	27.051	1109.0
4	9.12	0.0013	0.56429	0.05615	0.35702	0.35702	27.052	1109.0
5	14.2	0.0024	0.56429	0.05615	0.35703	035703	27.052	1109.0
6	20.7	0.0041	0.56430	0.05615	0.35703	0.35703	27.054	1108.9
8	42.6	0.0104	0.56434	0.05615	0.35706	0.35706	27.059	1108.7
10	69.6	0.0216	0.56440	0.05615	0.35710	0.35710	27.068	1108.3
12	95.3	0.0381	0.56450	0.05614	0.35717	0.35717	27.081	1107.8
14	125	0.0600	0.56462	0.05612	0.35726	0.35726	27.099	1107.0
15	145	0.0736	0.56470	0.05611	0.35731	0.35721	27.110	1106.6
16	161	0.0889	0.56478	0.05611	0.35737	0.35737	27.123	1106.1
18	197	0.125	0.56498	0.05609	0.35751	0.35751	27.152	1104.9
20	244	0.169	0.56523	0.05606	0.35768	0.35768	27.188	1103.5
22	278	0.221	0.56553	0.05603	0.35789	0.35789	27.230	1101.7
24	314	0.280	0.56586	0.05600	0.35813	0.35813	27.278	1099.8
25	334	0.313	0.56604	0.05598	0.35826	0.35826	27.305	1098.7
26	357	0.347	0.56624	0.05596	0.35839	0.35839	27.333	1097.6
28	408	0.424	0.56667	0.05592	0.35870	0.35870	27.396	1095.1
30	473	0.512	0.56717	0.05587	0.35905	0.35905	27.468	1092.2
32	554	0.615	0.56775	0.05581	0.35945	0.35945	27.553	1088.8
34	655	0.737	0.56844	0.05574	0.35993	0.35993	27.653	1084.9
35	714	0.805	0.56883	0.05571	0.36021	0.36021	27.709	1082.7
35.68	758	0.856	0.56911	0.05568	0.36041	0.36041	27.751	1081.0

Table 7i. Crystallographic properties of beta nitrogen (^{15}N)

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 ε_0 avr
35.68	947	61.0	652	1.179
36	922	95.2	647	1.200
38	794	281	623	1.329
40	707	423	612	1.454
42	657	527	613	1.578
44	638	598	625	1.704
45	639	624	634	1.768
46	646	644	645	1.838
48	674	670	673	1.967
50	718	683	706	2.108
52	772	687	744	2.256
54	831	690	784	2.412
55	861	693	805	2.493
56	890	698	826	2.577
58	943	716	867	2.751
60	985	751	907	2.933
62	1,011	809	944	3.124
63	1,016	848	960	3.222
63.19	1,017	856	963	3.241

Table 7j. Crystallographic properties of beta nitrogen (^{15}N)

T K	*a* nm	*c* nm	*c*/*a*	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
35.68	0.40370	0.65929	1.6331	28.019	1070.7
36	0.40382	0.65931	1.6327	28.036	1070.0
38	0.40451	0.65956	1.6305	28.143	1066.0
40	0.40512	0.66003	1.6292	28.247	1062.0
42	0.40567	0.66066	1.6286	28.358	1058.2
44	0.40619	0.66141	1.6283	28.457	1054.2
45	0.40645	0.66181	1.6283	28.511	1052.3
46	0.40671	0.66223	1.6283	28.565	1050.2
48	0.40725	0.66311	1.6283	28.678	1046.1
50	0.40781	0.66401	1.6282	28.797	1041.8
52	0.40842	0.66492	1.6280	28.923	1037.3
54	0.40908	0.66583	1.6276	29.055	1032.5
55	0.40942	0.66629	1.6274	29.125	1030.1
56	0.40978	0.66676	1.6271	29.196	1027.5
58	0.41053	0.66770	1.6264	29.345	1022.3
60	0.41133	0.66868	1.6257	29.501	1016.9
62	0.41215	0.66972	1.6249	29.666	1011.3
63	0.41257	0.67027	1.6246	29.751	1008.4
63.19	0.41265	0.67038	1.6246	29.767	1007.8

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8 OXYGEN O

Distinction is made between oxygen (O_2) and ozone (O_3).

Atomic Weight: 15.99903 to 15.99977 (Meija 2017)
Select 2007 value 15.9994 (3) (Wieser and Berglund 2009).

PART 8A. OXYGEN (O_2)

Allotropy: Alpha: Monoclinic (mS4)
Beta: Rhombohedral (hR2)
Gamma: Cubic (cP16)

The alpha-beta and beta-gamma transformation temperatures are secondary fixed points on ITS-90 at 23.868 (5) K and 43.796 (1) K respectively (Bedford et al. 1996) and the triple point is a primary fixed point on ITS-90 at 54.3584 K (Preston Thomas 1990).

A review on solid oxygen was carried out by Freiman and Jodl 2004. A previous review by Roder 1978 was hampered by apparent errors in the primary data sources.

The lattice parameter measurements of Krupskii et al. 1979 cover all three phases and are selected. All values were corrected from Å units to nm using the default ratio 0.100207697 / 1.00202.

8.1 Alpha Phase: Monoclinic (mS4: 0 K to 23.868 K.

Corrected measurements of Krupskii et al. (7-23.5 K) over the range 7 K to 20 K were combined with the enthalpy measurements as given in Part 8.6 and fitted to Equation B. Equations 8a, 8c and 8e were extrapolated to 0 K. From 20 K to 23.5 K the measurements were fitted to polynomial equations because of the ambiguous behavior of the specific heat above this temperature and were extrapolated to the transition temperature:

a axis

$$\text{0-20 K:} \quad \ln(a, \text{nm}) = (H_T - H_0)(-1.17416 \times 10^{-4} + 3.94212 \times 10^{-6} T + 1.43943 \times 10^{-3} / T) - 0.620819 \tag{8a}$$

$$\text{20-23.868 K:} \quad \ln(a, \text{nm}) = -0.571529 T + 4.02725 \times 10^{-2} T^2 - 1.26227 \times 10^{-3} T^3 + 1.48702 \times 10^{-5} T^4 + 2.42235 \tag{8b}$$

b axis

$$\text{0-20 K:} \quad \ln(b, \text{nm}) = (H_T - H_0)(-6.94446 \times 10^{-5} + 1.05023 \times 10^{-6} T + 1.11398 \times 10^{-3} / T) - 1.07165 \tag{8c}$$

$$\text{20-23.868 K:} \quad \ln(b, \text{nm}) = 0.260286 T - 1.81490 \times 10^{-2} T^2 + 5.62695 \times 10^{-4} T^3 - 6.54990 \times 10^{-6} T^4 - 2.47076 \tag{8d}$$

c axis

0-20 K: $\ln(c, \text{nm}) = (H_T - H_0)(-1.11614 \times 10^{-4} + 2.88407 \times 10^{-6} T + 1.42582 \times 10^{-3} / T) - 0.857581$ (8e)

20-23.868 K: $\ln(c, \text{nm}) = -0.295775 T + 2.13112 \times 10^{-2} T^2 - 6.82985 \times 10^{-4} T^3 + 8.22177 \times 10^{-6} T^4 + 0.683211$ (8f)

The angle β was smoothed by interpolation using low order polynomials. Different monoclinic cells give different values for the *c*-axis and the angle β and therefore selection followed Delone's rule (Delaunay 1933) in which the cell giving the lowest value of β was selected. The relationship between the different cells is given below.

Average length change and thermal expansion values take into account the angle β from the equation $r = (a\ b\ c \sin \beta)^{1/3}$:

0-20 K: $\ln(r, \text{nm}) = (H_T - H_0)(-9.95298 \times 10^{-5} + 2.56827 \times 10^{-6} T + 1.33377 \times 10^{-3} / T) - 0.890776$ (8g)

20-23.868 K: $\ln(r, \text{nm}) = -0.181346 T + 1.30117 \times 10^{-2} T^2 - 4.15208 \times 10^{-4} T^3 + 4.97892 \times 10^{-6} T^4 + 5.79857 \times 10^{-2}$ (8h)

Although given to five significant figures the measurements of Krupskii et al. 1979 are considered to be accurate to 0.06%, essentially ± 0.0003 nm, with the angle β having an accuracy of ± 0.03°. The values as given in Table 8c can therefore be compared to other determinations given in Table 8a in which the cell parameters have been orientated to correspond to the selected cell.

Table 8a. Other determinations of the lattice parameters of alpha oxygen

References	Temperature K	*a* nm	*b* nm	*c* nm	β°
Alikhanov 1967	20.4	0.5407	0.3448	0.4285	118.03
Barrett et al. 1967a	23	0.5403	0.3429	0.4232	117.67
Meier and Helmholdt 1984	22	0.5403	0.3433	0.4247	117.84
	6	0.5389	0.3433	0.4242	117.80

Monoclinic cell conversion for alpha oxygen

$c_2^2 = a_1^2 + c_1^2 - 2\, a_1\, c_1 \cos(180 - \beta_1)$ $c_1 \sin \beta_1 = c_2 \sin(180 - \beta_2)$

$c_1^2 = a_2^2 + c_2^2 - 2\, a_2\, c_2 \cos(180 - \beta_2$ $c_2 \sin \beta_2 = c_1 \sin(180 - \beta_1)$

Interatomic distances between molecular centres for alpha oxygen

$d1^{\,2} = a^{\,2}/\,4 + b^{\,2}/\,4 \quad d2 = b \quad d3^{\,2} = (a/2 + c\cos\beta)^{\,2} + (b/2)^{\,2} + c^2\sin^2\beta \quad d4 = c$

8.2 Beta Phase: Rhombohedral (hR2): 23.868 K to 43.796 K.

Corrected measurements of Krupkii et al. 1979 (24-43.5 K) were given in the alternative hexagonal cell form and were fitted to the following equations and extrapolated to the transition temperatures. These equations are considered as having accuracies of ± 0.0002 nm for the *a* axis and ± 0.0007 nm for the c axis. Equations for calculating interatomic distances in the beta phase are given below:

$$\ln (a_h\,, \text{nm}) = 1.33779 \times 10^{-3}\,T - 2.94829 \times 10^{-5}\,T^{\,2} + 4.44689 \times 10^{-7}\,T^{\,3} - 1.13834 \qquad (8i)$$

$$\ln (c_h\,, \text{nm}) = 5.51508 \times 10^{-4}\,T - 2.06856 \times 10^{-5}\,T^{\,2} + 1.94316 \times 10^{-7}\,T^{\,3} + 0.117819 \qquad (8j)$$

Lattice parameter measurements of Barrett et al. 1967b (26-42 K) vary from 0.0005 nm low to 0.0007 nm high along the *a* axis and from 0.0015 nm low to 0.0011 nm high along the *c* axis. Measurements of Meier and Helmholdt 1984 at 30 K are 0.0002 nm high for the *a* axis and 0.0004 nm low for the *c* axis. These values Therefore, agree with the selected values to within experimental accuracy. Hörl 1962 also measured the lattice parameters but the measuring temperature was only stated as being less than 28 K.

Calculation of interatomic distances for beta oxygen

$d1 = [\, a_h^2 / 3 + c_h^2\,(\tfrac{1}{3} - 2z)^{\,2}\,]^{\,\frac{1}{2}} \quad d2 = a_h \quad d3 = a_r$

where $2z = d_{\text{atom-atom}} / c_h$. Meier and Helmholdt 1984 determined $z = 0.05430$ for $c_h = 1.1281$ nm at 30 K from which $2z = 0.12251/\,c_h$ which has been used for all temperatures in the beta phase. The conversion factor is similar to $r_e = 0.12075358$ nm obtained for the bond length of the gas phase (Krupenie 1972).

8.3 The alpha–beta volume change on transition

From the above equations the alpha–beta volume change is only 0.025 $cm^3\ mol^{-1}$ compared to a value of 0.10 (4) $cm^3\ mol^{-1}$ determined by Prokhvatilov et al. 2001 by measuring lattice parameter values for both phases in the crossover region 22 K to 25.5 K. From high pressure curves Stevenson 1957 used the Clausius-Clapeyron equation to estimate a volume change of 0.117 $cm^3\ mol^{-1}$. From the measurements of Stewart 1959,

Roder 1978 estimated a volume change of 0.12_5 cm^3 mol^{-1} while Dundon 1977 obtained 0.135 cm^3 mol^{-1}. However, in all three cases the enthalpy of transition value determined by Giaque and Johnston 1929 at 93.8 J mol^{-1} was accepted. This value was later confirmed by Ancin 1975 and Szmyrka-Grzebyk 1998. However, Muijlwijk et al. 1969 and Fagerstroem and Hollis Hallett 1969 could find no evidence of an enthalpy of transition while Roder 1978 showed that the measurements of Kemp and Pickup 1972 lead to a value of only 10 J mol^{-1}. However, Szmyrka-Grzebyk et al. 1998 have suggested that unless the sample is first held at 20 K to remove hysteresis effects then an enthalpy of transition would not be detected. Therefore, if the enthalpy of transition is correct then the volume change discrepancies remain to be explained.

8.4 Gamma Phase: Cubic (cP16): 43.796 K to 54.3584 K.

Corrected lattice parameter measurements of Krupskii et al. 1979 (44-54 K) were fitted to the equation:

$$\ln (a, \text{nm}) = -1.64305 \times 10^{-4}\ T + 9.68590 \times 10^{-6}\ T^2 - 0.407884 \qquad (8k)$$

The accuracy of the lattice parameters is considered to be ± 0.0004 nm. Equations to calculate interatomic distances in gamma oxygen are given below. Low accuracy lattice parameter values were determined by Vegard 1935, Keesom and Taconis 1936 (50 K), Jordan et al. 1964 (50 K) and Cox et al. 1973 (46 K). Lattice parameter measurements of Barrett et al. 1967b (44-52 K) trend from 0.0014 nm to 0.0020 nm high.

Calculation of interatomic distances for gamma oxygen

$d1$ (II - II) (CN2) = a / 2 $d2$ (I – II) (CN 12) = $d3$ (II – II) (CN 4) = $\sqrt{5}a$ /4

$d4$ (II – II) (CN8) = $\sqrt{(3/8)}\ a$

Type I = spherically disordered; Type II = oblate spherical distribution in electron density

8.5 The beta–gamma volume changes on transition

The selected value for the volume change at the beta-gamma transition of 1.18 (5) cm^3 mol^{-1} agrees closely with values determined by Stewart 1959 as 1.18 (6) cm^3 mol^{-1} by extrapolation of ΔV to zero pressure and 1.16 (14) cm^3 mol^{-1} from the Clausius-Clapeyron equation.

8.6 Selected specific heat and enthalpy values for alpha oxygen

The measurements of Fagerstroem and Hollis Hallett 1969 were accepted to 9 K and fitted to a polynomial equation for measurements 10.918 to 21.806 K to cover the range from 9 K to 22 K. Above this temperature there is a rapid rise in specific heat which was not included and instead equation 8n was extrapolated to the transition temperature. Units of C_p are J mol^{-1} $K^{-1}$and $H_T - H_0$ in J mol^{-1}:

2 – 5 K: $C_p = 1.71998 \times 10^{-3} T^3 + 3.54053 \times 10^{-6} T^5 + 1.40017 \times 10^{-7} T^7$ (8l)

5 – 9 K: $C_p = -3.75 \times 10^{-2} T - 1.75 \times 10^{-3} T^2 + 2.75 \times 10^{-3} T^3 + 0.124400$ (8m)

9 – 22 K: $C_p = -4.39006 T + 0.502694 T^2 - 2.13286 \times 10^{-2} T^3 + 3.60521 \times 10^{-4} T^4 + 13.6255$ (8n)

Table 8b. Specific heat and enthalpy values for alpha oxygen

T K	1	2	3	4	5	6	7	8	9
C_p	0.00172	0.0139	0.0476	0.116	0.237	0.43	0.72	1.12	1.65
$H_T - H_0$	0.00043	0.00692	0.0353	0.114	0.285	0.61	1.18	2.09	3.46
T K	10	11	12	13	14	15	16	17	18
C_p	2.27	3.05	3.95	4.95	6.02	7.15	8.34	9.60	10.93
$H_T - H_0$	5.41	8.06	11.55	15.99	21.47	28.04	35.78	44.75	55.00
T K	19	20	21	22	23	23.5	23.868		
C_p	12.38	13.96	15.71	17.69	(19.96)	(21.22)	(22.21)		
$H_T - H_0$	66.65	79.80	94.62	111.30	(130.10)	(140.40)	(148.39)		

Table 8c. Crystallographic properties of alpha oxygen

T K	α_a x 10^6 K^{-1}	α_b x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}
0	0	0	0	0
1	1.7	1.3	1.7	1.6
2	6.0	4.9	6.0	5.7
3	12.3	10.2	12.2	11.6
4	20.1	16.9	19.9	19.1
5	29.8	25.2	29.1	28.2
6	40.9	34.4	39.2	38.4
7	53.4	44.3	49.9	49.4
8	66.6	53.4	59.9	60.1
9	80.9	61.3	69.1	70.4
10	93.2	64.4	74.2	76.9
11	109	66.6	79.9	84.3
12	127	64.9	84.1	90.3
13	147	59.4	87.2	95.3
14	171	50.0	90.0	99.8
15	201	37.7	94.1	105
16	237	23.5	101	113
17	283	8.3	113	125
18	339	- 7.3	130	142
19	409	- 22.5	155	166
20	494	- 37.1	188	197
21	785	- 161	274	264
22	997	- 211	406	349
23	1,487	- 342	781	571
23.868	2,414	- 644	1,456	968

Table 8d. Crystallographic properties of alpha oxygen

T K	100 ε_0 *a*	100 ε_0 *b*	100 ε_0 *c*	100 ε_0 avr
0	0	0	0	0
1	< 0.0001	< 0.0001	< 0.0001	< 0.0001
2	0.0004	0.0003	0.0004	0.0004
3	0.0013	0.0011	0.0013	0.0012
4	0.0029	0.0024	0.0029	0.0028
5	0.0054	0.0045	0.0054	0.0051
6	0.0089	0.0075	0.0087	0.0084
7	0.014	0.011	0.013	0.013
8	0.020	0.016	0.019	0.018
9	0.027	0.022	0.025	0.025
10	0.036	0.028	0.032	0.032
11	0.046	0.035	0.040	0.040
12	0.058	0.042	0.048	0.049
13	0.071	0.048	0.057	0.058
14	0.087	0.053	0.066	0.068
15	0.106	0.058	0.075	0.078
16	0.128	0.061	0.085	0.089
17	0.153	0.062	0.095	0.101
18	0.184	0.062	0.107	0.114
19	0.222	0.061	0.122	0.130
20	0.267	0.058	0.139	0.148
21	0.333	0.047	0.162	0.171
22	0.422	0.028	0.195	0.201
23	0.543	0.002	0.251	0.245
23.868	0.709	- 0.039	0.346	0.311

Table 8e. Crystallographic properties of alpha oxygen

T K	*a* nm	*b* nm	*c* nm	β °	c^1 nm	β^1 °	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.53750	0.34244	0.42419	117.760	0.50641	132.164	20.804	1538.1
1	0.53750	0.34244	0.42419	117.760	0.50641	132.164	20.804	1538.1
2	0.53751	0.34244	0.42419	117.760	0.50641	132.164	20.804	1538.1
3	0.53751	0.34245	0.42419	117.760	0.50642	132.164	20.805	1538.1
4	0.53752	0.34245	0.42420	117.760	0.50643	132.164	20.806	1538.0
5	0.53753	0.34246	0.42421	117.760	0.50644	132.164	20.807	1537.9
6	0.53755	0.34247	0.42422	117.760	0.50646	132.164	20.809	1537.7
7	0.53758	0.34248	0.42424	117.760	0.50648	132.164	20.812	1537.5
8	0.53761	0.34250	0.42427	117.760	0.50651	132.164	20.815	1537.3
9	0.53765	0.34252	0.42429	117.760	0.50655	132.165	20.819	1537.0
10	0.53770	0.34254	0.42432	117.760	0.50659	132.166	20.824	1536.6
11	0.53775	0.34256	0.42436	117.760	0.50664	132.167	20.829	1536.3
12	0.53781	0.34258	0.42439	117.761	0.50668	132.168	20.834	1535.9
13	0.53789	0.34261	0.42443	117.762	0.50674	132.170	20.840	1535.4
14	0.53797	0.34262	0.42447	117.763	0.50680	132.173	20.846	1535.0
15	0.53807	0.34264	0.42450	117.764	0.50687	132.177	20.853	1534.5
16	0.53819	0.34265	0.42455	117.766	0.50695	132.182	20.860	1534.0
17	0.53833	0.34266	0.42459	117.769	0.50704	132.188	20.867	1533.5
18	0.83850	0.34266	0.42464	117.772	0.50715	132.195	20.875	1532.8
19	0.53870	0.34265	0.42470	117.776	0.50728	132.205	20.885	1532.1
20	0.53894	0.26464	0.42477	117.782	0.50742	132.215	20.896	1531.3
21	0.53929	0.34260	0.42487	117.791	0.50763	132.232	20.911	1530.2
22	0.53977	0.34254	0.42501	117.804	0.50791	132.253	20.930	1528.9
23	0.54042	0.34245	0.42525	117.824	0.50829	132.276	20.958	1526.8
23.868	0.54131	0.34231	0.42565	117.848	0.50886	132.301	20.999	1523.9

Lattice parameter c^1 and angle β^1 are for the alternative monoclinic cell

Table 8f. Interatomic distances between molecular centres in alpha oxygen

T K	*d*1 nm	*d*2 nm	*d*3 nm	*d*4 nm	T K	*d*1 nm	*d*2 nm	*d*3 nm	*d*4 nm
0	0.31866	0.34244	0.41867	0.42419	13	0.31887	0.34261	0.41890	0.42443
1	0.31866	0.34244	0.41867	0.42419	14	0.31891	0.34262	0.41893	0.42447
2	0.31866	0.34244	0.41867	0.42419	15	0.31895	0.34264	0.41897	0.42450
3	0.31866	0.34245	0.41867	0.42419	16	0.31901	0.34265	0.41900	0.42455
4	0.31867	0.34245	0.41868	0.42420	17	0.31907	0.34266	0.41903	0.42459
5	0.31868	0.34246	0.41869	0.42421	18	0.31914	0.34266	0.41907	0.42464
6	0.31869	0.34247	0.41870	0.42422	19	0.31922	0.34265	0.41911	0.42470
7	0.31870	0.34248	0.41872	0.42424	20	0.31932	0.34264	0.41916	0.42477
8	0.31872	0.34250	0.41874	0.4247	21	0.31946	0.34260	0.41921	0.42487
9	0.31874	0.34252	0.41877	0.42429	22	0.31964	0.34254	0.41929	0.42501
10	0.31877	0.34254	0.41880	0.42432	23	0.31989	0.34245	0.41941	0.42525
11	0.31880	0.34256	0.41883	0.42436	23.868	0.32023	0.34231	0.41964	0.42565
12	0.31883	0.34258	0.41887	0.42439					

Table 8g. Crystallographic properties of beta oxygen

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 ε_0 avr	a_h nm	c_h nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
23.868	690	- 104	426	0.352	0.32721	1.12957	21.024	1522.0
24	691	- 106	425	0.358	0.37224	1.12956	21.028	1521.7
25	697	- 118	425	0.401	0.32747	1.12943	21.055	1519.8
26	707	- 130	428	0.444	0.32770	1.12929	21.082	1517.8
27	718	- 141	432	0.487	0.32793	1.12914	21.109	1515.9
28	733	- 150	438	0.531	0.32817	1.12897	21.137	1513.9
29	750	- 158	447	0.575	0.32841	1.12880	21.165	1511.9
30	769	- 165	458	0.621	0.32866	1.12862	21.193	1509.8
31	792	- 171	471	0.667	0.32892	1.12843	21.223	1507.7
32	817	- 175	486	0.715	0.32918	1.12823	21.253	1505.6
33	845	- 179	504	0.765	0.32945	1.12803	21.285	1503.4
34	875	- 181	523	0.817	0.32974	1.12783	21.318	1501.0
35	908	- 182	545	1.871	0.33003	1.12762	21.352	1498.6
36	944	- 182	569	0.927	0.33034	1.12742	21.388	1496.1
37	982	- 181	595	0.986	0.33066	1.12721	21.425	1493.5
38	1,023	- 179	623	1.047	0.33099	1.12701	21.464	1490.8
39	1,067	- 175	653	1.112	0.33133	1.12681	21.505	1488.0
40	1,114	- 171	686	1.179	0.33170	1.12662	21.548	1485.0
41	1,163	- 165	720	1.250	0.33207	1.12643	21.594	1481.8
42	1,215	- 158	757	1.325	0.33247	1.12625	21.642	1478.6
43	1,269	- 150	796	1.404	0.33288	1.12607	21.692	1475.1
43.796	1,314	- 142	829	1.469	0.33322	1.12594	21.734	1473.3

Table 8h. Crystallographic properties of beta oxygen

T K	a_r nm	α °	$d1$ nm	$d2$ nm	$d3$ nm
23.868	0.42126	45.706	0.31656	0.32721	0.42126
24	0.42126	45.710	0.31657	0.32724	0.42126
25	0.42128	45.741	0.31661	0.32747	0.42128
26	0.42130	45.773	0.31666	0.32770	0.42130
27	0.42132	45.806	0.31669	0.32793	0.42132
28	0.42133	45.840	0.31673	0.32817	0421333
29	0.42134	45.874	0.31677	0.32841	0.42134
30	0.42135	45.910	0.31681	0.32866	0.42135
31	0.42136	45.947	0.31685	0.32892	0.42136
32	0.42137	45.984	0.31689	0.32918	0.42137
33	0.42138	46.023	0.31693	0.32945	0.42138
34	0.42140	46.064	0.31697	0.32974	0.42140
35	0.42141	46.105	0.31702	0.33003	0.42140
36	0.42143	46.148	0.31707	0.33034	0.42143
37	0.42145	46.193	0.31713	0.33066	0.42145
38	0.42148	46.239	0.31719	0.33099	0.42148
39	0.42151	46.286	0.31725	0.33133	0.42151
40	0.42155	46.336	0.31734	0.33170	0.42155
41	0.42159	46.386	0.31741	0.33207	1.42159
42	0.42164	46.439	0.31751	0.33247	0.42164
43	0.42170	46.493	0.31760	0.33288	0.42170
43.795	0.42175	46.538	0.31768	0.33322	0.42175

Table 8i. Crystallographic properties of gamma oxygen

T K	α x 10^6 K^{-1}	100 ε_0	a nm	$d1$ nm	$d2 = d3$ nm	$d4$ nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
43.796	684	3.270	0.67267	0.33633	0.37603	0.41192	22.912	1396.6
44	688	3.285	0.67276	0.33638	0.37609	0.41198	22.922	1396.0
45	707	3.357	0.67323	0.33662	0.37635	0.41227	22.970	1393.1
46	727	3.431	0.67372	0.33686	0.37662	0.41256	23.019	1390.1
47	746	3.507	0.67421	0.33711	0.37690	0.41287	23.070	1387.0
48	766	3.585	0.67472	0.33736	0.37718	0.41318	23.123	1383.9
49	785	3.666	0.67525	0.33762	0.37747	0.41350	23.176	1380.7
50	804	3.748	0.67578	0.33789	0.37777	0.43183	23.232	1377.4
51	824	3.833	0.67633	0.33817	0.37808	0.41417	23.289	1374.0
52	843	3.919	0.67690	0.33845	0.37840	0.41451	23.347	1370.6
53	862	4.008	0.67747	0.33874	0.37872	0.41487	23.407	1367.1
54	882	4.098	0.67806	0.33903	0.37905	0.41523	23.468	1363.5
54.3584	889	4.131	0.67828	0.33914	0.37917	0.41536	23.490	1362.3

PART 8B. OZONE (O_3)

Structure: Orthorhombic (oP24)

A melting point of 80.6 K is selected as an average of the values of 80.5 (2) K determined by Thorp 1955 and 80.7 (4) K determined by Jenkins and DiPaulo 1956. Hanson and Mauersberger 1986 report a much lower triple point value of 79.6 (3) K.

8.7 Crystallographic Properties

Lattice parameter measurements of Marx and Ibberson 2001 were only shown graphically with actual data points being given by Ibberson 2007. The unpublished values are given in Section 8A.2 by permission of the author. The measurements show some scatter and because of this scatter the fitted equations given below do not always give a smooth derivative and therefore the *a* and *c* axis thermal expansion coefficients have been adjusted at 25 K and the *b* axis values at 15, 50, 55 and 60 K. The minimum in the *b* axis thermal expansion coefficient at 67.8 K is evident but there also appears to be a definate change in slope for the *a* axis at the same temperature. It is uncertain if this behavior is real or an artifact of the fitting process or due to sample purity:

a axis

$$0 - 12.5\ K: \quad \ln(a, nm) = 1.39496 \times 10^{-8} T^4 - 0.2499115 \tag{8o}$$

$$12.5 - 23.7\ K: \ln(a, nm) = -4.70571 \times 10^{-5} T + 7.70517 \times 10^{-6} T^2 - 0.2501867 \tag{8p}$$

$$23.7 - 67.8\ K: \ln(a, nm) = -2.64951 \times 10^{-4} T + 1.48253 \times 10^{-5} T^2 - 8.70438 \times 10^{-8} T^3 - 0.247861 \tag{8q}$$

$$67.8 - 80.6\ K: \ln(a, nm) = 4.73754 \times 10^{-4} T - 0.256915 \tag{8r}$$

b axis

0 – 12.5 K: $\ln(b, \text{nm}) = -1.11722 \times 10^{-8} T^4 - 0.4008752$ (8s)

12.5 – 23.7 K: $\ln(b, \text{nm}) = -7.62347 \times 10^{-5} T - 1.30758 \times 10^{-6} T^2 - 0.3999907$ (8t)

23.7 – 59.1 K: $\ln(b, \text{nm}) = -3.27959 \times 10^{-4} T + 4.38519 \times 10^{-6} T^2 - 2.87547 \times 10^{-8} T^3 - 0.396842$ (8u)

59.1 – 67.8 K: $\ln(b, \text{nm}) = -7.51327 \times 10^{-4} T + 5.41788 \times 10^{-6} T^2 - 0..381364$ (8v)

67.8 – 80.6 K: $\ln(b, \text{nm}) = 5.93614 \times 10^{-5} T - 0.4114155$ (8w)

c axis

0 – 12.5 K: $\ln(c, \text{nm}) = 2.93237 \times 10^{-9} T^4 - 0.3796146$ (8x)

12.5 – 23.7 K: $\ln(c, \text{nm}) = -4.34620 \times 10^{-5} T + 3.18617 \times 10^{-6} T^2 - 0.3794976$ (8y)

23.7 – 80.6 K: $\ln(c, \text{nm}) = -1.11559 \times 10^{-4} T + 4.66553 \times 10^{-6} T^2 - 1.27899 \times 10^{-8} T^3 - 0.378562$ (8z)

Streng and Grosse 1959 obtained a density of 1728 (2) kg m^{-3} at 77.4 K which is 8 kg m^{-3} (0.5 %) higher than the selected value.

8.8 Lattice parameter values of Marx and Ibberson 2001

The measurements were only shown graphically and are reproduced by permission of Ibberson 2007.

T K	*a* Å	*b* Å	*c* Å
4.7	7.78875 (17)	6.69730 (15)	6.84126 (15)
12.5	7.79135 (84)	6.69551 (57)	6.84174 (44)
18.2	7.79977 (83)	6.69107 (56)	6.84386 (44)
23.7	7.81161 (80)	6.68625 (53)	6.84725 (41)
28.9	7.83161 (82)	6.67797 (55)	6.84999 (43)
34.0	7.84544 (81)	6.67296 (53)	6.85563 (42)
40.5	7.86602 (65)	6.67062 (43)	6.86415 (35)
43.5	7.87798 (65)	6.66786 (42)	6.86855 (34)
46.7	7.89240 (60)	6.66658 (38)	6.87424 (32)
50.0	7.90490 (58)	6.66420 (38)	6.87932 (31)
52.8	7.91800 (52)	6.66179 (34)	6.88469 (28)
55.7	7.93343 (45)	6.65959 (29)	6.89082 (24)
59.1	7.94719 (41)	6.65771 (26)	6.89687 (22)
61.6	7.96140 (37)	6.65541 (24)	6.90288 (20)
64.4	7.97239 (35)	6.65488 (22)	6.90873 (19)
67.8	7.98673 (35)	6.65379 (22)	6.91637 (19)
72.0	8.00286 (35)	6.65560 (22)	6.92656 (19)
76.4	8.01934 (83)	6.65719 (52)	6.93836 (42)

Table 8j. Crystallographic properties of ozone

T K	α_a x 10^6 K^{-1}	α_b x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_0 a$	100 $\varepsilon_0 b$	100 $\varepsilon_0 c$	100 ε_0 avr
0	0	0	0	0	0	0	0	0
5	6.7	- 5.9	1.5	0.8	0.001	- 0.001	< 0.001	< 0.001
10	56	- 45	12	8	0.014	- 0.011	0.003	0.002
15	184	- 100	52	45	0.075	- 0.055	0.018	0.013
20	261	- 129	84	72	0.186	- 0.116	0.052	0.040
25	325	- 163	109	90	0.334	- 0.187	0.098	0.081
30	390	- 142	134	127	0.510	- 0.263	0.156	0.134
35	453	- 127	168	165	0.723	- 0.330	0.232	0.207
40	503	- 115	200	196	0.965	- 0.390	0.324	0.298
45	541	- 108	231	221	1.229	- 0.446	0.432	0.403
50	565	- 100	259	241	1.510	- 0.498	0.555	0.519
55	576	- 88	286	258	1.800	- 0.551	0.693	0.643
60	574	- 74	310	270	2.094	- 0.604	0.843	0.771
65	559	- 47	333	282	2.384	- 0.641	1.005	0.908
67.8	545	- 17	344	291	2.543	- 0.650	1.101	0.989
70	474	59	354	296	2.651	- 0.637	1.179	1.055
75	474	59	372	302	2.894	- 0.607	1.362	1.206
80	474	59	389	307	3.137	- 0.578	1.556	1.360
80.6	474	59	391	308	3.167	- 0.574	1.580	1.379

Table 8k. Crystallographic properties of ozone

T K	*a* nm	*b* nm	*c* nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
0	0.77887	0.66973	0.68413	26.864	1786.7
5	0.77888	0.66973	0.68413	26.864	1786.7
10	0.77898	0.66966	0.68415	26.865	1786.6
15	0.77946	0.66936	0.68425	23.874	1786.1
20	0.78032	0.66895	0.68448	26.896	1784.6
25	0.78147	0.66848	0.68480	26.929	1782.4
30	0.78285	0.66797	0.68519	26.972	1779.6
35	0.78450	0.66752	0.68571	27.051	1775.7
40	0.78638	0.66712	0.68634	27.104	1770.9
45	0.78844	0.66675	0.68708	27.190	1765.3
50	0.79063	0.66640	0.68792	27.284	1759.2
55	0.79289	0.66604	0.68886	27.385	1752.7
60	0.79518	0.66569	0.68989	27.490	1746.0
65	0.79744	0.66544	0.69100	27.602	1738.9
67.8	0.79867	0.66538	0.69166	27.669	1734.7
70	0.79951	0.66547	0.69219	27.723	1731.3
75	0.80141	0.66567	0.69345	27.848	1723.6
80	0.80331	0.66587	0.69477	27.975	1715.8
80.6	0.80353	0.66589	0.69493	27.990	1714.8

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9 FLUORINE F

Atomic Weight: 18.998403163 (6) (Meija 2017)

Allotropy: Alpha phase: Monoclinic (mS8)
Beta phase: Cubic (cP16)

Hu et al. 1953 determined the alpha-beta transformation temperature to be 45.55 (2) K while the triple point determined by both Straty and Prydz 1970 and Prydz et al. 1970 corrects to 53.478 (2) K on ITS-90.

9.1 Beta Phase: Cubic (cP16): 45.55 K to 53.478 K.

Jordan et al. 1964a, 1964b determined the structure to be cubic, possible space group Pm3n, and determined a low accuracy value for the lattice parameter. Following the review by de Reuck 1990, then based on an initial slope of the melting curve of 10.21 MPa K^{-1} and an enthalpy of transition of 510.3 (2.0) J mol^{-1} as determined by Hu et al. 1953, a volume change on fusion of 0.934 cm^3 mol^{-1} was derived using the Clausius-Clapeyron equation. Based on the tables given by de Reuck the molar volume for the liquid at the triple point is 22.263 cm^3 mol^{-1} so the molar volume of the solid is calculated as 21.329 cm^3 mol^{-1}. Assuming that the thermal expansion coefficient is 800 x 10^{-6} K^{-1}, because this is similar to the actual value obtained for gamma-oxygen, then the lattice parameters of the beta phase can be represented by:

$$\ln (a, \text{nm}) = 8.00 \times 10^{-4} T - 0.463153 \quad (9a)$$

The lattice parameter determined at 50 K, 0.6550 nm, is notably lower than the experimental value of 0.667 (7) nm determined by Jordan et al. 1964a, 1964b.

Calculation of interatomic distances in beta fluorine

F I – F II (CN12) = $d_1 = \sqrt{5}\, a/4$ F II – F II (CN2) = $d_2 = a/2$

F II – F II (CN2) = $d_3 = \sqrt{5}\, a/4$ F II – F II (CN8) = $d_4 = \sqrt{(3/8)}\, a$

9.2 Alpha Phase: Monoclinic (mS8): 0 K to 43.55 K

Meyer et al. 1968 determined the structure to be monoclinic, space group C2/m, but later Pauling et al. 1970 reinterpreted the data to be space group C2/c and the lattice parameters determined by Meyer et al. 1968 at 23 K and 39 K were corrected to correspond to this structure using the formulae given below.

23 K: a 0.550 nm b 0.328 nm c 0.728 nm β 102.17° Molar volume: 19.33_8 cm^3 mol^{-1}

39 K: a 0.556 nm b 0.328 nm c 0.732 nm β 102.81° Molar volume: 19.60_8 cm^3 mol^{-1}

The molar volumes were calculated from the original lattice parameters as given by Meyer et al. 1968 for the C2/m structure to avoid the rounding errors in the space group conversion. Meyer et al. 1968 also determined the structure at 4.2 K and obtained virtually the same lattice parameters as at 23 K but this would appear to be unlikely in view of the very large molar volume expansion between 23 K and 39 K. Based on a molar volume for the beta phase of 20.927 cm^3 mol^{-1} at the transition temperature and a volume of transition of 1.10 (1) cm^3 mol^{-1}, as determined by Jahnke 1967, then the volume for the alpha phase at the transition temperature is 19.827 cm^3 mol^{-1}. Combining this molar volume with those at 23 K and 39 K and reducing to equivalent length change values then in combination with the enthalpy values selected in Part 9.3 then a modified form of Equation B is used to represent the thermal expansion for the whole of the alpha range as:

$$\ln (L_T) = (H_T - H_0) (2.17587 \times 10^{-7} T + 1.42227 \times 10^{-6}) + 0.986537 \quad (9b)$$

Relationships between lattice parameters for different monoclinic structures for alpha fluorine

a_1 , b_1 , c_1 and β_1 correspond to C2/m and a_2 , b_2 , c_2 and β_2 correspond to C2/c

$c_2^2 = a_1^2 + c_1^2 + 2\, a_1\, c_1 \cos (180 - \beta_1)$ $\quad c_1 \sin \beta_1 = c_2 \sin (180 - \beta_2)$ $\quad a_1 = a_2$ $\quad b_1 = b_2$

9.3 Specific heat and enthalpy values for alpha fluorine

In order to interpolate to obtain enthalpy values corresponding to the experimental temperatures 23 K and 39 K and the transition temperature 45.55 K, the values of specific heat selected by Hu et al. 1953 between 20 K to 45.55 K were fitted to equation 9c with enthalpy values derived directly from this equation:

$$C_p\,(J\ mol^{-1}\ K^{-1}) = -17.0085 + 1.75934\ T - 1.55521 \times 10^{-2}\ T^2 + 1.29038 \times 10^{-4}\ T^3 \quad (9c)$$

$$H_T - H_0\ (J\ mol^{-1}) = -17.0085\ T + 0.879670\ T^2 - 5.18403 \times 10^{-3}\ T^3 + 3.22595 \times 10^{-5}\ T^4 + 107.58 \quad (9d)$$

Specific heat and enthalpy values at 15 K selected by Hu et al. 1953 were fitted to a Debye equation in order to extrapolate below this temperature:

$$C_p\,(J\ mol^{-1}\ K^{-1}) = 3.44786 \times 10^{-3}\ T^3 - 5.70925 \times 10^{-6}\ T^5 \quad (9e)$$

$$H_T - H_0\ (J\ mol^{-1}) = 5.61965 \times 10^{-4}\ T^4 - 9.51417 \times 10^{-7}\ T^6 \quad (9f)$$

Table 9a. Specific heat and enthalpy values for alpha fluorine

T K	5	10	15	20	23	25
C_p	0.413	2.877	7.301	12.99	16.80	19.27
$H_T - H_0$	0.524	7.668	32.80	82.97	127.7	163.8
T K	30	35	39	40	45	45.55
C_p	25.26	31.05	35.61	36.74	42.47	43.06
$H_T - H_0$	275.2	416.0	549.3	585.5	783.4	806.9

Table 9b. Crystallographic properties of alpha fluorine

All values are estimated

T K	$\alpha \times 10^6$ K^{-1}	100 ε_0 avr	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	0	19.29_0	1970
5	1.2	< 0.001	19.29_0	1970
10	12.0	0.003	19.29_2	1970
15	41.3	0.015	19.29_9	1969
20	93.1	0.048	19.31_8	1967
25	168	0.112	19.35_6	1963
30	261	0.219	19.41_7	1957
35	371	0.377	19.50_9	1948
40	499	0.595	19.63_7	1935
45	647	0.882	19.80_6	1918
45.55	664	0.919	19.82_7	1916

Table 9c. Crystallographic properties of beta fluorine

All values are estimated

T K	100 ε_0	*a* nm	*d*1 = *d*3 nm	*d*2 nm	*d*4 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
45.55	2.751	0.6527	0.3648	0.3263	0.3997	20.92_7	1816
46	2.788	0.6529	0.3650	0.3264	0.3978	20.94_9	1814
47	2.871	0.6534	0.3653	0.3267	0.4001	21.00_0	1809
48	2.953	0.6539	0.3656	0.3270	0.4004	21.05_0	1805
49	3.035	0.6545	0.3658	0.3272	0.4008	21.10_1	1801
50	3.118	0.6550	0.3661	0.3275	0.4011	21.15_2	1796
51	3.200	0.6555	0.3664	0.3278	0.4014	21.20_2	1792
52	3.283	0.6560	0.3667	0.3280	0.4017	21.25_3	1788
53	3.365	0.6566	0.3670	0.3283	0.4021	21.30_4	1784
53.478	3.405	0.6568	0.3672	0.3284	0.4022	21.32_9	1781

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10 NEON Ne

10A. NATURAL NEON

Atomic weight: 20.1797 (6) (Meija 2017)

Structure: Face-centered cubic (cF4)

The triple point is a primary fixed point on ITS-90 at 24.5561 K (Preston-Thomas 1990).

Smoothed values derived from the lattice parameter measurements of Batchelder et al. 1967 (3-23.5 K) were combined with dilatometric measurements of Holste and Swenson 1975 (2-14 K). The measurements were extrapolated to the triple point. The lattice parameter determined by Batchelder and Simmons 1965 at 4.25 K corrects to 0.446385 (7) nm and the determination of Batchelder et al. 1967 at the same temperature corrects to 0.446384 (8) nm. The average value of 0.446384 (8) nm was selected. Other lattice parameter determinations are of much lower accuracy with, for example, Henshaw 1958 obtaining 0.4429 (10) nm at 4.2 K and Bolz and Mauer 1963 obtaining 0.4460 (1) nm at 4 K. Lattice parameter measurements of Mauer and Bolz 1961 (4.2-21.6 K) were shown only graphically with equivalent length change values given by Touloukian et al. 1977. These trend to be higher than the selected values and on the basis $100\Delta\varepsilon_0$ are on average 0.027 higher above 8.9 K. Similar measurements by Bolz and Mauer 1963 (4.2-21.6 K) were also shown only graphically and on the basis $100\Delta\varepsilon$ trend to be on average 0.035 higher above 8.9 K

10B. ISOTOPES NEON 20 AND NEON 22

Natural neon consists of 90.48(3) at% of ^{20}Ne, 0.27 (1) at% of ^{21}Ne and 9.25 (3) at% of ^{22}Ne (Meija et al. 2016).

Atomic mass of ^{20}Ne: 19.9924401762 (17) (Wang et al. 2017)

Atomic mass of ^{22}Ne: 21.991385110 (19) (Wang et al. 2017)

On ITS-90 the triple point of ^{20}Ne is 24.5423 K and the triple point of ^{22}Ne is 24.6889 K (Pavese et al. 2011, Hill and Fahr 2011)

Smooth values derived from the lattice parameter measurements of Batchelder et al. 1968 (3-24.5 K) were accepted and extrapolated to the triple points. Lattice parameter values at 4.25 K determined by these authors correct to 0.446456 (8) nm for ^{20}Ne and 0.445605 (8) nm for ^{22}Ne were also accepted. Other lattice parameter measurements on both isotopes are of much lower accuracy with Kogan et al. 1961 obtaining 0.4480 (4) nm and 0.4464 (4) nm respectively at 4.2 K and Bolz and Mauer 1963 obtaining 0.4462 (1) nm and 0.4454 (1) nm respectively at 4 K. Lattice parameter measurements of Bolz and Mauer 1963 over the ranges 4.2 to 24.0 K for ^{20}Ne and 4.2 to 23.8 K for ^{22}Ne were only shown graphically with equivalent length change values being given by Touloukian et al. 1977.

Based on $100\Delta\varepsilon_0$ the trend away from the selected values for ^{20}Ne can be averaged to 0.048 higher above 9 K while for ^{22}Ne the trend can be averaged to 0.041 higher above 14 K.

Table 10a. Crystallographic properties of natural neon

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_0$	a nm	d nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	< 0.0001	0.44637	0.31563	13.390	1507.1
0.5	0.0335	< 0.0001	0.44637	0.31563	13.390	1507.1
1.0	0.269	< 0.0001	0.44637	0.31563	13.390	1507.1
1.5	0.911	< 0.0001	0.44637	0.31563	13.390	1507.1
2.0	2.18	0.0001	0.44637	0.31563	13.390	1507.1
2.5	4.34	0.0003	0.44637	0.31563	13.390	1507.0
3.0	7.73	0.0006	0.44638	0.31564	13.390	1507.0
3.5	12.78	0.0011	0.44638	0.31564	13.391	1507.0
4.0	19.99	0.0019	0.44638	0.31564	13.391	1507.0
4.5	29.85	0.0032	0.44639	0.31564	13.391	1506.9
5.0	42.77	0.0049	0.44640	0.31565	13.392	1506.8
6	78.80	0.0109	0.44642	0.31567	13.395	1506.6
7	127.9	0.0211	0.44647	0.31570	13.399	1506.1
8	189.0	0.0369	0.44654	0.31575	13.405	1505.4
9	260.8	0.0593	0.44664	0.31582	13.414	1504.4
10	340.0	0.0893	0.44677	0.31592	13.426	1503.0
11	423.0	0.1275	0.44694	0.31604	13.441	1501.3
12	514.0	0.1743	0.44715	0.31618	13.460	1499.3
13	605.7	0.2304	0.44740	0.31636	13.483	1496.7
14	702.7	0.2960	0.44769	0.31657	13.509	1493.8
15	803	0.3715	0.44803	0.31681	13.540	1490.4
16	900	0.4570	0.44841	0.31708	13.575	1486.6
17	999	0.5524	0.44884	0.31738	13.613	1482.4
18	1104	0.6581	0.44931	0.31771	13.656	1477.7
19	1218	0.7750	0.44983	0.37808	13.704	1472.6
20	1337	0.9038	0.45041	0.31849	13.756	1466.9
21	1462	1.045	0.45104	0.31893	13.814	1460.8
22	1595	1.200	0.45173	0.31942	13.878	1554.1
23	1728	1.368	0.45248	0.31995	13.947	1446.9
24	1861	1.550	0.45329	0.32053	14.022	1439.1
24.5561	1934	1.657	0.45377	0.32086	14.067	1434.5

$$d = a/\sqrt{2}$$

Table 10b. Crystallographic properties of isotope ^{20}Ne

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_0$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	< 0.0001	0.44645	0.31569	13.397	1492.3
3.0	6	< 0.0001	0.44645	0.31569	13.397	1492.3
3.5	10	0.0001	0.44645	0.31569	13.397	1492.3
4.0	16	0.0012	0.44645	0.31569	13.397	1492.3
4.5	28	0.0023	0.44646	0.31569	13.398	1492.2
5.0	43	0.0044	0.44647	0.31570	13.399	1492.1
6	81	0.0101	0.44649	0.31572	13.401	1491.9
7	132	0.0208	0.44654	0.31575	13.405	1491.4
8	197	0.0372	0.44661	0.31580	13.412	1490.7
9	266	0.0604	0.44672	0.31588	13.421	1489.6
10	341	0.0907	0.44685	0.31597	13.433	1488.3
11	423	0.1291	0.44702	0.31609	13.449	1486.6
12	509	0.1753	0.44723	0.31624	13.467	1484.5
13	599	0.2312	0.44748	0.31642	13.490	1482.0
14	694	0.2962	0.44777	0.31662	13.516	1479.2
15	789	0.3708	0.44810	0.31686	13.546	1475.9
16	885	0.4550	0.44848	0.31712	13.580	1472.1
17	986	0.5484	0.44889	0.31742	13.618	1468.0
18	1095	0.6529	0.44936	0.31775	13.661	1463.5
19	1215	0.7691	0.44988	0.31811	13.708	1458.4
20	1339	0.8979	0.45046	0.31852	13.761	1452.8
21	1471	1.040	0.45109	0.31897	13.819	1446.7
22	1613	1.196	0.45178	0.31946	13.883	1440.1
23	1764	1.367	0.45255	0.32000	13.954	1432.8
24	1923	1.554	0.45338	0.32059	14.031	1424.9
24.5423	2010	1.662	0.45387	0.32093	14.076	1420.3

$$d = a/\sqrt{2}$$

Table 10c. Crystallographic properties of isotope ^{22}Ne

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_0$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	< 0.0001	0.44560	0.31508	13.320	1651.0
3.0	6	< 0.0001	0.44560	0.31508	13.320	1651.0
3.5	11	0.0001	0.44560	0.31509	13.320	1650.9
4.0	21	0.0013	0.44561	0.31509	13.321	1650.9
4.5	35	0.0026	0.44561	0.31509	13.321	1650.8
5.0	51	0.0048	0.44562	0.31510	13.322	1650.7
6	93	0.0120	0.44565	0.31512	13.325	1650.4
7	146	0.0239	0.44570	0.31516	13.330	1649.8
8	208	0.0416	0.44578	0.31521	13.337	1648.9
9	277	0.0663	0.44589	0.31529	13.347	1647.7
10	355	0.0978	0.44603	0.31539	13.359	1646.1
11	439	0.1372	0.44621	0.31552	13.375	1644.2
12	530	0.1854	0.44642	0.31567	13.395	1641.8
13	625	0.2433	0.44668	0.31585	13.418	1639.0
14	723	0.3111	0.47698	0.31606	13.445	1635.7
15	821	0.3885	0.44733	0.31631	13.476	1631.9
16	921	0.4759	0.44772	0.31658	13.511	1627.6
17	1022	0.5736	0.44815	0.31689	13.551	1622.9
18	1124	0.6814	0.44863	0.31723	13.594	1617.7
19	1235	0.8001	0.44916	0.31760	13.643	1612.0
20	1349	0.9302	0.44974	0.31801	13.695	1605.7
21	1471	1.073	0.45038	0.31846	13.754	1599.0
22	1601	1.228	0.45107	0.31895	13.817	1591.6
23	1739	1.397	0.45182	0.31949	13.886	1583.7
24	1890	1.581	0.45264	0.32006	13.962	1575.1
24.6889	2004	1.717	0.45325	0.32049	14.018	1568.8

$$d = a/\sqrt{2}$$

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11 SODIUM Na

Atomic Weight: 22.98976928 (2) (Meija 2017)

Allotropy: Alpha: Hexagonal close-packed (hP2)
Beta: Body-centered cubic (cI2)

The transition is martensitic with Alcock et al. 1994 selecting M_S = 35 (3) K for the direct transformation beta to alpha; A_S = 45 (5) K for the reverse transformation and 75 (10) K for the end of the reverse transformation and an "equilibrium" transition temperature of 60 K although the beta phase can be retained at the lowest temperatures. The freezing point is a secondary fixed point on ITS-90 at 370.944 (5) K (Bedford et al. 1996).

11.1 Beta Phase: Body-centered cubic (cI2): 60 K to 370.944 K.

For the range 0 K to 140 K length change values at 4 K and 77 K derived from the volume ratios of Anderson and Swenson 1983 were combined with length change values of Siegel and Quimby 1938 (80 to 290 K but specifically 110 to 190 K) and fitted to Equation B using the enthalpy values selected by Alcock et al. 1994:

$$\ln (L_T) = (H_T - H_0) (2.16626 \times 10^{-6} + 7.97991 \times 10^{-10} T + 9.71719 \times 10^{-6} /T) - 1.53094 \times 10^{-2} \quad (11a)$$

For the range 140 to 293.15 K length change values of Siegel and Quimby 1938 over the full range 80 to 290 K were also fitted to Equation B:

$$\ln (L_T) = (H_T - H_0) (3.00481 \times 10^{-6} - 6.84732 \times 10^{-10} T - 1.96849 \times 10^{-4} /T) - 1.34172 \times 10^{-2} \quad (11b)$$

Above 293.15 K selected values are based on length changes derived from the lattice parameter measurements of Sullivan and Weymouth 1964 (241-371 K), Feder and Charbnau 1966 (248-371 K) and Adlhart et al. 1974, 1975 (305-371 K), but specifically measurements above 310 K. The measurements of Feder and Charbnau 1966 were only shown graphically with actual length change values being given by Touloukian 1975. The lattice parameter measurements of Adlhart et al. 1974, 1975 are systematically low because they are based on a value of 0.429315 nm at 313.3 K estimated from the graphical representation of Feber and Charbnau 1966 whereas the actual length change values as given by Touloukian et al. 1975 suggest a value 0.00018 nm higher:

$$\varepsilon_T = 1.25398 \times 10^{-4} T - 2.12436 \times 10^{-7} T^2 + 2.67883 \times 10^{-10} T^3 - 2.52530 \times 10^{-2} \quad (11c)$$

This equation was used to calculate the high temperature crystallographic properties of the beta phase as given in Table 11f.

Based on 100Δε, other volume ratios of Anderson and Swenson 1983 reduced to length change values show poor agreement with the selected values drifting from 0.033 high at

149 K to trend towards the selected values but a single data point at 350 K is 0.027 high. There have been a significant number of individual measurements of the lattice parameter below room temperature and these are tabulated below to indicate the scatter.

Table 11a. A comparison of additional length change values.

Authors	T K	*a* nm	Δ*a* nm	Note
Barrett 1956	4	0.4225	+ 0.0003	
	78	0.4235	+ 0.0004	
Elliott and Datar 1982	4	0.4226_3	+ 0.0004	a
Berliner et al. 1989	20	0.422140	– 0.0001	
Smith et al. 1991	20	0.4212	– 0.0011	
Berliner et al. 1992	32	0.4244	+ 0.0021	
Abe et al. 1994	20	0.4227	+ 0.0005	b

Notes for Table 11a

a. Lattice parameter calculated from De Haas-van Alphen (dHvA) measurements using the free electron model

b. Estimated from graph

Table 11b. Lattice parameter of sodium at 293.15 K

References	Original Temperature K	*a* nm
Aruja and Perlitz 1938	RT	0.42909
Sullivan and Weymouth 1964	298	0.428740
Feder and Charbnau 1966	298	0.428739
	Selected	0.42874(3)

At 293.15 K: Density 968.8 (2) kg m^{-3} Molar volume 23.730 (5) cm^3 mol^{-1}.

11.2 Alpha Phase: Hexagonal close-packed (hP2): 0 K to 60 K.

Using X-ray diffraction Barrett 1956 initially identified the structure as being hexagonal close-packed and this was confirmed by Stedman 1976. However, neutron diffraction measurements of Berliner et al. 1989, Smith et al. 1991 and Berliner et al. 1992 all suggested that the structure was in fact rhombohedral, the same as alpha-samarium, the so called *9R* structure. However, Schwarz et al. 1992 using diffuse-neutron-scattering found the low temperature phase to be a mixture of both the hexagonal close-packed and the *9R* structures contaminated with the high temperature body-centered cubic phase. Because the presence of the *9R* structure did not appear to be due to stacking faults, Sankaran et al. 1992 suggested that the hexagonal close-packed structure was the stable low temperature phase but that the transition from the body-centered cubic phase initially required the production of an intermediate rhombohedral distortion which because of the sluggish nature of the transition would also be observed. Based on these suggestions the structure is assumed to ideally be hexagonal close-packed.

Lattice parameter measurements on the *9R* structure by Berliner et al. 1989, and Smith et al. 1991 at 20 K and by Berliner et al. 1992 at 32 K show relatively poor agreement. Therefore, in order to obtain a set of reference values for the alpha phase the molar volume difference from the beta phase is determined and assumed to be constant between 0 and 60 K. The *c*/*a* ratio for the hexagonal structure is then also assumed to be constant at the ideal value of 1.6330 so that the *a*-axis lattice parameter is equal to both of the interatomic distances *d*1 and *d*2. Vaks et al. 1989 determined the initial slope of the pressure transition curve at dT/dP = – 0.170 K MPa^{-1} at a temperature between M_s and A_s. If the actual temperature is assumed to be about 40 K and the enthalpy of transition of 42 J/mol determined by Alcock et al. 1994 at the actual equilibrium temperature is retained then from the Clausius-Clapeyron equation the molar volume difference is equal to the value $V_\alpha - V_\beta = + 0.179$ cm^3 mol^{-1} which is selected at all temperatures up to the equilibrium transition at 60 K. This molar volume difference can be compared with other determinations where the molar volume values for the *9R* structure have been reduced by 4.5.

Table 11c. Molar volume differences between the alpha and beta phases

References	V_α cm^3 mol^{-1}	V_β cm^3 mol^{-1}	$V_\alpha - V_\beta$ cm^3 mol^{-1}	Notes
Barrett 1956	22.71	22.77	– 0.06	a
Basinskii and Verdi 1959	-	-	+ 0.07	
Berliner et al. 1989	22.65	22.72_5	– 0.07	b
Smith et al. 1991	22.50	22.64	– 0.14	b
Berliner et al. 1992	23.02	22.87	+ 0.15	b
Vaks et al. 1989	-	-	+ 0.179	

Notes for Table 11c

a. Hexagonal close-packed structure.

b. *9R* structure reduced.

Based on the accuracy of the volume change the *a*-axis values are considered to be accurate to ± 0.0005 nm and the *c*-axis to ± 0.0008 nm. In comparison the lattice parameter values for the hexagonal phase obtained by Barrett 1956 at 5 K are 0.0005 nm low along both axes while the measurements of Stedman 1976 at 35.7 K are also 0.0005 nm low along the *a*-axis but 0.0009 nm low along the *c*-axis. These differences may, to a certain extent, be reflected in the relatively low accuracy of the selected volume change on transition. Estimated crystallographic properties of the alpha phase are given in Table 11d.

11.3 Bulk properties of sodium

Ho 1973 has indicated the difficulties in interpreting the thermal vacancy effects because of the possible presence of divacancies. However, for this review only monovacancy effects are considered. Based on their lattice parameter values and the dilatometric measurements of Feder and Charbnau 1966, Adlhart et al. 1975 calculated $H_V = 0.354$

(25) eV and S_V/k = 3.9 (7) while based on the dilatometric measurements of Ritter et al. 1970 they calculated H_V = 0.36 (3) eV and S_V/k = 4.0 (9). Bulk properties as given in Table 11e are calculated by averaging these values to H_V = 0.357 (30) eV and S_V/k = 3.95 (90) and assuming that the vacancy effect is negligible below 270 K.

On the basis 100Δε dilatometric measurements of Sullivan and Weymouth 1964 (247-371 K) vary from up to 0.002 high in the region 330 K to 340 K but then trend to 0.009 low at the freezing point.

Table 11d. Crystallographic Properties of alpha sodium

T K	100 ε_T	*a* nm	*c* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	- 1.261	0.37715	0.61588	22.844	1006.4
5	- 1.261	0.37715	0.61588	22.844	1006.4
10	- 1.260	0.37715	0.61588	22.844	1006.4
15	- 1.259	0.37716	0.61589	22.845	1006.3
20	- 1.255	0.37717	0.61591	22.848	1006.2
25	- 1.249	0.37719	0.61595	22.852	1006.0
30	- 1.241	0.37723	0.61601	22.858	1005.8
40	- 1.216	0.37732	0.61616	22.875	1005.0
50	- 1.182	0.37745	0.61637	22.899	1004.0
60	- 1.144	0.37759	0.61661	22.925	1002.8

Table 11e. Bulk properties of sodium

$3\ (\varepsilon_T L - \varepsilon_T a) = \exp\ (3.95 - 4142.8\ /T)$ $\quad \alpha_L - \alpha_a = (1380.9/\ T^{\ 2}) \exp(3.95 - 4142.8\ /\ T)$

T K	$\alpha \times 10^6$ K^{-1}	100 ε_T	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
270	68.90	- 0.161	23.616	973.5
280	69.68	- 0.091	23.666	971.4
290	70.30	- 0.021	23.715	969.4
293.15	70.52	0.001	23.731	968.8
300	71.03	0.050	23.766	967.4
310	72.00	0.121	23.816	965.3
320	73.27	0.194	23.869	963.2
330	74.85	0.268	23.922	961.0
340	76.77	0.344	23.976	958.9
350	79.07	0.422	24.032	956.6
360	81.79	0.503	24.090	954.3
370	84.97	0.587	24.150	951.9
370.944	85.29	0.595	24.156	951.7

This Table is assumed to be identical to Table 11f below 270 K.

Table 11f. Crystallographic properties of beta sodium

T K	$\alpha \times 10^6$ K^{-1}	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	- 1.519	0.42223	0.36566	22.665	1014.3
5	0.29	- 1.519	0.42223	0.36566	22.665	1014.3
10	1.70	- 1.519	0.42223	0.36566	22.665	1014.3
15	4.94	- 1.517	0.42223	0.36567	22.666	1014.3
20	9.57	- 1.514	0.42225	0.36568	22.669	1014.2
25	14.86	- 1.508	0.42228	0.36570	22.673	1014.0
30	20.18	- 1.499	0.42231	0.36573	22.679	1013.7
40	29.30	- 1.475	0.42242	0.36582	22.696	1012.9
50	35.90	- 1.440	0.42265	0.36595	22.720	1011.9
60	41.09	- 1.402	0.42273	0.36609	22.746	1010.7
70	45.02	- 1.360	0.42291	0.36625	22.775	1009.4
80	48.09	- 1.314	0.42311	0.36642	22.807	1008.0
90	50.51	- 1.265	0.42332	0.36660	22.841	1006.5
100	52.44	- 1.214	0.42354	0.36679	22.876	1005.0
110	54.03	- 1.161	0.42376	0.36699	22.913	1003.3
120	55.38	- 1.107	0.42399	0.36719	22.951	1001.7
130	56.61	- 1.052	0.42423	0.36739	22.989	1000.0
140	58.07	- 0.996	0.42447	0.36760	23.028	998.3
150	59.58	- 0.939	0.42471	0.36781	23.068	996.4
160	60.99	- 0.879	0.42497	0.36804	23.110	994.8
170	62.22	- 0.818	0.42523	0.36826	23.153	993.0
180	63.26	- 0.756	0.42550	0.36849	23.196	991.1
190	64.17	- 0.692	0.42577	0.36873	23.241	989.2
200	64.96	- 0.628	0.42605	0.36897	23.286	987.3
210	65.67	- 0.563	0.42632	0.36921	23.331	985.4
220	66.31	- 0.498	0.42661	0.36945	23.378	983.4
230	66.89	- 0.431	0.42689	0.36970	23.424	981.4
240	67.64	- 0.365	0.42718	0.36995	23.472	979.4
250	67.95	- 0.297	0.42747	0.37020	23.519	977.5
260	68.42	- 0.229	0.42776	0.37045	23.568	975.5
270	68.90	- 0.161	0.42805	0.37070	23.616	973.5
280	69.34	- 0.092	0.42835	0.37096	23.665	971.5
290	69.77	- 0.022	0.42865	0.37122	23.715	969.4
293.15	69.91	0	0.42874	0.37130	23.730	968.8
300	70.23	0.048	0.42895	0.37148	23.764	967.4
310	70.83	0.119	0.42925	0.37174	23.815	965.4
320	71.60	0.190	0.42955	0.37200	23.866	963.7
330	72.52	0.262	0.42986	0.37227	23.917	961.2
340	73.60	0.335	0.43018	0.37255	23.970	959.1
350	74.83	0.410	0.43050	0.37282	24.023	957.0
360	76.23	0.486	0.43081	0.37310	24.078	954.8
370	77.78	0.563	0.43115	0.37339	24.133	952.6
370.944	77.93	0.570	0.43119	0.37342	24.139	952.4

$$d = \sqrt{3}a/2$$

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12 MAGNESIUM Mg

Atomic Weight: 24.304 to 24.307 (Meija 2017)
Select 2009 value 24.3050(6) (Wieser and Coplen 2011)

Structure: Hexagonal close-packed (hP2)

Alcock et al. 1993 selects 923 (1) K for the melting point

12.1 Crystallographic Properties

Up to 14 K thermal expansion coefficients of McCammon and White 1965 (5-283 K) were fitted to Debye equations and at 20 K and above were combined with the specific heat values selected by Alcock et al. 1993 and fitted to equation A. Values were extrapolated to 293.15 K:

a axis

$$0\text{-}14\ \text{K}: \quad \alpha_a\,(\text{K}^{-1}) = 1.73191 \times 10^{-9}\,T + 1.64072 \times 10^{-11}\,T^{3} + 2.20928 \times 10^{-13}\,T^{5} - 5.88987 \times 10^{-16}\,T^{7} \qquad (12a)$$

$$20\text{-}293.15\ \text{K}: \quad \alpha_a\,(\text{K}^{-1}) = Cp\,(9.15148 \times 10^{-7} + 3.47127 \times 10^{-10}\,T + 2.80024 \times 10^{-6}/T) \qquad (12b)$$

c axis

$$0\text{-}14\ \text{K}: \quad \alpha_c\,(\text{K}^{-1}) = 1.02811 \times 10^{-9}\,T + 1.45364 \times 10^{-11}\,T^{3} + 8.61665 \times 10^{-14}\,T^{5} - 1.86515 \times 10^{-16}\,T^{7} \qquad (12c)$$

$$20\text{-}293.15\ \text{K}: \quad \alpha_c\,(\text{K}^{-1}) = Cp\,(1.06219 \times 10^{-6} + 1.43096 \times 10^{-10}\,T - 2.82799 \times 10^{-6}/T) \qquad (12d)$$

Intermediate values in the range 14 to 20 K were given by McCammon and White 1965. On the basis $100\Delta\varepsilon$ length changes derived by an X-ray method by Goens and Schmid 1936 (21-473 K) in the low temperature region are on average only 0.002 lower along the *a* axis and 0.002 higher along the *c* axis.

In the high temperature region length change values derived from the lattice parameter values of Janot et al. 1970a, 1970b (633-924 K) were fitted to the equations:

$$\varepsilon_T\,a = 1.98894 \times 10^{-5}\,T + 1.25095 \times 10^{-8}\,T^{2} - 1.01964 \times 10^{-11}\,T^{3} + 7.49261 \times 10^{-15}\,T^{4} - 6.70407 \times 10^{-3} \qquad (12e)$$

$$\varepsilon_T\,c = 2.79128 \times 10^{-5}\,T - 7.61104 \times 10^{-9}\,T^{2} + 1.60334 \times 10^{-11}\,T^{3} - 5.49824 \times 10^{-15}\,T^{4} - 7.89188 \times 10^{-3} \qquad (12f)$$

On the basis $100\Delta\varepsilon$ X-ray values of Goens and Schmid 1936 (21-473 K) in the high temperature region trend to only 0.007 high along the *a* axis and 0.008 high along the *c* axis while earlier measurements of Goens and Schmid 1931 (293-473 K) trend to 0.001

and 0.004 low respectively. Similar measurements by Shinoda 1934 (297-373 K) trend to 0.019 low and 0.029 low respectively while those of Hanawalt and Frevel 1937 trend to 0.017 and 0.024 low respectively. Length change values actually derived from the published lattice parameter measurements of Busk 1952 (298-473 K) trend to 0.033 low and 0.051 low respectively while for the measurements of Raynor and Hume–Rothery 1939 (283-870 K) the trend is to 0.024 high and 0.040 high respectively.

Table 12a. Lattice parameter values of magnesium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm
Stenzel and Weerts 1932	293	0.32089	0.52099
Jette and Foote 1935	298	0.32092	0.52103
Owen et al. 1935	291	0.32088	0.52112
Ievinš et al. 1938	298	0.32091	0.52099
Raynor and Hume-Rothery 1939	283/303	0.32093	0.52109
Raynor 1940	293	0.32092	0.52108
Raynor 1942	293	0.32092	0.52105
Busk 1950	298	0.32086	0.52095
Swanson and Tatge 1953	298	0.32092	0.52099
Von Batchelder and Raeuchle 1957	298	0.32092	0.52103
Hardie and Parkins 1959	298	0.32097	0.52104
Morris et al. 1985	298	0.32089	0.52105
	Selected	0.32091 (3)	0.52103 (5)

At 293.15 K: Density 1737.1 (4) kg m^{-3} Molar volume 13.992 (2) cm^3 mol^{-1}.

12.2 Bulk Properties

Anisotropic dilatometric measurements of Janot et al. 1970a, 1970b (633-924 K) were adjusted so as to to be identical with average values derived from the lattice parameter values at 630 K and above this temperature were represented by a bulk length change equation:

$$\varepsilon_T = -1.12098 \times 10^{-4} T + 2.77382 \times 10^{-7} T^2 - 2.44249 \times 10^{-10} T^3 + 8.47159 \times 10^{-14} T^4 + 1.78104 \times 10^{-2} \quad (12g)$$

Bulk density measurements of Stankus and Khairulin 1990 (293-923 K) converted to average length change values on the basis $100\Delta\varepsilon$ trend to 0.043 lower than the selected value at the melting point. Other dilatometric measurements summarized by Touloukian et al. 1975 were not considered because of the possibility of preferred orientation effects. Bulk properties are given in Table 12d.

12b. Crystallographic properties of magnesium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
0	0	0	0	- 0.483	- 0.518	- 0.495
10	0.05	0.03	0.04	- 0.483	- 0.518	- 0.495
20	0.36	0.31	0.34	- 0.483	- 0.518	- 0.495
30	1.35	1.35	1.35	- 0.483	- 0.517	- 0.494
40	3.40	3.40	3.40	- 0.480	- 0.515	- 0.492
50	5.64	5.78	5.69	- 0.476	- 0.510	- 0.487
60	7.95	8.28	8.06	- 0.469	- 0.503	- 0.480
70	10.18	10.73	10.36	- 0.460	- 0.494	- 0.471
80	12.23	12.98	12.48	- 0.449	- 0.482	- 0.460
90	13.97	14.91	14.28	- 0.436	- 0.468	- 0.447
100	15.51	16.41	15.81	- 0.421	- 0.453	- 0.432
110	16.61	17.86	17.03	- 0.405	- 0.436	- 0.415
120	17.69	19.05	18.14	- 0.388	- 0.417	- 0.398
130	18.60	20.07	19.09	- 0.370	- 0.398	- 0.379
140	19.40	20.94	19.91	- 0.351	- 0.377	- 0.360
150	20.09	21.70	20.63	- 0.331	- 0.356	- 0.339
160	20.71	22.37	21.26	- 0.311	- 0.334	- 0.319
170	21.26	22.96	21.83	- 0.290	- 0.311	- 0.297
180	21.76	23.49	22.34	- 0.268	- 0.288	- 0.275
190	22.21	23.96	22.79	- 0.247	- 0.265	- 0.253
200	22.62	24.39	23.21	- 0.224	- 0.240	- 0.229
210	22.99	24.77	23.58	- 0.201	- 0.216	- 0.206
220	23.34	25.12	23.93	- 0.178	- 0.191	- 0.182
230	23.66	25.44	24.25	- 0.155	- 0.166	- 0.159
240	23.96	25.73	24.55	- 0.131	- 0.140	- 0.134
250	24.24	26.00	24.83	- 0.107	- 0.114	- 0.109
260	24.51	26.26	25.09	- 0.083	- 0.088	- 0.085
270	24.77	26.50	25.35	- 0.058	- 0.062	- 0.059
280	25.02	26.73	25.59	- 0.033	- 0.035	- 0.034
290	25.27	26.96	25.83	- 0.008	- 0.009	- 0.008
293.15	25.35	27.03	25.91	0	0	0
300	25.45	27.08	25.99	0.017	0.019	0.018
350	26.15	27.49	26.59	0.146	0.155	0.149
400	26.85	28.03	27.24	0.279	0.294	0.284
450	27.57	28.67	27.94	0.416	0.436	0.423
500	28.34	29.41	28.70	0.556	0.582	0.565
550	29.18	30.21	29.52	0.701	0.732	0.711
600	30.11	31.07	30.43	0.850	0.887	0.862
630	30.72	31.60	31.01	0.942	0.982	0.955
650	31.15	31.97	31.42	1.005	1.046	1.018
700	32.32	32.89	32.51	1.165	1.210	1.180
750	33.64	33.81	33.70	1.332	1.379	1.347
800	35.14	34.72	35.00	1.506	1.552	1.522
850	36.84	35.60	36.43	1.689	1.731	1.703
900	38.75	36.44	37.98	1.881	1.915	1.892
923	39.71	36.81	38.74	1.973	2.000	1.982

Table 12c. Crystallographic properties of magnesium

T K	*a* nm	*c* nm	*c*/*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.31936	0.51833	1.6230	0.31806	13.785	1763.1
10	0.31936	0.51833	1.6230	0.31806	13.785	1763.1
20	0.31936	0.51833	1.6230	0.31806	13.785	1763.1
30	0.31936	0.51834	1.6230	0.31806	13.786	1763.1
40	0.31937	0.51835	1.6230	0.31807	13.787	1763.0
50	0.31938	0.51837	1.6230	0.31809	13.788	1762.8
60	0.31940	0.51841	1.6230	0.31811	13.791	1762.3
70	0.31943	0.51846	1.6230	0.31814	13.795	1761.9
80	0.31947	0.51852	1.6231	0.31818	13.800	1761.3
90	0.31951	0.51859	1.6231	0.31822	13.805	1760.5
100	0.31956	0.51867	1.6231	0.31827	13.812	1759.8
110	0.31961	0.51876	1.6231	0.31832	13.818	1758.9
120	0.31966	0.51886	1.6231	0.31838	13.826	1757.9
130	0.31972	0.51896	1.6231	0.31844	13.833	1757.0
140	0.31978	0.51907	1.6232	0.31850	13.842	1755.9
150	0.31985	0.51918	1.6232	0.31857	13.850	1754.9
160	0.31991	0.51929	1.6232	0.31864	13.859	1753.8
170	0.31998	0.51941	1.6233	0.31871	13.868	1752.6
180	0.32005	0.51953	1.6233	0.31878	13.877	1751.5
190	0.32012	0.51965	1.6233	0.31885	13.886	1750.3
200	0.32019	0.51978	1.6233	0.31893	13.896	1749.1
210	0.32026	0.51990	1.6234	0.31901	13.906	1747.8
220	0.32034	0.52003	1.6234	0.31908	13.916	1746.6
230	0.32041	0.52017	1.6234	0.31916	13.926	1745.4
240	0.32049	0.52030	1.6235	0.31924	13.936	1744.1
250	0.32057	0.52044	1.6235	0.31932	13.946	1742.8
260	0.32064	0.52057	1.6235	0.31940	13.956	1741.5
270	0.32072	0.52071	1.6235	0.31949	13.967	1740.2
280	0.32080	0.52085	1.6236	0.31957	13.978	1738.8
290	0.32088	0.52098	1.6236	0.31965	13.989	1737.5
293.15	0.32091	0.52103	1.6236	0.31968	13.992	1737.1
300	0.32097	0.52113	1.6236	0.31974	13.999	1736.1
350	0.32138	0.52184	1.6237	0.32017	14.055	1729.3
400	0.32181	0.52256	1.6238	0.32060	14.112	1722.3
450	0.32224	0.52330	1.6239	0.32105	14.170	1715.2
500	0.32269	0.52406	1.6240	0.32151	14.230	1708.0
550	0.23216	0.52485	1.6241	0.32199	14.293	1700.5
600	0.32364	0.52565	1.6242	0.32248	14.357	1692.9
630	0.32393	0.52614	1.6242	0.32278	14.397	1688.2
650	0.32413	0.52648	1.6243	0.32298	14.424	1685.1
700	0.32465	0.52733	1.6243	0.32350	14.493	1677.0
750	0.32518	0.52821	1.6244	0.32404	14.565	1668.7
800	0.32574	0.52912	1.6243	0.32459	14.641	1660.1
850	0.32633	0.53005	1.6243	0.32517	14.719	1651.3
900	0.32695	0.53101	1.6241	0.32577	14.801	1642.1
923	0.32724	0.53145	1.6240	0.32605	14.841	1637.7

$$d1 = (a^2/3 + c^2/4)^{½} \quad d2 = a$$

12d. Bulk properties of magnesium

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
630	31.01	0.955	14.397	1688.2
650	31.65	1.019	14.424	1685.0
700	33.03	1.182	14.494	1676.9
750	34.30	1.353	14.568	1668.4
800	35.71	1.530	14.644	1659.7
850	37.50	1.716	14.725	1650.6
900	39.93	1.913	14.810	1641.1
923	41.33	2.008	14.852	1636.5

This Table is considered to be identical to Tables 12b and 12c below 630 K.

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13 ALUMINUM Al

Atomic weight: 26.9815384 (3) (Meija 2017)

Structure: Face-centered cubic (cF4)

The freezing point is a primary fixed point on ITS-90 at 933.473 K (Preston-Thomas 1990).

13.1 Low temperature

Up to 293.15 K the thermal expansion equations given by Kroeger and Swenson 1977 (0-320 K) were accepted. Thermal expansion values derived from these equations were also fitted to equation A and are given in Appendix A. The differences between the selected values and other experimental low temperature thermal expansion coefficients and length change values are compared with the selected values in Part 13.5, except for the lattice parameter measurements of Straumanis and Woodward 1971 (40-180 K) which cannot be directly connected to room temperature values. Low temperature lattice parameter measurements of Nicklow and Young 1963 (124-293 K) and Gupta and Singh 1970 (110-290 K) were only shown graphically with actual data points as length change values given by Touloukian et al. 1975.

13.2 High temperature

Lattice parameter measurements of Simmons and Balluffi 1960 (293-929 K), Nenno and Kauffman 1960 (298-924 K), Cornish and Burke 1965 (293-927 K) and King et al. 1966 (281-929 K) were combined with the lattice parameter and dilatometric measurements of Feder and Nowick 1958 (293-928 K), Bianchi et al. 1966 (293-926 K) and Von Guérard et al. 1974 (314-911 K), and the dilatometric measurements of Nix and MacNair 1941 (82-667 K). The various weightings applied to these measurements are given in Part 13.3. In order to represent only crystallographic properties no dilatometric measurements above 650 K were included in the evaluation. On the basis $\pm 100\varepsilon_T$ the overall fit to the data is ± 0.009:

$$\varepsilon_T = 1.85409 \times 10^{-5} T + 5.74131 \times 10^{-9} T^2 + 4.17674 \times 10^{-12} T^3 - 1.12986 \times 10^{-15} T^4 - 6.02553 \times 10^{-3} \quad (13a)$$

Lattice parameter measurements of Esser et al. 1938 (293-1273 K)) were only shown graphically. The deviations of other high temperature lattice and dilatometric measurements from the selected values are given in Part 13.5 except for the lattice parameter measurements of Straumanis and Cheng 1959-1960 (283-333 K) which lead to a derived thermal expansion coefficient of 22.8 – 22.9 x 10^{-6} K^{-1} and Otte et al. 1963 (292-312 K) which lead to 23.4 (2) x 10^{-6} K^{-1} in reasonable agreement with the selected values.

The present evaluation differs significantly to that of Wang and Reeber 2000 which appears to be due to the fact that while the present evaluation relied on a large number of

imput sources as given in Section 13.3, above 500 K Wang and Reeber 2000 appeared to have only considered the dilatometric measurements of Von Guérard et al. 1974.

Table 13a. Lattice parameter of aluminum at 293.15 K

References	Original Temperature K	*a* nm
Owen and Iball 1932	289.7	0.40493
Owen and Yates 1933	291	0.40492
Jette and Foote 1935	298	0.40493
Ievinš and Straumanis 1936a	298	0.40494
Ievinš and Straumanis 1936b	298	0.40494
Miller and DuMond 1940	298.2	0.40491
Wilson 1941	298	0.40493
Lu and Chang 1941	293	0.40493
Van Bergen 1941	293	0.40495
Wilson 1942	293	0.40493
Axon and Hume-Rothery 1948	298	0.40493
Owen et al. 1948	291	0.40492
Goniche and Graf 1948	291	0.40495
Ellwood and Silcock 1948	291	0.40495
Hardy and Heal 1948	298	0.40493
Hume-Rothery and Boultbee 1949	298	0.40493
Straumanis 1949	298	0.40494
Sully et al. 1949	298	0.40493
Kochanovska 1949	298	0.40493
Dorn et al. 1950	295	0.40492
Poole and Axon 1952	298	0.40491
Černohorský 1952	298	0.40493
Swanson and Tatge 1953	298	0.40492
Hill and Axon 1953	298	0.40491
Graf 1954	293.4	0.40493
Pearson 1954	298	0.40493
Smakula and Kalnajs 1955	298.2	0.40494
Figgins et al. 1956	298.7	0.40494
Weyerer 1956	298	0.40493
Zubenko and Umanskii 1956	283	0.40493
Feder and Nowick 1958	298	0.40492
Straumanis 1959	298	0.40493
Straumanis and Cheng 1959-1960	298	0.40493
Nenno and Kauffman 1960	298	0.40494
Otte 1961	297	0.40491
Cooper 1962	298.0	0.40494
Otte et al. 1963	297	0.40491
Delf 1963	298	0.40492
Batchelder and Simmons 1965	298	0.40494
Cornish and Burke 1965	293.2	0.40491
Kiendl and Witt 1966, Witt 1967	296	0.40492
King et al. 1966	293	0.40491
Adam-Vigneron et al. 1969	298	0.40495
Gupta and Singh 1970	290	0.40493
Seshadri and Downie 1979	300	0.40495
Langelaan and Saimoto 1999	293	0.40496
	Selected	0.40493 (2)

At 293.15 K for Al: Density 2699.2 (4) kg m^{-3} Molar volume 9.996 (1) cm^3 mol^{-1}

13.3 Weighting of the high temperature input values

X represents lattice parameter measurements and D dilatometric measurements.

Table 13b. Input data

References	Method	Actual range used K	Number of data points used	Notes
Simmons and Balluffi 1960	X	503-929	28	a
Nenno and Kauffman 1960	X	481-924	18	
Cornish and Burke 1965	X	408-927	15	
King et al. 1966	X	523-923	9	
Feder and Nowick 1958	X	494-928	40	b
	D	473-645	14	b
Bianchi et al. 1966	X	758-926	22	
	D	423-650	6	
Von Guérard et al. 1974	X	423-911	23	
	D	430-635	6	c
Nix and MacNair 1941	D	400-640	13	d
		Total	194	

Notes for Table 13b

a. The actual data points as give by Touloukian et al. 1975 were used in the fit not the smooth values given originally

b. Experimental values given by Touloukian et al. 1975

c. Values at 486 K and 610 K were not used in the evaluation

d. Experimental values 294 K to 667 K were fitted to a smooth curve and evaluated at 20 K intervals.

13.4 Bulk properties of aluminum

Because reported values for the thermal vacancy parameters were inconsistent, experimental values of the deviation of bulk length change measurements compared to the selected crystallographic values were smoothed by fitting the dilatometric measurements of Simmons and Balluffi 1960 over the range 723 to 923 K with those of Bianchi et al. 1966 over the range 758 to 926 K and those of Von Guérard et al. 1974 over the range 740 to 911 K (except for values at 740.17, 740.84, 792.69 and 826.06 K) and constraining at the crystallographic length change value at 650 K as given in Table 13h:

$$\varepsilon_T = 5.34970 \times 10^{-6} T + 3.73160 \times 10^{-8} T^2 - 2.91806 \times 10^{-11} T^3 + 1.10300 \times 10^{-14} T^4 + 1.31120 \times 10^{-18} T^5 - 3.94861 \times 10^{-3} \quad (13b)$$

The differences between this equation and equation 13a were used to derive thermal vacancy parameters as given in Table 13c which were then used to derive bulk properties

of aluminum. Fluss et al. 1978 summarized determinations of H_V using positron annihilation spectroscopy techniques which all appeared to lead to a distinctively different value of 0.66 eV compared to the value obtained from length change differences. Because this difference appears to be systematic it would appear that the formation of vacancies only in terms of monovacancies may be too simplified and the formation of divacancies may also be relevant. Bulk values are given in Table 13h.

Table 13c. Thermal vacancy parameters for aluminum

References	$10^4\ c_V$	H_V eV	S_V / k
Simmons and Balluffi 1960	9.4	0.76	2.4
Bianchi et al. 1966	(8.5)	0.71	1.76
Von Guérard et al. 1974	9.8	0.81	3.12
Mosig 1993	9.2	0.75	2.3
This Work	9.18	0.76	2.46

13.5 Deviations of experimental values from the selected values

Table 13d. Lattice parameter values on the basis $100\Delta\varepsilon$

References	Temperature Range K	Deviations $100\Delta\varepsilon$
Wilson 1941	273-923	Trends to 0.018 high
Wilson 1942	273-673	Unannealed sample trend to 0.017 high and annealed sample average bias 0.003 low
Elwood and Silcock 1948	291-862	Trends from 0.008 low to 0.008 high
Hume-Rothery and Boultbee 1949	213-298	Scatter 0.020 high at 213 K and 0.001 low at 223 K
Kochanovska 1949	295-560	Sample 1 trends to 0.070 low. Sample 2 to 0.043 low and sample 3 to 0.081 low
Figgins et al. 1956	20-299	Trends from 0.013 low to converge to the selected values
Zubenko and Umanskii 1956	227-375	Trends 0.017 low to 0.005 high
Nicklow and Young 1963	124-293	Average bias 0.001 low
Gupta and Singh 1970	110-290	Trends from 0.012 low to converge to the selected values
Seshadri and Downie 1979	300-693	Trends 0.005 high to 0.005 low at 624 K and then 0.042 low at 693 K
Langelaan and Saimoto 1999	303-659	Average bias 0.005 low

Table 13e. Dilatometric values on the basis 100Δε

References	Temperature Range K	Deviations 100Δε
Ayres 1905	86-373	Average trend 0.005 high to 0.004 low
Souder and Hidnert 1921	293-873	Sample 1 trends to 0.030 high and sample 2 to 0.047 high
Honda and Okubo 1924	334-621	Trends 0.008 high at 423 K to 0.005 low at 621 K
Buffington and Latimer 1926	87-315	Average bias 0.006 high below 160 K then converges to exactly agree with selected values above 270 K
Uffelmann 1930	373-803	Trends to 0.055 low
Taylor et al. 1938	293-773	Scatters 0.003 low to 0.002 high
Nix and MacNair 1941	82-667	Trends from 0.005 low to converge to selected values below 293.15 K. Above this temperature values were used in the evaluation
Esser and Eusterbrock 1941	273-873	Trends to 0.050 low
Richards 1942	82-896	Trends to 0.13 high
Hidnert and Krider 1952	293-573	Average bias 0.002 low as average of eight annealed samples
Altman et al. 1954	20-300	Agrees with selected values to within 0.001
Bijl and Pullan 1955	20-273	Average bias 0.006 low below 110 K then converges to selected values
Strelkov and Novikova 1957	84-342	Average bias 0.008 low below 200 K then trends to 0.006 high
Gibbons 1958	20-300	Average bias 0.001 high
Branchereau et al. 1962	273, 573	Average 0.005 low at 573 K
Rhodes et al. 1963	18-573	Initially 0.008 high then converges to selected values at 293 K then average bias 0.010 high above 450 K
Fraser and Hollis Hallet 1965	23-96	Average bias 0.002 high
Asay et al. 1968	173-473	Trend 0.041 high to average bias 0.022 low above 323 K
Ryabov et al. 1969	293-873	Trends to 0.017 low
Pathak and Vasavada 1970	300-900	Trends to 0.025 low

Table 13f. Thermal expansion coefficients

References	Temperature Range K	Deviations $\delta\alpha$ K^{-1}
Andres and Rohrer 1961	3-10.5	Agreement with selected values to better than 1×10^{-8} K^{-1}
Huzan et al. 1961	15-100	Scatter 2×10^{-8} K^{-1} high to 2.8×10^{-7} K^{-1} high
Abbiss et al. 1961	16-71	Scatter 1×10^{-8} K^{-1} high to 2.5×10^{-7} K^{-1} high
McLean 1969	4-27	Trend to 2×10^{-8} K^{-1} high
Awad and Gugan	10-75	Scatter 1×10^{-8} K^{-1} high to 3.1×10^{-7} K^{-1} high
Collins et al. 1973	3-85, 283	Agreement to better than 1×10^{-8} K^{-1} at 57.5 K and below. Average 8×10^{-8} K^{-1} low 65 to 85 K and 2.1×10^{-7} K^{-1} low at 283 K

Table 13g. Crystallographic properties of aluminum

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	- 0.414	0.40325	0.28514	9.872	2733.0
10	0.037	- 0.414	0.40325	0.28514	9.872	2733.0
20	0.230	- 0.414	0.40325	0.28514	9.873	2733.0
30	0.837	- 0.413	0.40326	0.28515	9.873	2733.0
40	2.03	- 0.413	0.40326	0.28515	9.873	2732.9
50	3.66	- 0.409	0.40327	0.28516	9.874	2732.6
60	5.50	- 0.405	0.40329	0.28517	9.875	2732.2
70	7.35	- 0.398	0.40332	0.28519	9.877	2731.7
80	9.11	- 0.390	0.40335	0.28521	9.880	2731.0
90	10.71	- 0.380	0.40339	0.28524	9.883	2730.2
100	12.16	- 0.369	0.40344	0.28527	9.886	2729.3
110	13.43	- 0.356	0.40349	0.28531	9.890	2728.2
120	14.55	- 0.342	0.40354	0.28535	9.894	2727.1
130	15.54	- 0.327	0.40361	0.28539	9.898	2725.9
140	16.42	- 0.311	0.40367	0.28544	9.903	2724.6
150	17.19	- 0.294	0.40374	0.28549	9.908	2723.2
160	17.88	- 0.277	0.40381	0.28554	9.913	2721.8
170	18.50	- 0.259	0.40388	0.28559	9.919	2720.3
180	19.06	- 0.240	0.40396	0.28564	9.924	2718.7
190	19.56	- 0.221	0.40404	0.28570	9.930	2717.2
200	20.01	- 0.201	0.40412	0.28575	9.936	2715.5
210	20.42	- 0.181	0.40420	0.28581	9.942	2713.9
220	20.80	- 0.160	0.40428	0.28587	9.948	2712.2
230	21.15	- 0.139	0.40437	0.28593	9.954	2710.5
240	21.48	- 0.118	0.40445	0.28599	9.961	2708.8
250	21.78	- 0.096	0.40454	0.28605	9.967	2707.0
260	22.06	- 0.075	0.40463	0.28612	9.976	2705.2
270	22.31	- 0.052	0.40472	0.28618	9.980	2703.4
280	22.56	- 0.030	0.40481	0.28624	9.987	2701.6
290	22.80	- 0.007	0.40490	0.28631	9.994	2699.8
293.15	22.87	0	0.40493	0.28633	9.996	2699.2
300	22.99	0.016	0.40499	0.28637	10.001	2697.9
350	23.87	0.133	0.40547	0.28671	10.036	2688.5
400	24.79	0.255	0.40596	0.28706	10.073	2678.7
450	25.74	0.381	0.40647	0.28742	10.111	2668.5
500	26.71	0.513	0.40701	0.28780	10.151	2658.1
550	27.71	0.650	0.40756	0.28819	10.192	2647.2
600	28.74	0.792	0.40814	0.28860	10.236	2636.1
650	29.78	0.940	0.40874	0.28902	10.281	2624.5
700	30.83	1.093	0.40936	0.28946	10.327	2612.6
750	31.90	1.251	0.41000	0.28991	10.376	2600.4
800	32.97	1.416	0.41066	0.29038	10.427	2587.7
850	34.04	1.586	0.41135	0.29087	10.479	2574.8
900	35.11	1.762	0.41206	0.29137	10.534	2561.4
933.473	35.83	1.882	0.41255	0.29172	10.571	2552.3

$$d = a/\sqrt{2}$$

Table 13h. Bulk properties of aluminum

$3\,(\varepsilon_T L - \varepsilon_T a) = \exp(2.46 - 8827/T)$ $\quad \alpha_L - \alpha_a = (2942/T^2)\exp(2.46 - 8827/T)$

T K	$\alpha \times 10^6$ K^{-1}	$100\,\varepsilon_T$	Molar Volume $cm^3\,mol^{-1}$	Density $kg\,m^{-3}$
650	29.88	0.940	10.281	2624.4
700	31.06	1.094	10.316	2612.5
750	32.36	1.254	10.377	2600.1
800	33.82	1.422	10.429	2587.3
850	35.49	1.598	10.483	2573.8
900	37.41	1.783	10.540	2559.8
933.473	38.86	1.913	10.581	2550.0

This Table is considered to be identical to Table 13g below 650 K.

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14 SILICON Si

Atomic weight: 28.084 to 28.086 (Meija 2017)
Select 2007 value 28.0855 (3) (Wieser and Berglund 2009).

Structure: Cubic (cF8)

Gurvich et al. 1991 selected 1690 K for the melting point.

14.1 Low temperature

The precision thermal expansion coefficients and length change values determined on single crystals by Middelmann et al. 2015 (7-293 K) were accepted. The deviations of other high precision thermal expansion measurements on single crystals by Karlmann et al. 2006 (35-305 K) and on polycrystals by Lyon et al. 1977 (6-340 K) are included in Table 14c. In addition, although only shown graphically, precision measurements of Yamada and Okaji 2000 (10-320 K) are stated to agree with selected values to within a value of 1 x 10^{-8} K^{-1} below room temperature. Other low temperature thermal expansion and length change values are compared with selected values in Part 14.4 except for the lattice parameter measurements of Shah and Straumanis 1972 (40-180 K) which were not connected to room temperature values for evaluation.

14.2 High temperature

Selected dilatomeric measurements of Watanabe et al. 2004 (293-1000 K) replace earlier measurements of Okaji 1988 (300-1300 K) and Watanabe et al. 2002 (700-1100 K). Thermal expansion coefficients derived from the precision lattice parameter measurements of Okado and Tokumaru 1984 (298-1513 K) are systematically lower than those of Watanabe et al. 2004 in the overlap region and therefore cannot be considerered to be compatible. Of other measurements in the high temperature region thermal expansion coefficients derived from lattice parameter measurements such as those of Skinner et al. 1953 (283-1591 K), Mauer and Bolz 1954 (298-1405 K), Mauer and Bolz 1955 (273-1406 K) and Mauer and Bolz 1957 (273-1612 K) are considered to be of too low a quality to be considered in the evaluation. Therefore, there does not appear to be any satisfactory thermal expansion measurements above 1000 K. In order to overcome this problem values of α^* and ε_T derived from the equations of Watanabe et al. 2004 at 25 K intervals from 300 K to 1000 K were converted to values of α which were combined in Equation A with specific heat (C_p) values derived from the equation of Gurvich et al. 1991 which covers the range from 298 K to the melting point:

$$C_p\,(\text{J mol}^{-1}\,\text{K}^{-1}) = 3.305 \times 10^{-3}\,T - 435100/T^{2} + 23.698 \qquad (14a)$$

The derived equation leads to an extraordinary correlation and fits to a standard deviation of only 2 x 10^{-9} K^{-1}:

$$\alpha\,(\text{K}^{-1}) = C_p\,(1.93601 \times 10^{-7} - 1.40756 \times 10^{-11}\,T - 1.71239 \times 10^{-5}/T) \qquad (14b)$$

This equation was integrated in order to obtain length change values relative to the fixed value at 1000 K and extrapolated values of α and ε_T at 25 K intervals from 1025 K to 1675 K and the melting point were combined in order to obtain values of α* which were then combined with values of α* from the equation of Watanabe et al. 2004 to give the following equations which represent the thermal expansion from 293.15 K to the melting point:

$$\alpha^* (K^{-1}) = 3.22196 \times 10^{-6} + 2.04774 \times 10^{-9} T - 1.06180 \times 10^{-12} T^2 + 2.20988 \times 10^{-16} T^3 - 0.101111/ T^2 \quad (14c)$$

$$\varepsilon_T = 3.22196 \times 10^{-6} T + 1.02387 \times 10^{-9} T^2 - 3.53935 \times 10^{-13} T^3 + 5.52473 \times 10^{-17} T^4 + 0.101111/ T - 1.36891 \times 10^{-3} \quad (14d)$$

Lattice parameter measurements of Dismukes et al. 1964 (298-1073 K) and dilatometric measurements of Dolino-Dobrovol'skaya et al. 1973 (293-875 K) were only shown graphically. Other dilatometric measurements such as those of Fine 1953 (97-426 K), Zhdanova et al. 1967 (293-1073 K) and Burkhardt and Marvel 1969 (293-1186 K) were also only shown graphically but with actual data points given by Touloukian et al. 1977. These and other measurements in the high temperature region are compared with selected values in Part 14.4.

14.3 Lattice parameter of silicon

Earlier determinations of the lattice parameter were tabulated by Donohue 1974 and in graphical form by Okada and Tokumaru 1984. However, these values are not involved in the evaluation and are therefore considered to be only of historical interest and are not listed. Later ultra precision measurements were evaluated in the CODATA reviews on the fundamental constants in 1998 (Mohr and Taylor 2000), 2002 (Mohr and Taylor 2005), 2006 (Mohr et al. 2008a, 2008b), 2010 (Mohr et al. 2012a, 2012b) and 2014 (Mohr et al. 2016a, 2016b) with the following selected values:

Table 14a. Selected lattice parameter of silicon at 295.65 K

Year	*a* nm
1998	0.543102088 (16)
2002	0.543102122 (20)
2006	0.543102064 (14)
2010	0.5431020504 (89)
2014	0.5431020504 (89)

The derived crystallographic properties in vacuum at 293.15 K corresponding to the 2014 selected value are:

At 293.15 K: Lattice parameter: 0.543098566 (16) nm
Density: 2329.085 (25) kg m^{-3}
Molar volume: 12.0586000 (11) cm^3 mol^{-1}

14.4 Deviations of experimental values from the selected values

Table 14b. Thermal expansion coefficients in the room temperature region

References	Temperature Range K	Deviations δα K^{-1}
Straumanis and Aka 1952	283-323	1.59 x 10^{-6} K^{-1} high at 293 K
Lisoivan and Dikovskaya 1969	293.15-303.15	5 x 10^{-8} K^{-1} low at average temperature 298.15 K
Bhalla and White 1971	298-314	Average 3.3 x 10^{-7} K^{-1} low
Norton et al. 1976	308.372-316.028	Average bias 1.2 x 10^{-8} K^{-1} low
Wagenbreth 1981	295.65	2 x 10^{-8} K^{-1} low
Bergamin et al. 1997	294.15-296.65	Trends 1.2 x 10^{-8} K^{-1} low to 6 x 10^{-9} K^{-1} high
Sacconi et al. 1997	293.15	1.1 x 10^{-8} K^{-1} high

Table 14c. Other thermal expansion coefficients

References	Temperature Range K	Deviations δα K^{-1}
Fine 1953	97-426	Trends from initially 2.5 x 10^{-7} K^{-1} high to 3.1 x 10^{-7} K^{-1} low at 300 K to 4 x 10^{-8} K^{-1} low at 426 K
Novikova and Strelkov 1959	26-340	Shows scatter but average bias 1.1 x 10^{-7} K^{-1} high above 50 K
Novikova 1964	81-343	Shows scatter but average bias 4 x 10^{-8} K^{-1} high
Carr et al. 1965	16-280	Shows scatter 4 x 10^{-8} K^{-1} low to 5 x 10^{-8} K^{-1} high
Sparks and Swenson 1967	2-32	Trends to 3 x 10^{-8} K^{-1} high
Nasekovskii 1967	52-800	Trends from 4.4 x 10^{-7} K^{-1} high at 100 K to 8.2 x 10^{-7} K^{-1} low at 300 K to 2.1 x 10^{-7} K^{-1} low at 800 K
Zhdanova et al. 1967	293-1073	Trends from maximum 2.3 x 10^{-7} K^{-1} low at 473 K to 4.1 x 10^{-7} K^{-1} high at 1073 K
Ibach 1969	20-850	Below room temperature maximum deviation 5 x 10^{-8} K^{-1} high at 70 K. At 250 K and above average bias 5 x 10^{-8} K^{-1} low
White 1973	20-283	Scatter 5 x 10^{-8} K^{-1} low to 6 x 10^{-8} K^{-1} high up to 203 K. 1.1 x 10^{-7} K^{-1} low at 283 K
Lyon et al. 1977	6-340	Averaging 3 x 10^{-9} K^{-1} high between 20 and 240 K and then trending to 1 x 10^{-9} K^{-1} low above 250 K
Roberts 1981	300-840	Initially 1.5 x 10^{-8} K^{-1} low at 320 K trending to an average of 1.2 x 10^{-8} K^{-1} high above 700 K
Bennett 1984	293-723	Trends to 9.7 x 10^{-8} K^{-1} high
Okaji 1988	300-1300	Trends to a maximum of 7.3 x 10^{-8} K^{-1} low at 800 K increasing to 4.5 x 10^{-8} K^{-1} high at 1300 K
Watanabe et al. 2002	700-1100	Trends to a maximum of 1.5 x 10^{-8} K^{-1} low at 900 K increasing to 5 x 10^{-9} K^{-1} high at 1300 K
Karlmann et al. 2006	35-305	Initial deviation less than 1 x 10^{-9} K^{-1} trending to an average of 6 x 10^{-9} K^{-1} low between 110 and 150 K then to 3 x 10^{-9} K^{-1} high between 220 and 250 K and then trending to 3 x 10^{-9} K^{-1} low in the room temperature region

Table 14d. Dilatometric values

References	Temperature Range K	Deviations 100Δε
Erfling 1942	78-323	Trends from initially 0.008 high to converge to the selected values
Gibbons 1958	40-300	Agrees to within 0.001 over the whole temperature range
Birss and Horne 1960	79-394	Initially 0.003 low then convergies to the selected values but above room temperature trends to 0.005 low
Maissel 1960	323-1123	Trends to a maximum of 0.007 low at 600 K then increases to 0.008 high at 1123 K
Schlötterer 1968	323-1273	Trends to 0.010 low
Burkhardt and Marvel 1969	293-1186	Scatters 0.006 low to 0.014 high up to 600 K but average bias 0.011 low above this temperature
Blet 1975	295-648	0.014 low at 648 K
Shevchenko et al. 1986	373-1073	Trends to 0.033 low

Table 14e. Lattice parameter values

References	Temperature Range K	Deviations 100Δε
Skinner et al. 1953	273-1591	Trends to 0.030 low
Mauer and Bolz 1954	298-1405	First sample 298-896 K average bias 0.004 high and second sample 298-1405 K average bias 0.005 low
Mauer and Bolz 1955	273-1406	First sample 273-1303 K agreement to better than 0.001 up to 685 K then average bias 0.008 low. Second sample 273-1406 K trends to 0.025 low
Mauer and Bolz 1957	273-1612	Trends to 0.029 low
Hall 1961	293-773	Scatters 0.010 low to 0.010 high
Dayal and Singh 1960-1961	296-803	Trends to 0.038 high
Dutta 1962	298-1151	Trends to 0.056 high
Shaw and Liu 1964	303-1133	Trends to 0.073 high
Batchelder and Simmons 1964	6-323	Agrees to better than 0.001 over the whole range
King and Preece 1967	18-298	Scatters 0.007 low to 0.005 high
Yim and Paff 1974	298-1086	Trends to 0.024 low
Okado and Tokumaru 1984	298-1513	Trends to 0.005 low

14.5 A comparison with previous evaluations

The review by Touloukian et al. 1977 does not include any of the modern thermal expansion measurements but on the basis 100Δε shows excellent agreement with the selected values differing by only 0.002 low in the region 800 to 1000 K before trending to 0.002 high at 1600 K. In the very high temperature region Swenson 1990 appeared to have relied mainly on the now obsolete dilatometric measurements of Okaji 1988. However, the agreement is quite close with the thermal expansion coefficients deviating from a maximum of 2 x 10^{-8} K^{-1} low at 900 K to 6 x 10^{-8} K^{-1} high at 1300 K. Length change values average only 0.001 low above 1000 K.. In the high temperature region Glazov and Pahinkin 2001 again relied on the now obsolete measurements of Okaji 1988 as well as the lattice parameter measurements of Okada and Tokumaru 1984. The derived thermal expansion coefficients average 6 x 10^{-8} K^{-1} lower over the range 500 K to 1400

K. Reeber and Wang 1996 also appeared to have relied on the measurements of Okaji 1988 and Okada and Tokumaru 1984. Selected thermal expansion coefficients show a trend deviating up to 1.5 x 10^{-7} K^{-1} low at 1650 K but length change values appear to agree to better than 0.001 up to 1100 K and then deviate only to 0.006 low at 1650 K.

Table 14f. Low temperature crystallographic properties of silicon

T K	α x 10^6 K^{-1}	100 ε_T	*a* nm	*d*1 nm	*d*2 nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
0	0	- 0.0215	0.542982	0.235118	0.383946	12.0508	2330.6
5	< 0.0001	- 0.0215	0.542982	0.235118	0.383946	12.0508	2330.6
10	- 0.0003	- 0.0215	0.542982	0.235118	0.383946	12.0508	2330.6
15	- 0.0011	- 0.0215	0.542982	0.235118	0.383946	12.0508	2330.6
20	- 0.0046	- 0.0215	0.542982	0.235118	0.383946	12.0508	2330.6
25	- 0.0214	- 0.0215	0.542982	0.235118	0.383946	12.0508	2330.6
30	- 0.0559	- 0.0215	0.542982	0.235118	0.383946	12.0508	2330.6
35	- 0.106	- 0.0216	0.542981	0.235118	0.383946	12.0508	2330.6
40	- 0.167	- 0.0217	0.542981	0.235118	0.383946	12.0508	2330.6
45	- 0.232	- 0.0218	0.542980	0.235117	0.383945	12.0507	2330.6
50	- 0.295	- 0.0219	0.542980	0.235117	0.383945	12.0507	2330.6
60	- 0.400	- 0.0222	0.542978	0.235116	0.383943	12.0506	2330.6
70	- 0.463	- 0.0227	0.542975	0.235115	0.383942	12.0504	2330.7
80	- 0.474	- 0.0231	0.542973	0.235114	0.383940	12.0502	2330.7
90	- 0.432	- 0.0236	0.542970	0.235113	0.383938	12.0501	2330.7
100	- 0.343	- 0.0240	0.542968	0.235112	0.383937	12.0499	2330.8
110	- 0.216	- 0.0243	0.542967	0.235111	0.383935	12.0498	2330.8
120	- 0.060	- 0.0244	0.542966	0.235111	0.383935	12.0498	2330.8
130	0.115	- 0.0244	0.542966	0.235111	0.383935	12.0498	2330.8
140	0.302	- 0.0242	0.542967	0.235112	0.383936	12.0499	2330.8
150	0.493	- 0.0238	0.542969	0.235113	0.383937	12.0500	2330.7
160	0.685	- 0.0232	0.542973	0.235114	0.383940	12.0502	2330.7
170	0.874	- 0.0224	0.542977	0.235116	0.383943	12.0505	2330.7
180	1.058	- 0.0214	0.542982	0.235118	0.383946	12.0508	2330.6
190	1.234	- 0.0203	0.542988	0.235121	0.383951	12.0513	2330.5
200	1.402	- 0.0190	0.542995	0.235124	0.383956	12.0517	2330.4
210	1.560	- 0.0175	0.543004	0.235127	0.383961	12.0523	2330.3
220	1.710	- 0.0159	0.543012	0.235131	0.383968	12.0529	2330.2
230	1.851	- 0.0141	0.543022	0.235135	0.383975	12.0535	2330.1
240	1.984	- 0.0122	0.543033	0.235140	0.383982	12.0542	2329.9
250	2.107	- 0.0101	0.543044	0.235145	0.383990	12.0549	2329.8
260	2.223	- 0.0079	0.543055	0.235150	0.383998	12.0557	2329.6
270	2.332	- 0.0057	0.542068	0.235155	0.384007	12.0565	2329.5
280	2.433	- 0.0033	0.543081	0.235161	0.384016	12.0574	2329.3
290	2.528	- 0.0008	0.543094	0.235167	0.384026	12.0583	2329.1
293.15	2.556	0	0.543099	0.235169	0.384029	12.0586	2329.1

$d1 = \sqrt{3}a/4 \quad d2 = a/\sqrt{2}$

Table 14g. High temperature crystallographic properties of silicon

T K	$\alpha \times 10^6$ K^{-1}	100 ε_T	*a* nm	*d1* nm	*d2* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
293.15	2.56	0	0.54310	0.23517	0.38403	12.059	2329.1
300	2.62	0.002	0.54311	0.23517	0.38404	12.059	2329.0
350	2.99	0.016	0.54318	0.23521	0.38409	12.064	2328.0
400	3.25	0.032	0.54327	0.23524	0.38415	12.070	2326.9
450	3.45	0.048	0.54336	0.23528	0.38421	12.076	2325.7
500	3.60	0.066	0.54346	0.23532	0.38428	12.082	2324.5
550	3.73	0.084	0.54356	0.23537	0.38435	12.089	2323.2
600	3.83	0.103	0.54366	0.23541	0.38443	12.096	2321.9
650	3.92	0.123	0.54376	0.23546	0.38450	12.103	2320.5
700	4.00	0.142	0.54387	0.23550	0.38458	12.110	2319.2
750	4.07	0.163	0.54398	0.23555	0.38465	12.118	2317.8
800	4.13	0.183	0.54409	0.23560	0.38473	12.125	2316.3
850	4.18	0.204	0.54421	0.23565	0.38481	12.133	2314.9
900	4.23	0.225	0.54432	0.23570	0.38489	12.140	2313.4
950	4.28	0.246	0.54444	0.23575	0.38497	12.148	2312.0
1000	4.32	0.268	0.54455	0.23580	0.38506	12.156	2310.5
1050	4.35	0.290	0.54467	0.23585	0.38514	12.164	2309.0
1100	4.39	0.312	0.54479	0.23590	0.38523	12.172	2307.4
1150	4.42	0.334	0.54491	0.23595	0.38531	12.180	2305.9
1200	4.45	0.356	0.54503	0.23601	0.38540	12.188	2304.4
1250	4.47	0.378	0.54515	0.23606	0.38548	12.196	2302.9
1300	4.50	0.401	0.54528	0.23611	0.38557	12.204	2301.3
1350	4.52	0.423	0.54540	0.23616	0.38565	12.214	2299.7
1400	4.54	0.446	0.54552	0.23622	0.38574	12.221	2298.2
1450	4.56	0.469	0.54565	0.23627	0.38583	12.229	2296.6
1500	4.58	0.492	0.54577	0.23633	0.38592	12.237	2295.0
1550	4.60	0.515	0.54590	0.23638	0.38601	12.246	2293.5
1600	4.62	0.538	0.54602	0.23643	0.38610	12.254	2291.9
1650	4.64	0.562	0.54615	0.23649	0.38619	12.263	2290.3
1690	4.65	0.580	0.54625	0.23653	0.38626	12.270	2289.0

$$d1 = \sqrt{3}a/4 \qquad d2 = a/\sqrt{2}$$

14.6 Silicon 28

Measurement of the lattice parameters, molar volumes and atomic weights of individual silicon 28 spheres contributed to fixing the 2017 CODATA value of the Avogadro Constant at exactly $N_A = 6.02214076 \times 10^{23}\ mol^{-1}$ (Newell et al. 2018)

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15 PHOSPHORUS P

Atomic weight: 30.973761998 (5) (Meija 2017)

Allotropy: Black allotrope: Orthorhombic (oS8)
Violet allotrope: Monoclinic (mP84)
Beta white allotrope: Triclinic (aP24)
Alpha white allotrope: Cubic (cI232)

Of the significant number of allotropes reported for phosphorus (Donohue 1974), the black, violet and alpha and beta white allotropes are considered to be well characterized and are evaluated. The group of allotropes designated as red are considered to be a varying mixture of the white and violet phases. The black allotrope is considered to be the most stable phase but this is questioned by Stephenson et al. 1969 who notes that it transforms to the red phase (but presumably actually to the violet phase) at 820 K. Smits and Bokhorst 1916 determined the sublimation temperature of the violet phase to be 964 K while Stephenson et al. 1969 selected 195.4 K for the transformation from the low temperature beta white allotrope to the high temperature alpha white allotrope and 317.30 (10) K as the melting point.

PART 15A. BLACK PHOSPHORUS

Structure: Orthorhombic (oS8)

Thermal expansion coefficients have been determined from lattice parameter measurements . Those obtained on powdered samples (P) are considered to be of low quality due to line broadening, and only those on single crystals (SC) are accepted although because of the scatter in the measurements of Riedner et al. 1974 this selection is considered to be tentative.

Table 15a. Thermal expansion coefficients for black phosphorus

References	Temperature Range K	α_a x 10^6 K^{-1}	α_b x 10^6 K^{-1}	α_c x 10^6 K^{-1}	Sample Type
Keyes 1953	293-707	22 (2)	38 (4)	39 (4)	P
Faber 1974	293-573	8 (4)	11 (4)	5 (5)	P
Riedner et al. 1974	295-473	53 (5)	10 (2)	0 (5)	SC

Lattice parameters determined on powdered sample show satisfactory agreement but differ significantly from values obtained on single crystals by Riedner et al. 1974. However, because the latter show relatively poor correlation between values determined at 295, 373 and 473 K then this suggests the presence of significant systematic errors and therefore these measurements are rejected and the selected values are based on the agreement obtained for the powder samples.

Table 15b. Lattice parameter of black phosphorus at 293.15 K

References	Original Temperature K	*a* nm	*b* nm	*c* nm	Sample Type
Riedner et al. 1974	295	0.32884	1.04715	0.43693	SC
Hultgen et al. 1935	RT	0.332	1.052	0.439	P
Brown and Rundqvist 1965	295	0.33134	1.0478	0.43765	P
Riedner et al. 1974	295	0.33142	1.0478	0.43758	P
Cartz et al. 1979	RT	0.33135	1.0474	0.4374	P
	Selected	0.33137 (4)	1.0477 (3)	0.43755 (12)	

At 293.15 K: Density 2709 (1) kg m^{-3} Molar volume 45.74 (2) cm^3 mol^{-1}.

Positional parameters of black phosphorus

References	*y*	*z*
Brown and Rundqvist 1965	0.10168 (9)	0.08056 (28)
Riedner et al. 1974	0.1016 (2)	0.0813 (3)
Cartz et al. 1979	0.1034 (7)	0.0806 (4)
Selected	0.1017	0.0806

Calculation of interatomic distances in black phosphorus

Three closest neigbours within the same layer d_1 and d_2. Eight neighbors in the same layer at distances d_3, d_4 and d_5. Four neighbors in the adjacent layer at d_6 and d_7.

$d_1 = [(2yb)^2 + (2zc)^2]^{½} = 0.2245$ nm $\quad d_2 = [(0.5\ a)^2 + (0.5 - 2z)^2 c^2]^{½} = 0.2223$ nm

$d_3 = a = 0.3314$ nm $\quad d_4 = [(0.5\ a)^2 + (0.5 + 2z)^2 c^2]^{½} = 0.3334$ nm

$d_5 = [(0.5\ a)^2 + (2yb)^2 + (0.5\ c)^2]^{½} = 0.3475$ nm

$d_6 = [(0.5\ a)^2 + (0.5 - 2y)^2 b^2 + (2zc)^2]^{½} = 0.3592$ nm

$d_7 = [(0.5 - 2y)^2 b^2 + (0.5\ c)^2]^{½} = 0.3800$ nm

PART 15B. VIOLET PHOSPHORUS

Structure: Monoclinic (mP84)

Discovered by Hittorf 1865 and often described as Hittorf's Phosphorus. The structure parameters at room temperature were refined by Thurn and Krebs 1969 who also determined values for the positional parameters and calculated the interatomic distances. The average bond angle is 101° and the average interatomic distance 0.2219 nm.

Table 15c. Crystallographic properties of violet phosphorus at room temperature

a nm	*b* nm	*c* nm	*β*°	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0.921	0.915	2.260	106.1	52.47	2361

PART 15C. WHITE PHOSPHORUS

15.1 Beta White Phosphorus: 0 K to 195.4 K

Structure: Triclinic (aP24)

The structure was determined by Simon et al. 1987 at 158 K who also determined values for the positional parameters and calculated the interatomic distances. The structure is orientationally ordered. Intramolecular angles are within 0.5° of 60° and interatomic distances are within the range 0.2209 (5) nm.

Table 15d. Crystallographic properties of beta white phosphorus at 158 K

a nm	*b* nm	*c* nm	*α*°	*β*°	*γ*°	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1.1450	0.5503	1.1264	71.84	90.37	71.56	63.76	1943

The only additional measurement is that Sapper and Blitz 1931 who determined the density to be 1994 $kg\ m^{-3}$ at 78 K.

15.2 Alpha White Phosphorus: 195.4 K to 317.40 K

Structure: Cubic (cI232)

The structure is likely to be complex but is speculated as being body-centered cubic. The number of atoms in the unit cell can be calculated from values of density and lattice parameter and rationalized to correspond to the number of P_4 molecules (N) which is related to the number of atoms in the unit cell (Z) as N = Z/4.

The values given in Table 15e were fitted to a linear relationship with an overall fit as a standard deviation of ± 3.3 $kg\ m^{-3}$:

$$\text{Density } (kg\ m^{-3}) = 2006.75 - 0.610342\ T \qquad (15a)$$

Table 15e. Density values of alpha white phosphorus

T K	Density kg m^{-3}	References
194	1891	Sapper and Blitz 1931
273	1836.8	Pisati and De Franchis 1874
273	1836.8	Vicentini and Omodei 1887
291	1831	Böeseken 1907
292	1824	Sapper and Blitz 1931
293	1823.2	Pisati and De Franchis 1874
297.4	1828.0	Damian 1881
308	1823	Gladstone and Dale 1859
308.4	1820.6	Damian 1881
313.3	1817.3	Damian 1881
317.4	1814.0	Damian 1881
317.4	1812.1	Erman 1827

Table 15f. Lattice parameters of alpha white phosphorus

References	Temperature K	Lattice Parameter nm	Calculated Density kg m^{-3}	Z	N
Sugawara et al. 1949	273-293 ?	1.88	1834 (6)	236.9	59.2
Corbridge and Lowe 1952	238-243	1.851 (3)	1860 (3)	229.3 (1.2)	57.3 (3)
Frevell 1955	273-293 ?	1.866 (10)	1834 (6)	231.7 (3.8)	57.9 (1.0)
Clark and Zaug 2010	RT	1.868 (9)	1828 (3)	231.7 (3.4)	57.9 (8)
			Selected	232 (4)	58 (1)

Temperature values corresponding to the lattice parameter measurements of Sugawara et al. 1949 and Frevell 1955 were not given but are assumed to be within the range 273 to 293 K.

By fixing Z = 232 the lattice parameters and length change values from the transition temperature to the melting point are given by:

$$a\ (\text{nm}) = 2.04937 \times 10^{-4}\,T + 1.808889 \qquad (15b)$$

$$\varepsilon_T = 1.09653 \times 10^{-4}\,T - 3.21447 \times 10^{-2} \qquad (15c)$$

The derived thermal expansion coefficient is 110 x 10^{-6} K^{-1}. Based on a density value of 1828 (3) kg m^{-3} at 293.15 K the derived lattice parameter is 1.869 (1) nm and the molar volume 67.78 (12) cm^3 mol^{-1}.

Table 15g. Crystallographic properties of alpha white phosphorus

T K	100 ε_T	*a* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
195.4	- 1.072	1.849	65.63	1888
200	- 1.021	1.850	65.73	1885
210	- 0.912	1.852	65.95	1879
220	- 0.802	1.854	66.17	1872
230	- 0.692	1.856	66.39	1866
240	- 0.583	1.858	66.61	1860
250	- 0.473	1.860	66.83	1854
260	- 0.363	1.862	67.05	1848
270	- 0.254	1.864	67.27	1842
280	- 0.144	1.866	67.49	1836
290	- 0.035	1.868	67.71	1830
293.15	0	1.869	67.78	1828
300	0.075	1.870	67.94	1824
310	0.185	1.872	68.16	1818
317.30	0.265	1.874	68.32	1813

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16 SULFUR S

Atomic Weight: 32.059 to 32.076 (Meija 2017)
Select 2007 value 32.065 (5) (Wieser and Berglund 2009).

The allotropic modifications of sulfur were reviewed by Donohue 1974, Meyer 1976 and Steudel and Eckert 2003 and generally consist of either homocyclic rings or chains of indefinite length. Of the crystalline phases consisting as rings the thermodynamically stable *cyclo*-octasulfur (S_8) allotropes are discussed in Part 16A and the remainder in Part 16B.

PART 16A. THERMODYNAMICALLY STABLE *CYCLO*-OCTASULFUR ALLOTROPES

For alpha orthorhombic and beta monoclinic octasulfur allotropes, Ferreira and Lobo 2011 select 368.39 K for the alpha beta transformation temperature and 393.57 K for the triple point. The triple point value represents the direct melting to a liquid consisting entirely of S_8 ring molecules. However, on standing there is a partial auto dissociation of the rings and a lowering of the melting point to an equilibrium value of 388.31 K (corrected to ITS-90) as an average of the values of West 1959 and Montgomery 1975.

16.1 Alpha Orthorhombic Octasulfur: 0 K to 368.39 K

Structure: Orthorhombic (oF128): Space Group Number 70.

Lattice parameter values calculated from the *d* spacing values of Wallis et al. 1986 (98-297 K) were corrected to length change values and combined with enthalpy values selected by Montgomery 1975 (after correcting from cal mol^{-1} to J mol^{-1}) which lead to the following equations when fitted to Equation B:

$$\ln (L_a) = (H_T - H_0)\,(1.42333 \times 10^{-6} + 7.20087 \times 10^{-9}\,T - 2.67762 \times 10^{-4}/T) - 1.12803 \times 10^{-2} \quad (16a)$$

$$\ln (L_b) = (H_T - H_0)\,(4.47009 \times 10^{-7} + 9.90849 \times 10^{-9}\,T - 9.64054 \times 10^{-4}/T) - 2.71144 \times 10^{-4} \quad (16b)$$

$$\ln (L_c) = (H_T - H_0)\,(1.27684 \times 10^{-6} + 1.59517 \times 10^{-9}\,T + 3.76698 \times 10^{-4}/T) - 1.30220 \times 10^{-2} \quad (16c)$$

In the derivation of equations 16a to 16c the enthalpy values of Montomery 1975 were preferred to later value of Hemingway 1999 because they were given to a greater number of significant figures.

Equations 16d to 16f were extrapolated to the alpha-beta transition temperature and can be represented above 293.15 K by representative polynomials:

$$\varepsilon_T\, a = -1.59070 \times 10^{-5}\,T + 1.83501 \times 10^{-7}\,T^{2} + 4.61166 \times 10^{-11}\,T^{3} - 1.22682 \times 10^{-2} \quad (16d)$$

$$\varepsilon_T\, b = -8.69928 \times 10^{-5}\,T + 2.95408 \times 10^{-7}\,T^{2} + 2.34692 \times 10^{-11}\,T^{3} - 4.75761 \times 10^{-4} \quad (16e)$$

$$\varepsilon_T c = 4.06752 \times 10^{-5} T + 1.27304 \times 10^{-8} T^2 + 3.20911 \times 10^{-11} T^3 - 1.38264 \times 10^{-2} \quad (16f)$$

Because of the relatively poor correlation of the measurements of Wallis et al. 1986 then derived thermal expansion coefficients are only given as nominal values.

Table 16a. Lattice parameter values of alpha orthorhombic octasulfur at 293.15 K

References	Original Temperature K	*a* nm	*b* nm	*c* nm
Abrahams 1955	RT	1.0437	1.2845	2.4369
Swanson et al. 1960	298	1.0463	1.2865	2.448
Caron and Donohue 1961	298	1.0462	1.2865	2.4487
Coppens et al. 1977	298	1.0459	1.2873	2.4473
Hemingway 1999	RT	1.0454	1.2870	2.4472
Cooper et al. 1961	298.0	1.04600	1.28610	2.44809
	Selected	1.0460 (1)	1.2861 (1)	2.4481 (1)

At 293.15 K: Density 2069.4 (4) kg m^{-3} Molar volume 123.956 (16) cm^3 mol^{-1}.

Rettig and Trotter 1987 refined the positional parameters and determined the mean bond length to be 0.2046 (3) nm (uncorrected) and 0.2055 (2) nm (corrected for libration). Bond angle (S-S-S) 108.2 (6) ° and torsion angle (S-S-S-S) 98.5 (1.9) °.

The lattice parameter values of Coppens et al. 1977 (78-298 K) show very poor agreement with those of Wallis et al. 1986. On the basis 100Δε derived length change values at 100 K and 200 K are along the *a* axis 0.46 high and 0.40 high, along the *b* axis are 0.32 low and 0.18 high and along the *c* axis are 0.69 high and 0.39 high.

16.2 Beta Monoclinic Octasulfur: 368.39 K to 393.57 K

Structure: Monoclinic (mP48): Space Group Number 14.

The phase is easily retained in a metastable condition to very low temperatures. Specific heat measurements of Montgomery 1974 revealed an order-disorder transformation at 198 K. Neutron diffraction lattice parameter measurements of David et al. 2006 (40-250 K) were shown only graphically with actual data points given by Ibberson 2007. Extrapolation to 293.15 K was obtained by combining with the 297 K lattice parameters of Templeton et al. 1976. Thermal expansion coefficients were not derived because of the effects on the smooth values of considerable scatter in the measurements of David et al. 2006.

Table 16b. Lattice parameter values of beta monoclinic octasulfur at 293.15 K

References	Original Temperature K	*a* nm	*b* nm	*c* nm	*β*°
Sands 1971	RT	0.10934	1.0844	1.0778	95.80
Templeton et al. 1976	297	0.10923	1.0851	1.0787	95.905
	Selected	1.0923 (2)	1.0851 (2)	1.0787 (3)	95.905 (20)

The lattice parameter values given by Sands 1971 were rearranged to give the sequence *a*>*b*>*c*

At 293.15 K: Density 2009.5 (8) kg m^{-3} Molar volume 127.651 (49) cm^3 mol^{-1}.

Templeton et al. 1976 gives the average bond length as 0.2045 (1) nm and the average bond angle as 107.9 (1)°. Lattice parameter values of Goldsmith and Strouse 1977 (113-218 K) average 0.0005 nm low along the *a* axis, 0.0014 nm low along the *b* axis, 0.0011 nm low along the *c* axis and 0.04° low for the angle β.

In the high temperature region Crapanzano 2005 determined the lattice parameter values at 392 K. While the value for the angle β shows excellent agreement with an extrapolation of the selected lower temperature data and is accepted, the lattice parameters show poor agreement and all appear to be too low. The molar volume of the alpha phase at the transition temperature is 126.74_1 cm^3 mol^{-1} and when combined with a volume expansion on transition of 3.4032 cm^3 mol^{-1} as determined by Crapanzano 2005 leads to a value for the beta phase at the transition temperature of 130.14_4 cm^3 mol^{-1} and in combination with the lower temperature data extrapolates to a value of 130.93_0 cm^3 mol^{-1} at 392 K which compares to the much lower value of 129.734 cm^3 mol^{-1} determined from the lattice parameter values. In order to obtain representative lattice parameter values the selected values from 260 K to 293.15 K for all three axes were linearly extrapolated to 368.39 K and 392 K. Fixing the values of the angle β at both temperatures then very small but equal adjustments were applied to the extrapolated values until the above molar volume values were matched. The selected rounded values are then derived as *a* 1.0986 nm *b* 1.0936 nm *c* 1.0857 nm and *β* 96.240° at 368.39 K and *a* 1.1006 nm *b* 1.0963 nm *c* 1.0879 nm and *β* 96.366° at 392 K. In combination with measurements 270 to 293.15 K the lattice parameters above 293.15 K and up to the triple point can be represented by the equations:

$$a\ (\text{nm}) = 8.06237 \times 10^{-5}\,T + 4.47128 \times 10^{-9}\,T^2 + 1.06826 \qquad (16g)$$

$$b\ (\text{nm}) = 1.10222 \times 10^{-4}\,T + 4.66648 \times 10^{-9}\,T^2 + 1.05241 \qquad (16h)$$

$$c\ (\text{nm}) = 9.00359 \times 10^{-5}\,T + 4.12996 \times 10^{-9}\,T^2 + 1.05196 \qquad (16i)$$

$$\beta^\circ = -1.52647 \times 10^{-3}\,T + 9.03040 \times 10^{-6}\,T^2 + 95.5767 \qquad (16j)$$

Burwell 1937 determined the lattice parameters at 376 K which lead to a molar volume of 132.04 cm^3 mol^{-1} which is notably higher than the selected value of 130.40 cm^3 mol^{-1}.

16.3 Lattice parameter values of David et al. 2006

The measurements for the beta monoclinic phase were originally only shown graphically and are reproduced by permission of Ibberson 2007.

Table 16c. Experimental lattice parameter values for beta monoclinic sulfur

T K	*a* Å	*b* Å	*c* Å	*β*°
40	10.79478 (12)	10.64853 (10)	10.64783 (12)	95.6859 (10)
45	10.49499 (31)	10.65019 (26)	10.64836 (32)	95.6857 (26)
50	10.79492 (32)	10.65234 (27)	10.64930 (33)	95.6862 (27)
55	10.79540 (34)	10.65500 (28)	10.65037 (34)	95.6897 (28)
60	10.79544 (34)	10.65943 (28)	10.65211 (34)	95.6905 (28)
65	10.79604 (34)	10.66213 (29)	10.65380 (34)	95.6953 (29)
70	10.79676 (34)	10.66519 (28)	10.65504 (34)	95.6902 (28)
75	10.79828 (14)	10.67371 (12)	10.65930 (14)	95.6983 (11)
80	10.79908 (31)	10.67660 (26)	10.66084 (31)	95.7019 (26)
85	10.79873 (30)	10.67874 (26)	10.66173 (30)	95.7019 (26)
90	10.79981 (31)	10.68084 (26)	10.66322 (31)	95.7046 (27)
95	10.80017 (30)	10.68393 (25)	10.66458 (30)	95.7037 (25)
100	10.80271 (13)	10.69111 (11)	10.66888 (13)	95.7124 (11)
105	10.80418 (29)	10.69457 (25)	10.67101 (30)	95.7165 (25)
110	10.80453 (28)	10.69736 (25)	10.67242 (29)	95.7194 (24)
115	10.80575 (28)	10.69986 (25)	10.67383 (29)	95.7211 (25)
120	10.80686 (28)	10.70255 (25)	10.67605 (29)	95.7259 (25)
125	10.80964 (12)	10.70989 (11)	10.68042 (13)	95.7317 (11)
130	10.81135 (28)	10.71351 (25)	10.68245 (29)	95.7340 (25)
135	10.81241 (27)	10.71574 (24)	10.68420 (29)	95.7339 (24)
140	10.81373 (28)	10.71807 (25)	10.68550 (30)	95.7330 (25)
145	10.81512 (27)	10.72137 (24)	10.68761 (29)	95.7393 (24)
150	10.81914 (12)	10.72822 (11)	10.69240 (13)	95.7377 (11)
155	10.82242 (29)	10.73232 (25)	10.69512 (30)	95.7349 (26)
160	10.82356 (28)	10.73399 (25)	10.69683 (30)	95.7327 (26)
165	10.82537 (29)	10.73651 (26)	10.69819 (30)	95.7306 (26)
170	10.82836 (30)	10.73967 (27)	10.70015 (32)	95.7359 (27)
175	10.83531 (13)	10.74622 (12)	10.70542 (14)	95.7281 (12)
180	10.83869 (31)	10.74907 (28)	10.70756 (33)	95.7239 (28)
182	10.84104 (31)	10.75090 (28)	10.70874 (33)	95.7233 (28)
184	10.84338 (33)	10.75177 (29)	10.70981 (34)	95.7252 (29)
186	10.84477 (34)	10.75326 (30)	10.71087 (35)	95.7134 (30)
188	10.84748 (35)	10.75421 (31)	10.71161 (36)	95.7080 (31)
190	10.84923 (35)	10.75526 (31)	10.71258 (36)	95.7060 (31)
192	10.85186 (36)	10.75661 (32)	10.71328 (37)	95.7004 (32)
194	10.85516 (36)	10.75772 (33)	10.71417 (38)	95.6922 (32)
196	10.85776 (40)	10.75870 (36)	10.71481 (41)	95.6801 (36)
198	10.86195 (43)	10.76005 (39)	10.71575 (44)	95.6755 (38)
200	10.86473 (42)	10.76029 (38)	10.71678 (43)	95.6711 (37)
	10.86453 (41)	10.76033 (38)	10.71677 (43)	95.6719 (36)
202	10.86746 (42)	10.76195 (38)	10.71787 (43)	95.6719 (37)
	10.86742 (41)	10.76191 (38)	10.71781 (43)	68.6722 (37)
204	10.86972 (41)	10.76344 (37)	10.71931 (42)	95.6717 (36)
	10.86957 (40)	10.76340 (37)	10.71929 (42)	95.6715 (36)
206	10.87100 (44)	10.76557 (40)	10.72003 (46)	95.6733 (39)
	10.87075 (44)	10.76552 (41)	10.72016 (47)	95.6735 (39)

Table 16c. Experimental lattice parameter values for beta monoclinic sulfur (Continued)

208	10.87197 (42)	10.76680 (37)	10.72171 (44)	95.6690 (37)
	10.87187 (41)	10.76687 (38)	10.72177 (44)	95.6683 (37)
210	10.87293 (41)	10.76889 (38)	10.72329 (43)	95.6743 (37)
	10.87278 (40)	10.76892 (38)	10.72341 (43)	95.6739 (36)
215	10.87530 (41)	10.77195 (38)	10.72459 (44)	95.6826 (37)
220	10.87689 (41)	10.77499 (37)	10.72747 (44)	95.6884 (37)
225	10.88115 (17)	10.78266 (16)	10.73349 (19)	95.7059 (16)
230	10.88287 (42)	10.78577 (40)	10.73587 (46)	95.7133 (39)
235	10.88464 (42)	10.78970 (39)	10.73790 (46)	95.7250 (38)
240	10.88603 (40)	10.79296 (37)	10.74172 (44)	95.7319 (37)
245	10.88890 (42)	10.79648 (40)	10.74506 (47)	95.7461 (39)
250	10.89307 (17)	10.80476 (17)	10.75043 (20)	95.7662 (16)

Table 16d. Crystallographic properties of alpha orthorhombic octasulfur

T K	α_a x 10^6 K^{-1}	α_b x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 ε_T *a*	100 ε_T *b*	100 ε_T *c*	100 ε_T avr
100	17	- 31	42	9	- 1.157	- 0.591	- 0.939	- 0.896
110	21	- 25	42	13	- 1.139	- 0.619	- 0.897	- 0.885
120	26	- 18	43	17	- 1.116	- 0.640	- 0.855	- 0.870
130	30	- 12	44	21	- 1.088	- 0.655	- 0.812	- 0.852
140	35	- 6	44	25	- 1.056	- 0.664	- 0.769	- 0.830
150	39	1	45	28	- 1.019	- 0.667	- 0.724	- 0.803
160	44	7	46	32	- 0.978	- 0.663	- 0.679	- 0.774
170	48	14	47	36	- 0.932	- 0.652	- 0.633	- 0.739
180	53	20	48	40	- 0.882	- 0.636	- 0.586	- 0.701
190	57	27	48	44	- 0.828	- 0.613	- 0.538	- 0.660
200	62	33	49	48	- 0.768	- 0.583	- 0.490	- 0.614
210	66	39	50	52	- 0.705	- 0.547	- 0.440	- 0.564
220	71	46	51	56	- 0.636	- 0.505	- 0.390	- 0.510
230	75	52	51	60	- 0.564	- 0.456	- 0.340	- 0.453
240	80	59	52	64	- 0.505	- 0.401	- 0.288	- 0.392
250	84	65	53	67	- 0.405	- 0.339	- 0.235	- 0.326
260	89	71	54	71	- 0.318	- 0.271	- 0.182	- 0.257
270	93	78	54	75	- 0.228	- 0.197	- 0.128	- 0.184
280	98	84	55	79	- 0.132	- 0.116	- 0.073	- 0.107
290	102	90	56	83	- 0.032	- 0.029	- 0.018	- 0.026
293.15	104	92	56	84	0	0	0	0
300	107	97	57	87	0.072	0.065	0.039	0.059
310	111	103	58	91	0.181	0.164	0.096	0.147
320	115	109	59	94	0.294	0.271	0.154	0.240
330	120	115	59	98	0.412	0.383	0.214	0.326
340	124	121	60	102	0.535	0.502	0.274	0.437
350	129	128	61	106	0.662	0.627	0.335	0.541
360	133	134	62	110	0.794	0.759	0.396	0.650
368.39	137	139	63	113	0.908	0.875	0.449	0.744

Table 16e. Crystallographic properties of alpha orthorhombic octasulfur

T K	*a* nm	*b* nm	*c* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
100	1.0339	1.2785	2.4251	120.65	2126.1
110	1.0341	1.2781	2.4261	120.69	2125.4
120	1.0343	1.2779	2.4272	120.75	2124.5
130	1.0346	1.2777	2.4282	120.81	2123.3
140	1.0350	1.2776	2.4293	120.90	2121.8
150	1.0353	1.2775	2.4304	120.99	2120.1
160	1.0358	1.2776	2.4315	121.10	2118.2
170	1.0362	1.2777	2.4326	121.23	2116.0
180	1.0368	1.2779	2.4338	121.37	2113.6
190	1.0373	1.2782	2.4349	121.52	2110.9
200	1.0380	1.2786	2.4361	121.69	2108.0
210	1.0386	1.2791	2.4373	121.87	2104.9
220	1.0393	1.2796	2.4385	122.07	2101.5
230	1.0401	1.2802	2.4398	122.28	2097.8
240	1.0409	1.2809	2.4411	122.50	2094.0
250	1.0418	1.2817	2.4423	122.75	2089.8
260	1.0427	1.2826	2.4436	123.00	2085.5
270	1.0436	1.2836	2.4450	123.27	2080.9
280	1.0446	1.2846	2.4463	123.56	2076.1
290	1.0457	1.2857	2.4477	123.86	2071.1
293.15	1.0460	1.2861	2.4481	123.96	2069.4
300	1.0468	1.2869	2.4490	124.17	2065.8
310	1.0479	1.2882	2.4505	124.50	2060.3
320	1.0491	1.2896	2.4519	124.85	2054.6
330	1.0503	1.2910	2.4533	125.21	2048.7
340	1.0516	1.2926	2.4548	125.59	2042.6
350	1.0529	1.2942	2.4563	125.98	2036.2
360	1.0543	1.2959	2.4578	126.39	2029.6
368.39	1.0555	1.2974	2.4591	126.74	2024.0

16f. Crystallographic properties of beta monoclinic octasulfur

T K	100 ε_T *a*	100 ε_T *b*	100 ε_T *c*	100 ε_T avr
40	- 1.174	- 1.867	- 1.291	- 1.432
50	- 1.171	- 1.832	- 1.277	- 1.415
60	- 1.165	- 1.772	- 1.251	- 1.384
70	- 1.156	- 1.714	- 1.218	- 1.351
80	- 1.144	- 1.657	- 1.182	- 1.316
90	- 1.128	- 1.554	- 1.144	- 1.264
100	- 1.111	- 1.483	- 1.104	- 1.221
110	- 1.089	- 1.412	- 1.062	- 1.171
120	- 1.063	- 1.343	- 1.019	- 1.131
130	- 1.032	- 1.275	- 0.975	- 1.084
140	- 0.995	- 1.208	- 0.930	- 1.034
150	- 0.951	- 1.142	- 0.884	- 0.982
160	- 0.900	- 1.077	- 0.837	- 0.928
170	- 0.840	- 1.013	- 0.791	- 0.871
180	- 0.772	- 0.950	- 0.744	- 0.812
190	- 0.674	- 0.887	- 0.698	- 0.762
198	- 0.560	- 0.840	- 0.661	- 0.675
200	- 0.532	- 0.831	- 0.651	- 0.658
210	- 0.459	- 0.760	- 0.600	- 0.593
220	- 0.423	- 0.684	- 0.544	- 0.538
230	- 0.370	- 0.603	- 0.484	- 0.474
240	- 0.336	- 0.518	- 0.419	- 0.414
250	- 0.292	- 0.429	- 0.349	- 0.349
260	- 0.240	- 0.337	- 0.276	- 0.277
270	- 0.178	- 0.240	- 0.197	- 0.200
280	- 0.107	- 0.139	- 0.115	- 0.117
290	- 0.027	- 0.034	- 0.028	- 0.029
293.15	0	0	0	0
300	0.052	0.071	0.059	0.059
310	0.129	0.176	0.145	0.146
320	0.205	0.280	0.230	0.232
330	0.281	0.384	0.316	0.318
340	0.358	0.489	0.402	0.404
350	0.435	0.593	0.489	0.490
360	0.511	0.698	0.575	0.576
368.39	0.576	0.786	0.647	0.649
370	0.588	0.803	0.661	0.662
380	0.665	0.907	0.747	0.748
390	0.742	1.012	0.834	0.834
393.57	0.769	1.050	0.865	0.865

* $\varepsilon_{avr} = [(V_{m\,(T)} / V_{m\,(293.15)})^{⅓} - 1]$ where V_m = molar volume

16g. Crystallographic properties of beta monoclinic octasulfur

T K	*a* nm	*b* nm	*c* nm	β°	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
40	1.0795	1.0648	1.0648	95.686	122.24	2098
50	1.0795	1.0652	1.0649	95.686	122.30	2097
60	1.0796	1.0659	1.0652	65.691	122.42	2095
70	1.0797	1.0665	1.0656	95.695	122.54	2093
80	1.0798	1.0671	1.0660	95.700	122.67	2091
90	1.0800	1.0682	1.0664	95.706	122.86	2088
100	1.0802	1.0690	1.0668	95.713	123.02	2085
110	1.0804	1.0698	1.0675	95.720	123.21	2082
120	1.0807	1.0705	1.0677	95.726	123.36	2079
130	1.0810	1.0713	1.0682	95.732	123.54	2076
140	1.0814	1.0720	1.0687	95.737	123.72	2073
150	1.0819	1.0727	1.0692	95.736	123.92	2070
160	1.0825	1.0734	1.0697	95.733	124.12	2067
170	1.0831	1.0741	1.0702	95.731	124.34	2063
180	1.0839	1.0748	1.0707	95.731	124.56	2059
190	1.0849	1.0755	1.0712	95.724	124.82	2055
198	1.0862	1.0760	1.0716	95.704	125.08	2501
200	1.0865	1.0761	1.0717	95.672	125.15	2050
210	1.0873	1.0769	1.0722	95.674	125.39	2046
220	1.0877	1.0777	1.0728	95.692	125.60	2042
230	1.0883	1.0786	1.0735	95.712	125.84	2038
240	1.0886	1.0795	1.0742	95.736	126.07	2035
250	1.0891	1.0805	1.0749	95.763	126.32	2031
260	1.0897	1.0815	1.0757	95.792	126.59	2026
270	1.0904	1.0825	1.0766	95.823	126.88	2022
280	1.0911	1.0836	1.0775	95.857	127.20	2017
290	1.0920	1.0848	1.0784	95.894	127.54	2011
293.15	1.0923	1.0851	1.0787	95.905	127.65	2010
300	1.0928	1.0859	1.0793	95.932	127.87	2006
310	1.0937	1.0870	1.0803	95.971	128.20	2001
320	1.0945	1.0882	1.0812	96.013	128.53	1996
330	1.0954	1.0893	1.0821	95.056	128.87	1991
340	1.0962	1.0904	1.0830	96.101	129.20	1985
350	1.0970	1.0916	1.0840	96.149	129.53	1980
360	1.0979	1.0927	1.0849	96.198	129.87	1975
368.39	1.0986	1.0936	1.0857	96.240	130.14	1971
370	1.0987	1.0938	1.0858	96.248	130.20	1970
380	1.0995	1.0950	1.0868	96.301	130.53	1965
390	1.1004	1.0961	1.0877	96.355	130.87	1960
393.57	1.1007	1.0965	1.0880	96.374	130.99	1958

PART 16B. OTHER *CYCLO* ALLOTROPES

Crystal structure parameters including bond lengths, bond angles and torsion angles as well as melting points have been reviewed for all of these allotropes by Steudel and Eckert 2003. The tables below include Pearson symbols and molar volumes which were not included by Steudel and Eckert 2003. Although Steudel and Holz 1978 identified four allotropes for S_7 from infrared and Raman spectroscopy only γ-S_7 and δ-S_7 have been

characterized. Similarly, from Raman spectroscopy, Steudel et al. 1985 and Steudel et al. 1996 identified two allotropic modifications for S9 but only α-S9 has been characterized. The crystal structure of S15 has not been determined.

16.4 S6: *Cyclo*- hexasulfur

Structure: Rhombohedral (hR6): Space Group Number 148.

Lattice parameters of the equivalent hexagonal cell at room temperature are from Caron and Donohue 1960 and Donohue et al. 1961. Values for the equivalent rhombohedral cell have also been included. In addition Steidel et al. 1978 determined the lattice parameters at 183 K.

Table 16h. Crystallographic properties of S6

T K	a_h nm	c_h nm	a_r nm	$\alpha°$	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
RT	1.0818	0.4280	0.6407	115.19	87.08	2209

16.5 γ-S7: Gamma *cyclo*-heptasulfur

Structure: Monoclinic (mP28): Space Group Number 14.

Lattice parameters at 163 K are from Steudel et al. 1980:

Table 16i. Crystallographic properties of γ-S7

T K	*a* nm	*b* nm	*c* nm	$\beta°$	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
163	0.9680	0.7641	0.9409	102.08	102.46	2191

16.6 δ-S7: Delta *cyclo*-heptasulfur

Structure: Monoclinic (mP56): Space Group Number 14.

The actual space group $P2_1/n\text{-}C_{2h}^2$ represents an alternative setting of the no. 14 space group $P2_1/c\text{-}C_{2h}^5$. Lattice parameters at 163 K are from Steudel et al. 1977 and Steudel et al. 1980:

Table 16j. Crystallographic properties of γ-S7

T K	*a* nm	*b* nm	*c* nm	$\beta°$	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
163	1.5105	0.5998	1.5096	92.15	102.88	2182

16.7 γ-S8: Gamma *cyclo*-octasulfur

Structure: Monoclinic (mP32): Space Group Number 13.

Lattice parameters at 294 K are from Gallacher and Pinkerton 1993:

Table 16k. Crystallographic properties of γ-S8

T K	*a* nm	*b* nm	*c* nm	*β*°	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
294	0.8455	1.3052	0.9267	124.89	126.29	2031

16.8 α-S9: Alpha *cyclo*-nonasulfur

Structure: Monoclinic (mP72): Space Group Number 14.

The actual space group $P2_1/n\text{-}C_{2h}^2$ represents an alternative setting of the no. 14 space group $P2_1/c\text{-}C_{2h}^5$. Lattice parameters at 173 K are from Steudel et al. 1996:

Table 16l. Crystallographic properties of α-S9

T K	*a* nm	*b* nm	*c* nm	*β*°	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
163	0.7902	1.3908	1.6948	103.2	136.51	2114

16.9 S10: *Cyclo*-decasulfur

Structure: Monoclinic (mS40): Space Group Number 15.

Lattice parameters at 163 K are from Reinhardt et al. 1978 and Steudel et al. 1983:

Table 16m. Crystallographic properties of S10

T K	*a* nm	*b* nm	*c* nm	*β*°	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
163	1.2533	1.0275	1.2776	37.98	152.45	2103

An alternative definition of this structure as $a = 0.8240$ nm and $\beta = 110.59°$.

16.10 Compound $S_6.S_{10}$

Structure: Monoclinic (mS64): Space Group Number 12.

The actual space group I2/a represents an alternative setting of the no. 12 space group C2/n-C_{2h}^3. Lattice parameters at 163 K are from Steudel et al. 1983:

Table 16n. Crystallographic properties of S6.S10

T K	*a* nm	*b* nm	*c* nm	*β*°	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
163	1.9541	0.9431	0.8831	105.11	236.55	2169

16.11 S11: *Cyclo*-undecasulfur

Structure: Orthorhombic (oP88): Space Group Number 29.

Lattice parameters at 163 K are from Steidel and Steudel 1982 and Steudel et al. 1986:

Table 16o. Crystallographic properties of S11

T K	*a* nm	*b* nm	*c* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
163	1.4933	0.8321	1.8086	169.17	2085

16.12 S12: *Cyclo*- dodecasulfur

Structure: Orthorhombic (oP24): Space Group Number 58.

Lattice parameters at room temperature are from Steidel et al. 1981:

Table 16p. Crystallographic properties of S12

T K	*a* nm	*b* nm	*c* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
RT	0.4725	0.9104	1.4532	188.23	2044

16.13 S13: *Cyclo*- tridecasulfur

Structure: Monoclinic (mP104): Space Group Number 14.

Lattice parameters at 163 K are from Steudel et al. 1986:

Table 16q. Crystallographic properties of S13

T K	*a* nm	*b* nm	*c* nm	*β*°	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
163	1.295	1.236	1.761	110.41	198.86	2096

16.14 S14: *Cyclo*-tetradecasulfur

Structure: Triclinic (aP28): Space Group Number 2.

Lattice parameters at 173 K are from Steudel et al. 1998:

Table 16r. Crystallographic properties of S14

T K	*a* nm	*b* nm	*c* nm	*α*°	*β*°	*γ*°	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
173	0.5469	0.9662	1.4331	95.97	98.96	100.43	219.45	2046

16.15 α-S18: Alpha *cyclo*-octadecasulfur

Structure: Orthorhombic (oP72): Space Group Number 19.

Lattice parameters at room temperature are from Debaerdemaeker and Kotoglu 1974 and Schmidt et al. 1974:

Table 16s. Crystallographic properties of α-S18

T K	*a* nm	*b* nm	*c* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
RT	2.1152	1.1441	0.7581	276.21	2090

16.16 β-S18: Beta *cyclo*-octadecasulfur

Structure: Monoclinic (mP36): Space Group Number 11.

Lattice parameters at room temperature are from Debaerdemaeker and Kotoglu 1974 and Schmidt et al. 1974:

Table 16t. Crystallographic properties of β-S18

T K	*a* nm	*b* nm	*c* nm	*β*°	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
RT	1.075	0.725	1.225	92.3	287.25	2009

16.17 S20: *Cyclo*-eicosasulfur

Structure: Orthorhombic (oP80): Space Group Number 60.

Lattice parameters at room temperature are from Schmidt et al. 1974:

Table 16u. Crystallographic properties of S20

T K	*a* nm	*b* nm	*c* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
RT	1.8580	1.3181	0.8600	317.10	2022

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17 CHLORINE Cl

Atomic Weight: 35.446 to 35.457 (Meija 2017)
Select 2007 value 35.453 (2) (Wieser and Berglund 2009).

Structure: Orthorhombic (oS8)

After correction for temperature scale the triple point determined by Giauque and Powell 1939 becomes 172.17 (5) K on ITS-90.

Keesom and Taconis 1936 and Hawes and Cheesman 1959 both indexed the structure as being tetragonal. Collins 1952, 1956 correctly identified the structure as being orthorhombic, isostructural with both bromine (Vonnegut and Warren 1936) and iodine (Harris et al. 1928) and gave low accuracy lattice parameter values at 113 K.

17.1 Crystallographic Properties

Powell et al. 1984 determined the lattice parameters at 22 K, 55 K, 100 K and 160 K but for the *a*-axis one of the values would appear to be in error otherwise a major distortion of the derived thermal expansion coefficient occurs. It would appear that the value at 55 K may be considered to be in error and was rejected with the other three values fitted to equation:

$$a\ (\text{nm}) = 8.66328 \times 10^{-5}\,T + 1.11669 \times 10^{-7}\,T^{2} + 0.612570 \qquad (17a)$$

In order for a realistic thermal expansion curve to be derived equation 17a was fitted to Equation B over three temperature intervals using the enthalpy values selected by Arblaster 2013. For the *b* and *c* axes all four data points were fitted to Equation B:

a axis

$$0 - 39\ \text{K:}\quad \ln(a, \text{nm}) = (H_T - H_0)(-1.95155 \times 10^{-5} + 2.30255 \times 10^{-7}\,T + 8.70012 \times 10^{-4}/T) - 0.488406 \qquad (17b)$$

$$40 - 99\ \text{K:}\quad \ln(a, \text{nm}) = (H_T - H_0)(1.68762 \times 10^{-6} + 8.67160 \times 10^{-9}\,T + 2.76959 \times 10^{-4}/T) - 0.487491 \qquad (17c)$$

$$100 - 172.17\ \text{K:}\quad \ln(a, \text{nm}) = (H_T - H_0)(5.36930 \times 10^{-6} - 5.84342 \times 10^{-9}\,T - 7.70319 \times 10^{-5}/T) - 0.484237 \qquad (17d)$$

b axis

$$\ln(b, \text{nm}) = (H_T - H_0)(2.73535 \times 10^{-7} + 2.36097 \times 10^{-8}\,T + 3.25697 \times 10^{-4}/T) - 0.822964 \qquad (17e)$$

c axis

$$\ln(c, \text{nm}) = (H_T - H_0)(1.04024 \times 10^{-7} - 6.69693 \times 10^{-9}\,T + 2.00610 \times 10^{-4}/T) - 0.204659 \qquad (17f)$$

Values of the positional parameters determined by Powell et al. 1984 were fitted to the following equations where the *y* parameter is assumed to be fixed at 0.1219 above 100 K:

$$y = -8.053 \times 10^{-5} T + 6.2513 \times 10^{-7} T^2 - 1.4832 \times 10^{-9} T^3 + 0.12519 \quad (0 \text{ to } 100 \text{ K}) \qquad (17g)$$

$$z = 2.9838 \times 10^{-6} T - 1.9597 \times 10^{-7} T^2 + 6.3892 \times 10^{-10} T^3 + 0.10252 \qquad (17i)$$

Lattice parameters determine by Stevens 1979 at 90 K are 0.0006 nm lower for the *a*-axis, 0.0005 nm lower for the *b*-axis and 0.0062 nm lower for the *c*-axis.

Calculation of interatomic distances in chlorine

Cl (1) – Cl (2) = $d1 = [(2yb)^2 + (2zc)^2]^{½}$ (Bond length r_e)

Cl (1) – Cl (3) = $d2 = [b^2/4 + (0.5 - 2z)^2 c^2]^{½}$

Cl (1) – Cl (4) = $d3 = [(1 - 2y)^2 b^2 + (2zc)^2]^{½}$

Cl (1) – Cl (5) = $d4 = [a^2/4 + b^2/4]^{½}$

Cl (1) – Cl (6) = $d5 = [a^2/4 + (0.5 - 2y)^2 b^2 + (2zc)^2]^{½}$

Cl (1) – Cl (7) = $d6 = [a^2/4 + (0.5 - 2z)^2 c^2]^{½}$

$d1$ is the bond length (r_e).

Table 17a. Crystallographic properties of chlorine

T K	α_a x 10^6 K^{-1}	α_b x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}
0	0	0	0	0
5	17.7	7.77	4.75	10.1
10	58.1	30.0	18.0	35.4
15	103	62.3	36.7	67.3
20	137	97.4	55.3	96.6
25	151	124	67.4	114
30	152	142	72.0	122
40	154	152	67.5	127
50	160	166	55.5	127
60	162	173	41.9	126
70	165	183	28.7	125
80	168	195	16.4	126
90	171	209	4.91	129
100	174	227	- 5.69	132
110	178	247	- 15.6	136
120	182	269	- 25.1	142
130	185	293	- 34.4	148
140	188	320	- 43.6	155
150	191	349	- 52.8	162
160	194	381	- 62.3	171
170	198	415	- 72.0	180
172.17	198	422	- 74.2	182

Table 17b. Crystallographic properties of chlorine

T K	100 ε_0 *a*	100 ε_0 *b*	100 ε_0 c	100 ε_0 avr
0	0	0	0	0
5	1.3 x 10^{-3}	8.0 x 10^{-4}	8.2 x 10^{-4}	1.7 x 10^{-3}
10	0.022	0.010	6.2 x 10^{-3}	0.013
15	0.062	0.033	0.020	0.038
20	0.123	0.073	0.043	0.079
25	0.196	0.129	0.074	0.132
30	0.272	0.196	0.109	0.192
40	0.425	0.348	0.180	0.318
50	0.583	0.511	0.242	0.445
60	0.745	0.681	0.291	0.572
70	0.909	0.860	0.326	0.698
80	1.077	1.051	0.349	0.825
90	1.249	1.255	0.359	0.953
100	1.425	1.476	0.359	1.085
110	1.604	1.716	0.348	1.221
120	1.788	1.979	0.328	1.362
130	1.975	2.265	0.298	1.508
140	2.165	2.578	0.259	1.662
150	2.359	2.922	0.210	1.824
160	2.556	3.298	0.153	1.993
170	2.758	3.710	0.086	2.173
172.17	2.802	3.804	0.070	2.213

Table 17c. Crystallographic properties of chlorine

T K	*a* nm	*b* nm	*c* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.61360	0.43913	0.81493	33.059	2145
5	0.61363	0.43913	0.81493	33.061	2145
10	0.61374	0.43917	0.81498	33.071	2144
15	0.61398	0.43927	0.81509	33.097	2142
20	0.61436	0.43945	0.81527	33.138	2140
25	0.61480	0.43969	0.81553	33.191	2136
30	0.61527	0.43999	0.81581	33.256	2133
40	0.61621	0.44066	0.81639	33.375	2125
50	0.61718	0.44137	0.81690	33.502	2116
60	0.61817	0.44212	0.81730	33.629	2108
70	0.61918	0.44291	0.81758	33.756	2101
80	0.62021	0.44374	0.81777	33.884	2093
90	0.62127	0.44464	0.81785	34.014	2085
100	0.62235	0.44561	0.81785	34.147	2076
110	0.62345	0.44666	0.81776	34.285	2068
120	0.62457	0.44782	0.81760	34.428	2060
130	0.62572	0.44907	0.81735	34.578	2051
140	0.62689	0.45045	0.81703	34.735	2041
150	0.62808	0.45196	0.81664	34.901	2032
160	0.62929	0.45361	0.81617	35.076	2022
170	0.63053	0.45542	0.81562	35.261	2011
172.17	0.63080	0.45583	0.81549	35.302	2009

Table 17d. Inter-atomic distances for chlorine

T K	*y*	*z*	*d*1 nm	*d*2 nm	*d*3 nm	*d*4 nm	*d*5 nm	*d*6 nm
0	0.1252	0.1025	0.2000	0.3256	0.3692	0.3773	0.3661	0.3897
5	0.1248	0.1025	0.1999	0.3255	0.3695	0.3773	0.3663	0.3897
10	0.1244	0.1025	0.1997	0.3256	0.3698	0.3773	0.3664	0.3898
15	0.1241	0.1025	0.1996	0.3256	0.3701	0.3775	0.3666	0.3899
20	0.1238	0.1025	0.1994	0.3258	0.3705	0.3777	0.3669	0.3901
25	0.1235	0.1025	0.1994	0.3259	0.3709	0.3779	0.3672	0.3904
30	0.1233	0.1025	0.1993	0.3261	0.3713	0.3782	0.3674	0.3906
40	0.1229	0.1024	0.1992	0.3266	0.3720	0.3788	0.3680	0.3912
50	0.1225	0.1023	0.1990	0.3271	0.3727	0.3794	0.3685	0.3918
60	0.1223	0.1021	0.1989	0.3275	0.3734	0.3800	0.3690	0.3924
70	0.1221	0.1020	0.1988	03280	0.3740	0.3806	0.3695	0.3930
80	0.1220	0.1018	0.1986	0.3286	0.3746	0.3813	0.3699	0.3936
90	0.1219	0.1017	0.1985	0.3291	0.3751	0.3820	0.3703	0.3942
100	0.1219	0.1015	0.1984	0.3296	0.3756	0.3827	0.3707	0.3948
110	0.1219	0.1013	0.1983	0.3302	0.3762	0.3835	0.3711	0.3953
120	0.1219	0.1012	0.1982	0.3307	0.3769	0.3847	0.3716	0.3959
130	0.1219	0.1010	0.1981	0.3313	0.3776	0.3851	0.3720	0.3965
140	0.1219	0.1009	0.1980	0.3319	0.3784	0.3860	0.3725	0.3970
150	0.1219	0.1007	0.1980	0.3324	0.3793	0.3869	0.3729	0.3976
160	0.1219	0.1006	0.1980	0.3330	0.3803	0.3879	0.3735	0.3981
170	0.1219	0.1005	0.1980	0.3336	0.3814	0.3889	0.3740	0.3986
172.17	0.1219	0.1005	0.1980	0.3338	0.3817	0.3891	0.3741	0.3987

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18 ARGON Ar

Atomic weight: 39.792 to 39.963 (Meija 2017)
Select 2015 value 39.948 (1) (CIAAW 2015)

Structure: Face-centered cubic (cF4)

The triple point is a primary fixed point on ITS-90 at 83.8058 K (Preston-Thomas 1990).

18.1 Crystallographic properties

Smoothed values derived from the lattice parameter measurements of Peterson et al. 1966 (4-83 K) were combined with dilatometric measurements of Tilford and Swenson 1972 (1-35 K). The measurements were extrapolated to the triple point. The lattice parameter determined by both Batchelder and Simmons 1965 and Peterson et al. 1966 at 4.25 K corrects to 0.531113 (8) nm and is selected. Urvas et al. 1967 obtained a slightly higher value of 0.531127 nm at 4.25 K. However, depending on the method of production, Peterson et al. 1965 found variations of 0.531111 (8) nm to 0.531137 (8) nm for different crystals. Lattice parameter measurements of Schwalbe and Wilkins 1980 (70-83 K) are systematically 1 x 10^{-5} nm higher than the selected values and this may also be due to the origin of the samples being used while similar measurements of Barrett and Meyer 1964 (4.2-81 K) can be considered as varying by ± 9 x 10^{-5} nm around the selected values. Lattice parameter measurements along the melting line by Macrander and Crawford 1977 and Macrander 1978 leads to a value which is 6 x 10^{-5} nm higher at the triple point but this is within experimental accuracy.

18.2 Bulk properties

Schwalbe 1976 could not detect thermal vacancy effects when trying to measure differences between lattice parameter and bulk determinations of thermal expansion, and wide variations are found with other methods. However, there have been numerous theoretical estimates of the thermal vacancy parameters and these are listed by Schwalbe 1976 and from which consensus vacancy values of H_V = 80 (20) eV and S_V/k = 3 (2) have been derived and which were used to derived the bulk properties in Table 18b with the assumption that crystallographic and bulk properties are equal at 60 K. Lattice parameter measurements of Dobbs et al. 1956 at 20 K and 40 K and direct density measurements at 60 K and 80 K on average agree with the selected values of density to within 1 kg m^{-3}. Direct density measurements on solids obtained from the vapour by Smith and Chapman 1967 at 77.25 and 77.40 K lead to values 1 kg m^{-3} higher than the selected values while measurements on solids obtained from the liquid 77.45 to 81.70 K are on 1 kg m^{-3} lower. Measurements of Smith 1961 (77-83 K), which were only shown graphically, appear to trend from 5 to 1 kg m^{-3} low. Bulk volume thermal expansion coefficients determined by Manzhelii et al. 1967 (15-48 K) trend from 14% lower to 0.2% higher than the selected values.

Table 18a. Crystallographic properties of argon

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_0$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	0	0.53111	0.37555	22.555	1771.1
1	0.0347	< 0.0001	0.53111	0.37555	22.555	1771.1
2	0.280	< 0.0001	0.53111	0.37555	22.555	1771.1
3	0.983	0.0001	0.53111	0.37555	22.555	1771.1
4	2.45	0.0002	0.53111	0.37555	22.555	1771.1
5	5.10	0.0006	0.53111	0.37555	22.556	1771.1
6	9.48	0.0013	0.53112	0.37556	22.556	1771.1
7	15.84	0.0026	0.53112	0.37556	22.557	1771.0
8	24.23	0.0046	0.53114	0.37557	22.558	1770.9
9	34.47	0.0075	0.53115	0.37558	22.560	1770.7
10	46.20	0.0115	0.53117	0.37560	22.563	1770.5
11	58.93	0.0168	0.53120	0.37562	22.567	1770.2
12	72.46	0.0233	0.53123	0.37564	22.571	1769.8
13	86.50	0.0313	0.53128	0.37567	22.576	1769.5
14	100.8	0.0407	0.53133	0.37570	22.583	1769.0
15	115.2	0.0514	0.53138	0.37575	22.590	1768.4
16	129.5	0.0637	0.53145	0.37579	22.598	1767.7
18	158.3	0.0925	0.53160	0.37590	22.618	1766.6
20	183.7	0.127	0.53178	0.37603	22.641	1764.4
25	240.0	0.233	0.53235	0.37643	22.713	1758.8
30	285.4	0.365	0.53305	0.37692	22.803	1751.9
35	323.0	0.517	0.53386	0.37750	22.907	1743.9
40	356.0	0.689	0.53477	0.37814	23.024	1735.0
45	388.0	0.875	0.53576	0.37884	23.153	1725.4
50	418.0	1.079	0.53684	0.37960	23.293	1715.0
55	449.7	1.299	0.53801	0.38043	23.446	1703.9
60	483.3	1.535	0.53926	0.38132	23.610	1692.0
65	521.0	1.790	0.54062	0.38228	23.789	1679.3
70	566.3	2.067	0.54209	0.38332	23.983	1665.7
75	618.3	2.369	0.54370	0.38445	24.197	1651.0
80	677.0	2.701	0.54546	0.38570	24.433	1635.0
83	715.7	2.916	0.54660	0.38650	24.586	1624.8
83.8058	726.5	2.975	0.54691	0.38673	24.629	1622.0

$$d = a/\sqrt{2}$$

Table 18b. Bulk properties of argon

$3\ (\varepsilon_0 L - \varepsilon_0 a) = \exp(3.0 - 928.4/T)$ $\quad \alpha_L - \alpha_a = (309.5/T^2) \exp(3.0 - 928.4/T)$

T K	$\alpha \times 10^6$ K	$100\ \varepsilon_0$	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
60	483.3	1.535	23.610	1692.0
65	521.9	1.791	23.789	1679.3
70	568.5	2.068	23.984	1665.6
75	623.0	2.372	24.199	1650.8
80	685.9	2.707	24.437	1634.7
83	728.2	2.925	24.593	1624.4
83.8058	736.7	2.985	24.636	1621.5

This Table is considered to be identical to Table 18a below 60 K.

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19 POTASSIUM K

Atomic weight: 39.0983 (1) (Meija 2017)

Structure: Body-centered cubic (cI2)

Alcock et al. 1994 select 336.6 (2) K for the melting point.

19.1 Crystallographic properties

Initially the dilatometric thermal expansion measurements of Schouten and Swenson 1974 (0-320 K) and the lattice parameter measurements of Stetter et al. 1978 (279-336 K) appear to be incompatible. This problem was overcome by selecting 250 K (i.e. 0.74 T_M) as the point of onset of thermal vacancy effects. The thermal expansion at 250 K and its derivative derived from the equations of Schouten and Swenson 1974 were then combined with the fixed values $\varepsilon_T = 0$ at 293.15 K and $\varepsilon_T = 3.455 \times 10^{-3}$ at the melting point as derived from the lattice parameter equation given by Stetter et al. 1978 to produce an equation to represent the "crystallographic" properties up to the melting point as:

$$\varepsilon_T = 5.26084 \times 10^{-5} T + 3.57358 \times 10^{-8} T^2 + 1.47818 \times 10^{-11} T^3 - 1.88656 \times 10^{-2} \quad (19a)$$

At 250 K this equation leads to $\varepsilon_T = -3.249 \times 10^{-3}$ and this value was used as a fixed point to calculate length change values below this temperature using three point integration of the thermal expansion coefficients measured by Schouten and Swenson 1974.

On the basis $100\Delta\varepsilon$, the actual lattice parameters values of Stetter et al. 1978, when smoothed, show an average bias of only 0.001 lower than the selected values**.** On the same basis length change values derived from the volume ratios of Anderson and Swenson 1983 (4-297 K) scatter from 0.027 low to 0.006 high while the earlier molar volume values of Montfort and Swenson 1965 (0-300 K) reduced to length change values are initially 0.056 high, but above 100 K only show an average bias of 0.005 high. Lattice parameter measurements of Simon et al. 1976 (108-238 K) initially agree but then trend to 0.0011 nm low. A number of individual measurements in the low temperature region are compared with selected values as follows:

Table 19a. A comparison of additional length change values.

References	T K	*a* nm	Δ*a* nm	Note
Barrett 1956	4	0.5225	- 0.0011	
	66	0.5236	- 0.0011	
	78	0.5247	- 0.0033	
Thomas and Turner 1968	1.1	0.5234_8	- 0.0001	a
Templeton 1972	(4)	0.5234_6	- 0.0001	a
Altounian and Datars 1980	1.3	0.5234_4	- 0.0001	a
Werner et al. 1969	5.2	0.52295	- 0.0006	
Berliner et al. 1989	20	0.52334	- 0.0002	

Notes for Table 19a

a. Lattice parameter calculated from De Haas-van Alphen (dHvA) measurements using the free electron model

Table 19b. Lattice parameter of potassium at 293.15 K

References	Original Temperature K	*a* nm	Notes
Stokes 1966	293	0.532686	a
Stetter et al. 1978	293	0.532691	
	Selected	0.53269(3)	

Notes for Table 19b

a. Calculated from interpolated molar volume 45.513 $cm^3\ mol^{-1}$

At 293.15 K: Density 859.0 (1) kg m^{-3} Atomic volume 45.514 (8) $cm^3\ mol^{-1}$

19.2 Bulk properties

Above 250 K the thermal expansion coefficients of Schouten and Swanson 1974 are considered as representing the bulk properties as given in Table 19c. Based on the fixed length change value at 250 K the bulk thermal expansion is represented by:

$$\varepsilon_T = -3.20179 \times 10^{-5} T + 5.33262 \times 10^{-7} T^2 - 1.30715 \times 10^{-9} T^3 + 1.33959 \times 10^{-12} T^4 - 1.33820 \times 10^{-2} \quad (19b)$$

The net defect concentration $\Delta N/ N_0 = 4.3 \times 10^{-4}$ is similar to the value of 4.4×10^{-4} obtained for lithium from a direct comparison between dilatometric and lattice parameter measurements determined by Feder 1970 but differs from the value of 7.3×10^{-4} obtained for sodium from a combination of several sets of measurements.

On the basis $100\Delta\varepsilon$, molar volume measurements of Stokes 1966 reduced to length change values which only show a scatter of 0.010 low to 0.005 high.

Table 19c. Crystallographic properties of potassium

T K	α x 10^6 K^{-1}	100 ε_T	*a* nm	*d* nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
0	0	- 1.714	0.52356	0.45341	43.213	0.9048
5	0.95	- 1.714	0.52356	0.45341	43.213	0.9048
10	6.01	- 1.713	0.52357	0.45342	43.215	0.9047
15	13.57	- 1.708	0.52359	0.45344	43.221	0.9046
20	21.72	- 1.699	0.52364	0.45348	43.233	0.9044
25	29.24	- 1.687	0.52370	0.45354	43.249	0.9040
30	35.53	- 1.671	0.52379	0.45362	43.271	0.9036
40	44.11	- 1.631	0.52400	0.45380	43.323	0.9025
50	49.08	- 1.585	0.52425	0.45401	43.384	0.9012
60	52.46	- 1.535	0.52451	0.45424	43.450	0.8998
70	54.96	- 1.482	0.52479	0.45449	43.520	0.8984
80	56.85	- 1.427	0.52509	0.45474	43.593	0.8969
90	58.32	- 1.370	0.52539	0.45500	43.669	0.8953
100	59.52	- 1.312	0.52570	0.45527	43.746	0.8938
110	60.56	- 1.253	0.52603	0.45554	43.825	0.8922
120	61.49	- 1.192	0.52634	0.45582	43.905	0.8905
130	62.39	- 1.131	0.52666	0.45610	43.987	0.8889
140	63.27	- 1.069	0.52700	0.45639	44.070	0.8872
150	64.14	- 1.006	0.52733	0.45668	44.154	0.8855
160	65.00	- 0.942	0.52767	0.45698	44.240	0.8838
170	65.85	- 0.877	0.52802	0.45728	44.327	0.8821
180	66.69	- 0.812	0.52837	0.45758	44.415	0.8803
190	67.50	- 0.745	0.52872	0.45789	44.504	0.8785
200	68.32	- 0.678	0.52908	0.45820	44.595	0.8767
210	69.35	- 0.609	0.52944	0.45851	44.687	0.8749
220	70.42	- 0.540	0.52982	0.45883	44.781	0.8731
230	71.37	- 0.469	0.53019	0.45916	44.876	0.8712
240	72.43	- 0.398	0.53057	0.45949	44.973	0.8694
250	73.49	- 0.325	0.53096	0.45982	45.072	0.8675
260	74.38	- 0.251	0.53135	0.46016	45.172	0.8655
270	75.27	- 0.177	0.53175	0.46051	45.273	0.8636
280	76.17	- 0.101	0.53215	0.46086	45.376	0.8616
290	77.08	- 0.024	0.53256	0.46121	45.481	0.8597
293.15	77.37	0	0.53269	0.46132	45.514	0.8590
295	77.54	0.014	0.53277	0.46146	45.553	0.8583
300	78.00	0.053	0.53297	0.46157	45.587	0.8577
305	78.46	0.092	0.53318	0.46174	45.640	0.8567
310	78.92	0.132	0.53339	0.46193	45.694	0.8557
315	79.39	0.171	0.53360	0.46211	45.748	0.8546
320	79.85	0.211	0.53381	0.46230	45.803	0.8536
325	80.32	0.251	0.53403	0.46248	45.858	0.8526
330	80.79	0.292	0.53424	0.46267	45.914	0.8516
335	81.26	0.332	0.53446	0.46286	45.969	0.8505
336.6	81.41	0.345	0.53453	0.46292	45.987	0.8502

$$d = \sqrt{3}a/2$$

Table 19d. Bulk properties of potassium

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
250	73.49	- 0.325	45.072	0.8675
260	74.55	- 0.251	45.172	0.8655
270	75.67	- 0.176	45.274	0.8636
280	76.87	- 0.100	45.378	0.8616
290	78.18	- 0.023	45.483	0.8596
293.15	78.62	0.002	45.517	0.8590
300	79.64	0.056	45.591	0.8576
310	81.27	0.137	45.701	0.8555
320	83.11	0.219	45.814	0.8534
330	85.19	0.304	45.930	0.8513
336.6	86.71	0.360	46.008	0.8498

This Table is considered to be identical to Table 19c below 250 K.

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20 CALCIUM Ca

Atomic Weight: 40.078 (4) (Meija 2017)

Allotropy: Alpha phase: Face-centered cubic (cF4)
Beta phase: Body-centered cubic (cI2)

Both Melsert et al. 1956 and Schottmiller et al. 1958 reported an intermediate hexagonal close-packed (hP2) structure but Peterson and Fattore 1961 showed that this was due to hydrogen contamination. Alcock et al. 1993 selected 716 (3) K for the alpha-beta transition temperature and 1115 (2) K for the melting point.

20.1 Alpha Phase: Face-centered cubic (cF4): 0 K to 716 K.

Up to 16 K thermal expansion coefficients of White 1972 (3-85 K and 283 K) were fitted to a Debye equation and extrapolated to 0 K. At 20 K and above they were combined with the selected specific heat values of Alcock et al. 1993 and fitted to Equation A which was extrapolated to 293.15 K:

$$0\text{–}16\ \text{K}: \quad \alpha\ (\text{K}^{-1}) = 1.36795 \times 10^{-10}\,T + 7.63219 \times 10^{-11}\,T^{3} + 1.76764 \times 10^{-13}\,T^{5} - 1.12009 \times 10^{-16}\,T^{7} \qquad (20a)$$

$$20 - 293.15\ \text{K}: \quad \alpha\ (\text{K}^{-1}) = Cp\,(\,8.82472 \times 10^{-7} + 3.35920 \times 10^{-12}\,T - 5.13532 \times 10^{-6}\,/T) \qquad (20b)$$

Equation 20a has an accuracy of ± 6 x 10^{-10} K^{-1} and equation 20b ± 2.7 x 10^{-8} K^{-1}. Intermediate values in the range 16 K to 20 K were given by White 1972. On the basis $100\Delta\varepsilon$ length change values derived from the volume ratios of Anderson et al. 1990 (4-295 K) show a scatter of only 0.008 low to 0.005 high while dilatometric measurements of Erfling 1942 (57-313 K) trend from being only 0.010 high at the lowest temperature and then converge to the selected values.

In the high temperature region, in agreement with Touloukian et al. 1975, it is considered that the mean thermal expansion coefficients as given by Bernstein and Smith 1959 (299-644 K) are not compatible with the low temperature data and therefore instead the provisional length change values suggested by Touloukian et al. 1975 over the range 400 K to 625 K were accepted and were refitted to the following equation:

$$\varepsilon_T = 1.89249 \times 10^{-5}\,T + 6.56809 \times 10^{-9}\,T^{2} - 1.96836 \times 10^{-12}\,T^{3} - 6.06269 \times 10^{-3} \qquad (20c)$$

The equation was extrapolated to the transition temperature. On the basis $100\Delta\varepsilon$ the measurements of Bernstein and Smith 1959 trend up to 0.044 low while measurements of Schulze 1935 (293-814 K), in what could be considered as being the alpha region, show scatter but can be considered as trending to 0.39 low.

Table 20a. Lattice parameter measurements of alpha calcium at 293.15 K

References	Original Temperature K	*a* nm	Notes
Klemm and Mika 1941	RT	0.5577	a
Smith et al. 1956	291	0.5583	
Schottmiller et al. 1958	298	0.5601	a
Berstein and Smith 1959	299	0.55880	
Peterson and Fattore 1961	RT	0.5590	
Bruzzone 1971	RT	0.5585	a
	Selected	0.5588 (5)	

Notes for Table 20a

a. Not included in the average

At 293.15 K: Density 1526 (4) kg m^{-3} Atomic volume 26.27 (7) cm^3 mol^{-1}.

20.2 Beta Phase: Body-centered cubic (cI2): 716 K to 1115 K.

Jayaraman et al. 1963 determined the transition pressure to be 0.033 K MPa^{-1} which together with an enthalpy of transition of 930 (100) J mol^{-1}, as selected by Alcock et al. 1993, leads to a molar volume of transition of 0.043 cm^3 mol^{-1} using the Clausius-Clapeyron equation and from the alpha phase, a molar volume of 27.12_0 cm^3 mol^{-1} for the beta phase. This value, together with a thermal expansion coefficient of 33.6 (1.6) x 10^{-6} K^{-1}, as determined by Bernstein and Smith 1959 over the range 740 K to 876 K, were used to derive the equations:

$$a \text{ (nm)} = 1.47074 \times 10^{-5} T + 0.437720 \quad (20d)$$

$$\varepsilon_T = 3.31606 \times 10^{-5} T - 1.30769 \times 10^{-2} \quad (20e)$$

The actual lattice parameter determined by Bernstein and Smith 1959 at 740 K is 0.0006 nm lower than the selected value while the earlier value of Smith et al. 1956 at 773 K is 0.0014 nm lower. The measurement by Schottmiller et al. 1958 at 888 K is 0.0020 nm lower but the samples used were almost certainly saturated with hydrogen. On the basis $100\Delta\varepsilon$ dilatometric measurements of Schulze 1935 (293-814 K) in what could be considered to be the beta region show scatter but are on average 0.72 low.

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Table 20b. Crystallographic properties of alpha calcium

T K	α x 10^6 K^{-1}	100 ε_T	*a* nm	*d* nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
0	0	- 0.479	0.5561	0.3932	25.89	1548
10	0.09	- 0.479	0.5561	0.3932	25.89	1548
20	1.00	- 0.478	0.5561	0.3932	25.90	1548
30	3.30	- 0.476	0.5561	0.3932	25.90	1548
40	6.21	- 0.472	0.5562	0.3933	25.90	1547
50	9.05	- 0.464	0.5562	0.3933	25.91	1547
60	11.45	- 0.454	0.5563	0.3933	25.91	1547
70	13.36	- 0.441	0.5563	0.3934	25.92	1546
80	14.86	- 0.427	0.5564	0.3934	25.93	1545
90	16.03	- 0.412	0.5565	0.3935	25.95	1545
100	16.95	- 0.396	0.5566	0.3936	25.96	1544
110	17.71	- 0.378	0.5567	0.3936	25.97	1543
120	18.34	- 0.360	0.5568	0.3937	25.99	1542
130	18.87	- 0.342	0.5569	0.3938	26.00	1541
140	19.30	- 0.323	0.5570	0.3939	26.02	1540
150	19.67	- 0.303	0.5571	0.3939	26.03	1540
160	19.99	- 0.284	0.5572	0.3940	26.05	1539
170	20.28	- 0.263	0.5573	0.3941	26.06	1538
180	20.54	- 0.243	0.5574	0.3942	26.08	1537
190	20.78	- 0.222	0.5576	0.3943	26.10	1536
200	20.98	- 0.202	0.5577	0.3943	26.11	1535
210	21.17	- 0.181	0.5578	0.3944	26.13	1534
220	21.32	- 0.159	0.5579	0.3945	26.14	1533
230	21.48	- 0.138	0.5580	0.3946	26.16	1532
240	21.61	- 0.117	0.5581	0.3947	26.18	1531
250	21.72	- 0.095	0.5583	0.3948	26.20	1530
260	21.84	- 0.073	0.5584	0.3948	26.21	1529
270	21.97	- 0.051	0.5585	0.3949	26.23	1528
280	22.11	- 0.029	0.5586	0.3950	26.25	1527
290	22.23	- 0.007	0.5588	0.3951	26.26	1526
293.15	22.27	0	0.5588	0.3951	26.27	1526
300	22.33	0.015	0.5589	0.3952	26.28	1525
350	22.77	0.128	0.5595	0.3956	26.37	1520
400	23.18	0.243	0.5602	0.3961	26.46	1515
450	23.56	0.360	0.5608	0.3966	26.56	1509
500	23.90	0.480	0.5615	0.3970	26.65	1504
550	24.22	0.601	0.5622	0.3975	26.75	1498
600	24.50	0.723	0.5628	0.3980	26.84	1493
650	24.76	0.847	0.5635	0.3985	26.94	1487
700	24.98	0.973	0.5642	0.3990	27.04	1482
716	25.05	1.013	0.5645	0.3991	27.08	1480

$$d = a/\sqrt{2}$$

Table 20c. Crystallographic properties of beta calcium

T K	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
716	1.067	0.4483	0.3882	27.12	1478
750	1.179	0.4488	0.3886	27.21	1473
800	1.345	0.4495	0.3893	27.34	1466
850	1.511	0.4502	0.3899	27.48	1459
900	1.677	0.4510	0.3905	27.61	1451
950	1.843	0.4517	0.3912	27.75	1444
1000	2.008	0.4524	0.3918	27.88	1437
1050	2.174	0.4532	0.3925	28.02	1430
1100	2.340	0.4539	0.3931	28.16	1423
1115	2.390	0.4541	0.3933	28.20	1421

$$d = \sqrt{3}a/2$$

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21 SCANDIUM Sc

Atomic weight: 44.955908 (5) (Meija 2017)

Allotropy: Alpha phase: Hexagonal close-packed (hP2)
Beta phase: Body-centered cubic (cI2)

Gschneidner 1990 selects 1610 K for the alpha-beta transformation temperature and 1814 K for the melting point.

21.1 Alpha Phase: Hexagonal close-packed (hP2): 0 K to 1610 K.

Up to 293.15 K selected values are based on the thermal expansion equations given by Swenson 1996 (0-300 K). On the basis $100\Delta\varepsilon$ length change values derived from the lattice parameter equations of Zhabko 1982 (80-360 K) trend from initially 0.035 high to then agree with selected values along the *a* axis while along the *c* axis the trend is from initially 0.005 low to a maximum of 0.004 high at 180 K.

In the high temperature region, length change values along the *a* and *c* axes derived by Touloukian et al. 1975 from the lattice parameter values of Spedding et al. 1961 (293-1282 K) were corrected to correspond to the selected thermal expansion coefficients at 293.15 K as equations 21a and 21c respectively. Above 900 K and 1050 K respectively these were combined with length change values derived from the lattice parameter measurements of Kammler et al. 2008 (298, 1473-1643 K in the alpha region). A certain degree of incompatibility between these two sets of measurements was resolved as given in Part 21.3 and above 293.15 K the thermal expansion can be represented by the equations:

a axis

293.15-900 K: $\varepsilon_T a = 6.26513 \times 10^{-6} T + 3.28335 \times 10^{-9} T^2 - 8.15152 \times 10^{-13} T^3 - 2.09825 \times 10^{-3}$ (21a)

900-1610 K: $\varepsilon_T a = 1.33487 \times 10^{-5} T - 5.37638 \times 10^{-9} T^2 + 2.69133 \times 10^{-12} T^3 - 4.01696 \times 10^{-3}$ (21b)

c axis

293.15-1050 K: $\varepsilon_T c = 1.25539 \times 10^{-5} T + 2.53237 \times 10^{-9} T^2 - 3.82544 \times 10^{-13} T^3 - 3.88816 \times 10^{-3}$ (21c)

1050-1610 K: $\varepsilon_T c = 4.78637 \times 10^{-5} T - 3.47717 \times 10^{-8} T^2 + 1.26533 \times 10^{-11} T^3 - 1.49403 \times 10^{-2}$ (21d)

For comparison purposes length change values have been derived from a number of sets of lattice parameter determinations. On the basis $100\Delta\varepsilon$ those of Schmitz-Pranghe and Dünner 1968 (293, 539-932 K) along the *a* axis scatter 0.011 to 0.073 high while along the *c* axis the trend is 0.060 low to 0.014 high. In the case of the measurements of Hájek

et al. 1973 (293-1773 K) the *a* axis values trend from 0.93 high at 773 K to 0.41 high at 1773 K, and the *c* axis values from 0.10 high at 773 K to 1.39 low at 1773 K where the highest temperature represents an extrapolation above the stability limit of the alpha phase. The measurements of Mardon et al. 1961 (290-1131 K) were only shown graphically with actual data points given by Touloukian et al. 1975. Along the *a* axis these show a trend to 0.15 high while along the *c* axis there is an average deviation of 0.044 low at 582 K and above. The selected values of Touloukian are based on the measurements of Spedding et al. 1961 and average 0.011 low along the *a* axis and along the *c* axis trend from 0.018 high at 600 K to 0.009 low at 1200 K.

Table 21a. Lattice parameter of alpha scandium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Notes
Spedding et al. 1956	RT	0.33092	0.52736	
Mardon et al. 1961	293	0.33087	0.52705	a
Spedding and Beaudry 1971	297	0.33089	0.52680	b
Zhabko et al. 1982	293	0.33061	0.52706	c
Kammler et al. 2008	298	0.33097	0.52660	
	Selected	0.33089 (2)	0.52680 (3)	

Notes for Table 21a

a. Values given by Touloukian et al. 1975

b. Temperature of measurements given by Gschneidner 1990

c. Derived from equations

In agreement with Gschneidner 1990 the values determined by Spedding and Beaudry 1971 for electropolished wires are selected.

At 293.15 K: Density 2989 (1) kg m^{-3} Molar volume 15.041 (2) cm^3 mol^{-1}

21.2 Beta Phase: Body-centered cubic (cI2): 1610 K to 1814 K.

Beaudry and Daane 1962 identified the structure from the formation of a continuous series of solid solutions between beta scandium and beta titanium at high temperatures while Petry et al. 1993 directly determined the lattice parameter at 1673 K. Lattice parameter measurements of Kammler et al. 2008 (1623-1673 K) over the range 1633 to 1673 K were fitted to the following equations and referenced directly to the selected values at 293.15 K. The lattice parameter values are considered to be accurate equal to $\pm$ 8 x 10^{-5} nm:

$$a \text{ (nm)} = 5.60000 \times 10^{-6} T + 0.366366 \quad (21e)$$

$$\varepsilon = 1.52057 \times 10^{-5} T - 5.20422 \times 10^{-3} \quad (21f)$$

The derived thermal expansion coefficient of 14.9 x 10^{-6} K^{-1} differs from the value of 16.1 x 10^{-6} K^{-1} suggested by Kammler et al. 2008. The molar volume increase through the alpha-beta transition is 0.35%.

21.3 Derivation of the high temperature equations for the alpha phase

For the lattice parameter measurements of Kammler et al. 2008 (298, 1473-1643 K in the alpha phase) the stabilization of the alpha phase 33 K above the alpha-beta transition temperature is considered as an indication of oxidation and a possible expansion of the lattice parameters which may explain the large difference between these values and an extension of the values of Spedding et al. 1961. For the *a* axis the incompatibility between the two sets of measurements was resolved by fixing the value 100 ε_T at *a* = 1.477 at 1610 K obtained by fitting the the selected measurements at 1583, 1593 and 1613 K to a linear relationship and interpolating. These values were combined with values 750 K to 950 K from equation 21a to derive equation 21b. For the *c* axis, values 800 K to 1100 K from equation 21c were combined with high temperature measurements at 1573, 1583, 1593 and 1623 K to derive equation 21d. On the basis 100ε the derived length change value at 1610 K is only 0.001 lower than a linear fit to the length change values at 1573, 1583, 1593 and 1623 K and interpolating. In order to retain their integrity the length change values of Kammler et al. 2008 were obtained by direct reference to the selected lattice parameter values at 293.15 K and not their actual values at 298 K.

Table 21b. Crystallographic properties of alpha scandium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T a$	100 ε_T avr
0	0	0	0	- 0.164	- 0.243	- 0.190
10	0.33	- 0.44	0.07	- 0.164	- 0.243	- 0.190
20	0.68	- 0.69	0.22	- 0.163	- 0.244	- 0.190
30	1.11	- 0.57	0.55	- 0.162	- 0.245	- 0.190
40	1.64	0.18	1.15	- 0.161	- 0.245	- 0.189
50	2.28	1.34	1.97	- 0.159	- 0.244	- 0.187
60	3.01	2.67	2.90	- 0.156	- 0.242	- 0.185
70	3.72	3.95	3.80	- 0.153	- 0.239	- 0.182
80	4.36	5.12	4.61	- 0.149	- 0.234	- 0.177
90	4.92	6.16	5.33	- 0.144	- 0.229	- 0.173
100	5.39	7.08	5.95	- 0.139	- 0.222	- 0.167
110	5.79	7.89	6.49	- 0.134	- 0.215	- 0.161
120	6.12	8.60	6.95	- 0.128	- 0.206	- 0.154
130	6.40	9.21	7.34	- 0.121	- 0.197	- 0.147
140	6.64	9.75	7.68	- 0.115	- 0.188	- 0.139
150	6.84	10.23	7.97	- 0.108	- 0.178	- 0.131
160	7.01	10.65	8.22	- 0.101	- 0.168	- 0.123
170	7.15	11.04	8.45	- 0.094	- 0.157	- 0.115
180	7.26	11.39	8.64	- 0.087	- 0.146	- 0.107
190	7.35	11.72	8.81	- 0.080	- 0.134	- 0.098
200	7.44	12.02	8.97	- 0.072	- 0.122	- 0.089
210	7.51	12.31	9.11	- 0.065	- 0.110	- 0.080
220	7.59	12.58	9.25	- 0.057	- 0.098	- 0.071
230	7.66	12.83	9.38	- 0.050	- 0.085	- 0.061
240	7.74	13.06	9.51	- 0.042	- 0.072	- 0.052
250	7.81	13.26	9.63	- 0.034	- 0.059	- 0.042
260	7.88	13.45	9.74	- 0.026	- 0.045	- 0.033
270	7.92	13.62	9.82	- 0.018	- 0.032	- 0.023
280	7.95	13.77	9.89	- 0.010	- 0.018	- 0.013
290	7.97	13.91	9.95	- 0.003	- 0.004	- 0.003
293.15	7.98	13.94	9.97	0	0	0
300	8.01	13.97	10.00	0.005	0.010	0.007
400	8.49	14.37	10.45	0.088	0.151	0.109
500	8.92	14.76	10.87	0.175	0.297	0.216
600	9.30	15.11	11.24	0.267	0.447	0.327
700	9.63	15.44	11.57	0.362	0.601	0.441
800	9.91	15.75	11.86	0.460	0.758	0.559
900	10.14	16.04	12.11	0.561	0.918	0.680
1000	10.60	16.29	12.50	0.665	1.082	0.804
1100	11.20	17.08	13.16	0.774	1.248	0.932
1200	11.97	18.81	14.25	0.891	1.429	1.070
1300	12.88	21.26	15.67	1.016	1.632	1.221
1400	13.96	24.45	17.46	1.152	1.864	1.389
1500	15.19	28.35	19.58	1.299	2.132	1.576
1600	16.57	32.97	22.04	1.460	2.445	1.787
1610	16.72	33.46	22.30	1.477	2.479	1.810

Table 21c. Crystallographic properties of alpha scandium

T K	*a* nm	*c* nm	*c*/*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.33035	0.52552	1.5908	0.32468	14.955	3006
10	0.33035	0.52552	1.5908	0.32468	14.955	3006
20	0.33035	0.52551	1.5908	0.32468	14.955	3006
30	0.33035	0.52551	1.5908	0.32468	14.955	3006
40	0.33036	0.52551	1.5907	0.32468	14.955	3006
50	0.33036	0.52551	1.5907	0.32469	14.956	3006
60	0.33037	0.52552	1.5907	0.32469	14.957	3006
70	0.33038	0.52554	1.5907	0.32470	14.959	3005
80	0.33040	0.52557	1.5907	0.32472	14.961	3005
90	0.33041	0.52560	1.5907	0.32474	14.963	3004
100	0.33043	0.52563	1.5907	0.32476	14.965	3004
110	0.33045	0.52567	1.5908	0.32478	14.968	3003
120	0.33047	0.52571	1.5908	0.32480	14.971	3003
130	0.33049	0.52576	1.5909	0.32483	14.974	3002
140	0.33051	0.52581	1.5909	0.32486	14.978	3001
150	0.33053	0.52586	1.5910	0.32488	14.981	3001
160	0.33056	0.52592	1.5910	0.32491	14.985	3000
170	0.33058	0.52597	1.5911	0.32495	14.989	2999
180	0.33060	0.52603	1.5911	0.32498	14.993	2999
190	0.33063	0.52609	1.5912	0.32501	14.996	2998
200	0.33065	0.52616	1.5913	0.32504	15.000	2997
210	0.33068	0.52622	1.5913	0.32508	15.005	2996
220	0.33070	0.52629	1.5914	0.32511	15.009	2995
230	0.33073	0.52635	1.5915	0.32515	15.013	2994
240	0.33075	0.52642	1.5916	0.32518	15.017	2994
250	0.33078	0.52649	1.5917	0.32522	15.021	2993
260	0.33080	0.52656	1.5918	0.32526	15.026	2992
270	0.33083	0.52663	1.5919	0.32530	15.030	2991
280	0.33086	0.52670	1.5919	0.32533	15.035	2990
290	0.33088	0.52678	1.5920	0.32537	15.039	2989
293.15	0.33089	0.52680	1.5921	0.32539	15.041	2989
300	0.33091	0.52685	1.5921	0.32541	15.044	2988
400	0.33118	0.52760	1.5931	0.32581	15.090	2979
500	0.33147	0.52837	1.5940	0.32622	15.138	2970
600	0.33177	0.52916	1.5949	0.32664	15.189	2960
700	0.33209	0.52997	1.5959	0.32707	15.241	2950
800	0.33241	0.53079	1.5968	0.32752	15.294	2939
900	0.33274	0.53164	1.5977	0.32797	15.349	2929
1000	0.33309	0.53250	1.5987	0.32844	15.406	2918
1100	0.33345	0.53337	1.5996	0.32892	15.465	2907
1200	0.33384	0.53433	1.6006	0.32943	15.529	2895
1300	0.33425	0.53540	1.6018	0.33001	15.598	2882
1400	0.33470	0.53662	1.6033	0.33065	15.676	2868
1500	0.33519	0.53803	1.6052	0.33139	15.763	2852
1600	0.33572	0.53968	1.6075	0.33224	15.862	2834
1610	0.33578	0.53986	1.6078	0.33233	15.872	2832

$$d1 = (a^2/3 + c^2/4)^{½} \quad d2 = a$$

Table 21d. Crystallographic properties of beta scandium

T K	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1610	1.928	0.37538	0.32509	15.927	2823
1625	1.951	0.37547	0.32516	15.938	2821
1650	1.989	0.37561	0.32528	15.956	2818
1675	2.027	0.37575	0.32541	15.974	2814
1700	2.065	0.37589	0.32553	15.992	2811
1725	2.103	0.37603	0.32565	16.009	2808
1750	2.141	0.37617	0.32577	16.027	2805
1775	2.179	0.37631	0.32589	16.045	2802
1800	2.217	0.37645	0.32601	16.063	2799
1814	2.238	0.37652	0.32608	16.073	2797

$$d = \sqrt{3}a/2$$

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22 TITANIUM Ti

Atomic Weight: 47.867 (1) (Meija 2017)

Allotropy: Alpha phase: Hexagonal close-packed (hP2)
Beta phase: Body-centered cubic (cI2)

A transition temperature of 1159 (7) K was selected as an average of 1166 K determined by Cezairliyan and Miiller 1978 on heating cycles and 1152 K determined by Kaschnitz and Reiter 2002 on cooling cycles. The melting point is a secondary fixed point on ITS-90 at 1943 (2) K (Bedford et al. 1996).

22.1 Alpha Phase: Hexagonal close-packed (hP2): 0 K to 1159 K.

Selected values of length change measurements derived from the lattice parameter measurements of Medoff and Cadoff 1959 (298-1033 K), Spreadborough and Christian 1959 (282-972 K in the alpha phase), Wasilewski 1961 (292-1008 K), Willens 1962 (293-920 K), Roberts 1962 (285-884 K) and Schmitz-Pranghe and Dünner 1968 (85-1150 K in the alpha range) were fitted to the following equations with accuracies expressed on the basis ± 100 ε_T of ± 0.018 and ± 0.030 respectively:

$$\varepsilon_T\, a = 9.08966 \times 10^{-6}\, T + 6.68342 \times 10^{-10}\, T^2 - 2.72207 \times 10^{-3} \quad (22a)$$

$$\varepsilon_T\, c = 8.98435 \times 10^{-6}\, T + 1.83885 \times 10^{-9}\, T^2 - 2.79179 \times 10^{-3} \quad (22b)$$

The input measurements showed a marked scatter. On the basis $100\Delta\varepsilon$ the *a*-axis values of Wasilewski 1961 over the range 381 to 716 K were rejected because they differed from the selected values by an average of 0.093 high. Similarly the *c*-axis values of Roberts 1962 were all rejected because they averaged 0.081 low. Certain of the values determined by Schmitz-Pranghe and Dünner 1968 were rejected for both axes. For the range 413 to 885 K, *a*-axis values averaged 0.070 low and for the range 900 to 1113 K *c*-axis values averaged 0.14 high. Of additional lattice parameter measurements those of Berry and Raynor 1953 (574-985 K) were all rejected because the *a*-axis values averaged 0.046 high and the *c*-axis values 0.097 high. Measurements of Pawar and Deshpande 1968 (301-428 K) trend 0.019 high to 0.003 low for the *a*-axis and 0.005 to 0.056 low for the *c*-axis. The measurements of Wasilewski 1961 and Berry and Raynor 1953 were only shown graphically with actual data points given by Touloukian et al. 1975.

In the low temperature region anisotropic dilatometric measurements of Nizhankovskii et al. 1994 suggested that the *c*-axis initially showed a negative thermal expansion reaching a value of - 9 x 10^{-6} K^{-1} at 160 K before increasing dramatically to 1 x 10^{-5} K^{-1} at 200 K. Souvatzis et al. 2007 suggested on theoretical grounds that this behavior was possible. However, lattice parameter measurements of both Schmitz-Pranghe and Dünner 1968 (85-1150 K in the alpha range) and Zhabko 1982 (80-360 K) showed no evidence of a negative thermal expansion for the *c*-axis while bulk dilatometric measurements of both Laquer 1952 (0-300 K) and Altman et al. 1954 (20-300K) showed only continuous

smooth length change values covering the region 160 to 200 K. On these grounds it is considered that further work is required to confirm the findings of Nizhankovskii et al. 1994 and selected values are therefore based on the assumption that the thermal expansion behaves normally.

Length change values along both the *a* and c axes derived from the lattice parameter equations of Zhabko 1982 were adjusted to conform the selected thermal expansion coefficients and their derivatives at 293.15 K as equations 22d and 22f below. For the *a* axis equation 22d was used to extrapolate below 100 K by fitting derived thermal expansion coefficient values over the range 100 to 230 K to Equation A using the specific heat values selected by Desai 1987 to derive equation 22c. For the *c* axis equation 22f leads to a minimum in the derived thermal expansion coefficient at 136 K but this is considered to be an artifact of the fitting process because the original equation of Zhabko 1982 did not show this behavior. Therefore, the derived thermal expansion coefficients from equation 22f were extrapolated below 160 K and estimated values were combined with specific heat values of Desai 1987 in Equation A and were adjusted until they gave a smooth fit as equation 22e:

a axis

$$0 - 100\ \text{K:} \qquad \alpha_a = Cp\,(4.04959 \times 10^{-7} - 2.80133 \times 10^{-11}\,T - 9.59818 \times 10^{-7}/T) \qquad (22c)$$

$$100 - 293.15\ \text{K:} \quad \varepsilon_T a = -2.04133 \times 10^{-6}\,T + 5.35642 \times 10^{-8}\,T^2 - 1.11061 \times 10^{-10}\,T^3 + 8.68403 \times 10^{-14}\,T^4 - 1.84816 \times 10^{-3} \qquad (22d)$$

c axis

$$0 - 160\ \text{K:} \qquad \alpha_c = Cp\,(-1.71982 \times 10^{-7} + 1.69105 \times 10^{-9}\,T + 7.70636 \times 10^{-6}/T) \qquad (22e)$$

$$160 - 293.15\ \text{K:} \quad \varepsilon_T c = 2.80835 \times 10^{-5}\,T - 2.22536 \times 10^{-7}\,T^2 + 7.98277 \times 10^{-10}\,T^3 - 9.26396 \times 10^{-13}\,T^4 - 2.37756 \times 10^{-3} \qquad (22f)$$

On the basis $100\Delta\varepsilon$ along the *a* axis the values of Ebneter 1967 average 0.012 high while the *c* axis values scatter from 0.013 low to 0.013 high. The measurements of Schmitz-Pranghe and Dünner 1968 below 293.15 K reach a maximum difference of 0.033 high for the *a*-axis at 180 K and for the *c*-axis trend from initially 0.070 low at 100 K to then agree with the selected values. The dilatometric measurements of Laquer 1952 average 0.006 higher than the selected values while the measurements of Altman et al. 1954 average 0.005 higher. These differences of these dilatometric measurements from the selected values are considered to be surprisingly small in view of the uncertainties that could arise due to the extrapolation of the measurements of Zabko 1982 below experimental limits.

Table 22a. Lattice parameter of alpha titanium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Notes
Clark 1949	298	0.29504	0.46833	
Berry and Raynor 1953	RT	0.29498	0.46825	
Spreadborough and Christian 1959	293	0.29505	0.46807	a
Makarov and Kuznetsov1960	RT	0.29512	0.46853	
Wasilewski 1961	293	0.29510	0.46841	b
Roberts 1962	285 to 296	0.29506	0.46835	
Wood 1962	298	0.29511	0.46843	
Willens 1962	293	0.29498	0.46825	
Ebneter 1967	300	0.29505	0.46830	
Schmitze-Pranghe and Dünner 1968	293	0.29505	0.46813	
Pawar and Deshpande 1968	301	0.29507	0.46854	
	Selected	0.29505 (5)	0.46833 (16)	

Notes for Table 22a

a. From a fit to the data 282 to 972 K

b. Values given by Touloukian et al. 1975

At 293.15 K: Density 4502 (2) kg m^{-3} Molar volume 10.632 (4) cm^3 mol^{-1}.

22.2 Beta Phase: Body-centered cubic (cI2): 1159 K to 1943 K

Length change values corresponding to the beta phase lattice parameter values of Spreadborough and Christian 1959 (1181-1340 K) and Schmitz-Pranghe and Dünner 1968 (1193-1720 K) were referenced to the selected values for the alpha phase at 293.15 K. This resulted in the following equations where equation 22h as an accuracy on the basis of $\pm 100\varepsilon_T$ of ± 0.011:

$$a \text{ (nm)} = 1.54538 \times 10^{-6} T + 1.09231 \times 10^{-9} T^2 + 0.327747 \quad (22g)$$

$$\varepsilon_T = 4.71061 \times 10^{-6} T + 3.32956 \times 10^{-9} T^2 - 9.65168 \times 10^{-4} \quad (22h)$$

Equation 22g extrapolates to 0.3283 nm at room temperature in excellent agreement with values of 0.3283 (2) nm determined by Aurelio and Fernández-Guillermet 2000 by extrapolating Ti-Mo alloys to pure Ti and 0.3282 (2) nm determined by Aurelio et al. 2002 by extrapolating Ti-V alloys. However, at the transition temperature the molar volume difference between the alpha and beta phases is a contraction of only 0.007 cm^3 mol^{-1} whereas from the Clausius-Clapeyron equation using a temperature-pressure slope of the transition curve of – 0.008 K Mpa^{-1} as determined by Jayaraman et al. 1963 and a transition enthalpy of 4170 J mol^{-1} as selected by Desai 1987, then the contraction should be 0.03 cm^3 mol^{-1}. The differences may simply be due to the scatter in the data, especially for the alpha phase. Senkov et al. 2001 obtain a lattice parameter of 0.331 nm at 1173 K which agrees with the selected values while the measurements of Petry et al. 1991 (1155-

1783 K) were initially 0.0002 nm low but agreed with the selected values to better than 0.0001 nm above 1250 K. Eppelsheimer and Penman 1950b obtained a lattice parameter 0.00039 nm low at 1173 K but the metal used was only 99.0% + pure. Touloukian et al. 1975 selected length change values for the beta phase based on a compromise between the discrepant dilatometric measurements of Williams 1961 (1255-1699 K in the beta region), Mal'ko et al. 1970 (1212-1431 K in the beta region) and the single measurement of Fratsevich et al. 1967 at 1473 K. The selected values showed a trend of 0.025 to 0.099 low compared to the presently selected values.

Table 22c. Crystallographic properties of alpha titanium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 ε_T *a*	100 ε_T *c*	100 ε_T avr
0	0	0	0	- 0.183	- 0.107	- 0.158
10	0.02	0.04	0.03	- 0.183	- 0.107	- 0.158
20	0.12	0.08	0.11	- 0.183	- 0.107	- 0.158
30	0.44	0.16	0.35	- 0.183	- 0.107	- 0.158
40	1.01	0.24	0.75	- 0.182	- 0.107	- 0.157
50	1.80	0.31	1.30	- 0.181	- 0.107	- 0.156
60	2.68	0.40	1.92	- 0.179	- 0.106	- 0.155
70	3.52	0.51	2.52	- 0.176	- 0.106	- 0.152
80	4.31	0.66	3.09	- 0.172	- 0.105	- 0.150
90	5.03	0.84	3.63	- 0.167	- 0.105	- 0.146
100	5.65	1.07	4.12	- 0.162	- 0.104	- 0.142
110	6.17	1.32	4.55	- 0.156	- 0.102	- 0.138
120	6.62	1.60	4.95	- 0.150	- 0.101	- 0.133
130	7.02	1.92	5.32	- 0.143	- 0.099	- 0.128
140	7.38	2.25	5.67	- 0.136	- 0.097	- 0.123
150	7.70	2.60	6.00	- 0.128	- 0.095	- 0.117
160	7.99	3.00	6.33	- 0.120	- 0.092	- 0.111
170	8.25	3.42	6.64	- 0.112	- 0.089	- 0.104
180	8.47	3.96	6.97	- 0.104	- 0.085	- 0.097
190	8.67	4.56	7.30	- 0.095	- 0.081	- 0.090
200	8.84	5.22	7.63	- 0.086	- 0.076	- 0.083
210	8.98	5.92	7.96	- 0.077	- 0.070	- 0.075
220	9.10	6.63	8.28	- 0.068	- 0.064	- 0.067
230	9.20	7.32	8.57	- 0.059	- 0.057	- 0.058
240	9.28	7.99	8.85	- 0.050	- 0.049	- 0.050
250	9.34	8.60	9.09	- 0.041	- 0.041	- 0.041
260	9.39	9.13	9.30	- 0.031	- 0.032	- 0.032
270	9.43	9.56	9.47	- 0.022	- 0.023	- 0.022
280	9.46	9.87	9.60	- 0.012	- 0.013	- 0.013
290	9.48	10.04	9.67	- 0.003	- 0.003	- 0.003
293.15	9.48	10.06	9.68	0	0	0
300	9.49	10.09	9.69	0.007	0.007	0.007
400	9.61	10.44	9.89	0.102	0.110	0.105
500	9.74	10.80	10.09	0.199	0.216	0.205
600	9.86	11.15	10.29	0.297	0.326	0.307
700	9.99	11.51	10.49	0.397	0.440	0.411
800	10.11	11.86	10.69	0.498	0.557	0.518
900	10.23	12.21	10.89	0.600	0.678	0.626
1000	10.35	12.56	11.09	0.704	0.803	0.737
1100	10.48	12.91	11.29	0.809	0.932	0.850
1159	10.55	13.11	11.40	0.871	1.009	0.917

Table 22d. Crystallographic properties of alpha titanium

T K	*a* nm	*c* nm	*c*/*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.29451	0.46783	1.5885	0.28918	10.581	4524
10	0.29451	0.46783	1.5885	0.28918	10.581	4524
20	0.29451	0.46783	1.5885	0.28918	10.581	4524
30	0.29451	0.46783	1.5885	0.28918	10.581	4524
40	0.29451	0.46783	1.5885	0.28919	10.581	4524
50	0.29452	0.46783	1.5885	0.28919	10.582	4524
60	0.29452	0.46783	1.5884	0.28919	10.582	4523
70	0.29453	0.46783	1.5884	0.28919	10.583	4523
80	0.29454	0.46784	1.5883	0.28920	10.584	4523
90	0.29456	0.46784	1.5883	0.28921	10.585	4522
100	0.29457	0.46784	1.5882	0.28921	10.586	4522
110	0.29459	0.46785	1.5881	0.28922	10.588	4521
120	0.29461	0.46786	1.5881	0.28923	10.589	4520
130	0.29463	0.46787	1.5880	0.28924	10.591	4520
140	0.29465	0.46788	1.5879	0.28925	10.592	4519
150	0.29467	0.46789	1.5878	0.28926	10.594	4518
160	0.29470	0.46790	1.5877	0.28928	10.596	4517
170	0.29472	0.46792	1.5877	0.28929	10.598	4516
180	0.29474	0.46793	1.5876	0.28931	10.600	4516
190	0.29477	0.46795	1.5875	0.28932	10.603	4515
200	0.29480	0.46798	1.5875	0.28934	10.605	4514
210	029482	0.46800	1.5874	0.28936	10.608	4513
220	0.29485	0.46803	1.5874	0.28938	10.610	4511
230	0.29488	0.46806	1.5873	0.28940	10.613	4510
240	0.29490	0.46810	1.5873	0.28943	10.616	4509
250	0.29493	0.46814	1.5873	0.28945	10.618	4508
260	0.29496	0.46818	1.5873	0.28948	10.621	4507
270	0.29499	0.46822	1.5873	0.28951	10.624	4505
280	0.29501	0.46827	1.5873	0.28953	10.627	4504
290	0.29504	0.46832	1.5873	0.28956	10.630	4503
293.15	0.29505	0.46833	1.5873	0.28957	10.632	4502
300	0.29507	0.46836	1.5873	0.28959	10.634	4501
400	0.29535	0.46884	1.5874	0.28988	10.665	4488
500	0.29564	0.46934	1.5876	0.29018	10.697	4475
600	0.29593	0.46986	1.5877	0.29049	10.730	4461
700	0.29622	0.47039	1.5880	0.29080	10.763	4447
800	0.29652	0.47094	1.5882	0.29113	10.797	4433
900	0.29682	0.47151	1.5882	0.29146	10.832	4419
1000	0.29713	0.47209	1.5889	0.29180	10.868	4404
1100	0.29744	0.47269	1.5892	0.29215	10.905	4390
1159	0.29762	0.47306	1.5895	0.29235	10.927	4381

$$d1 = (a^2/3 + c^2/4)^{½} \quad d2 = a$$

Table 22e. Crystallographic properties of beta titanium

T K	$\alpha \times 10^6$ K^{-1}	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1159	12.31	0.897	0.33101	0.28666	10.920	4383
1200	12.58	0.948	0.33117	0.28681	10.937	4377
1300	13.22	1.079	0.33160	0.28718	10.979	4360
1400	13.86	1.216	0.33205	0.28756	11.024	4342
1500	14.50	1.359	0.33252	0.28797	11.071	4324
1600	15.14	1.510	0.33302	0.28840	11.120	4304
1700	15.77	1.667	0.33353	0.28885	11.172	4285
1800	16.40	1.830	0.33407	0.28931	11.226	4264
1900	17.02	2.000	0.33463	0.28980	11.282	4243
1943	17.29	2.076	0.33487	0.29001	11.307	4233

$$d = \sqrt{3}a/2$$

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23 VANADIUM V

Atomic weight: 50.9415 (1) (Meija 2017)

Structure: Body-centered cubic (cI2)

The melting point selected by Desai 1986 corrects to 2201 K on ITS-90.

23.1 Allotropy

It was suggested by Westlake 1967a, 1967b that numerous anomalies found in the measurements of physical properties of vanadium between 180 K and 250 K were due to the precipitation of impurity hydrogen as vanadium hydride. Subsequently, Westlake et al. 1972 dehydrogenated samples at 1073 K in high vacuum and found that electrical resistivity and elastic constants measurements no longer showed evidence of such anomalies. However, based on dilatometric measurements on high purity materials containing low hydrogen levels Bollinger et al. 2011 suggested that all of the Group 5 metals did in fact show evidence of a structural distortion below 300 K which was martensitic in character and led to a structure which was not cubic. They further suggested that the vacuum used in the heat treatment process to remove hydrogen was not able to prevent a small amount of oxidation which led to the introduction of interstitial impurities which were enough to completely suppress the martensitic transformation and this was the reason for the removal of the anomalies and not the removal of hydrogen as suggested by Westlake 1967a, 1967b. However, in spite of this suggestion, earlier Jung et al. 1977 had carried out electrical resistivity measurements on samples containing less than 1 wt ppm hydrogen and less than a total of 100 at ppm of oxygen + carbon + nitrogen and found no evidence of anomalies between 6 K and 300 K. Further, Smirnov and Finkel' 1965 identified the structure as being body-centered cubic down to 112 K, Schmitz-Pranghe and Dünner 1968 down to 83 K and and Henry et al. 1970 at 99 K. Even an apparent transition to a tetragonal structure at 230 K observed by Finkel' et al. 1969 was shown by Westlake et al. 1972 to be due to a misinterpretation and the correct interpretation indicated that the structure remained in the body-centered cubic form down to 80 K. In view of these findings it is assumed that until the measurements of Bollinger et al. 2011 are independently verified and that the supposed new low temperature structure is fully characterized then the structure is considered to be body-centered cubic over the whole temperature range.

23.2 Low temperature

Thermal expansion coefficients determined by White 1962 (6-85, 283 K) were combined with thermal expansion coefficients derived from the length change equation of Westlake and Ockers 1970 (113-343 K) and fitted to Equation A using the specific heat (C_p) values selected by Desai 1986:

$$\alpha\ (K^{-1}) = C_p\ (3.67763 \times 10^{-7} - 2.36895 \times 10^{-11}\ T - 1.10181 \times 10^{-6} / T) \qquad (23a)$$

Deviations of low temperature lattice parameter values from the selected values are given in Table 24b and deviations of dilatometric values in Table 24c.

Lattice parameter values of Smirnov and Finkel' 1965 (112-398 K) and Finkel' et al. 1969 (76-297 K) were only shown graphically with actual data points as length change values given by Touloukian et al. 1975. The measurements of Finkel' et al. 1969 (76-297 K) show a transition to a tetragonal structure below 230 K which is not considered to be valid structure and therefore, only the values above this temperature are considered. Similaly the measurements of Suzuki and Miyahara 1966 (173-300 K which includes strain gauge measurements 185-300 K) showed anomalous behavior below 240 K suggesting a transition to an orthorhombic structure which is again not considered to be a valid structure and therefore only measurements above 240 K are considered. Lattice parameter measurements of James and Straumanis 1961 (283-333 K) lead to a mean thermal expansion coefficient of 8.96 x 10^{-6} K^{-1} in satisfactory agreement with the selected value while the value of Linkoaho and Rantavuori 1970 at 8.0 (4) x 10^{-6} K^{-1} at 300 K is in poorer agreement. Dilatometric measurements of Bolef et al. 1971a (4-300 K) and Bolef et al. 1971b (75-366 K) were shown only graphically with actual data points given by Touloukian et al. 1975.

23.3 High temperature

Length changes derived from the lattice parameter measurements of Schmitz-Prange and Dünner 1968 (83-1708 K), and Vasyutinskiy et al. 1966 (293-1900 K) were combined with dilatometric measurements of Mochalov and Ivanov 1969 (293-1934 K) and Brodskiy and Neymark 1971 (293-1672 K). The last three sets of measurements were only shown graphically with actual data points given by Touloukian et al. 1975. These were fitted to the following equation with an overall accuracy on the basis ± $100\varepsilon_T$ of only ± 0.031:

$$\varepsilon_T = 8.02389 \times 10^{-6} T + 1.07948 \times 10^{-9} T^2 + 4.39130 \times 10^{-13} T^3 - 2.45603 \times 10^{-3} \quad (23b)$$

Dilatometric measurements of Yagee and Styles 1966 (273-1273 K) and Yagee et al. 1969 (294-1205 K) were only shown graphically with actual data points given by Touloukian et al. 1975. Deviations of length change values derived from the direct density measurements of Stankus 1993 (293-2172 K) and the volume ratios of Hüpf and Pottlacher 2011 (1200-2199 K) were also included in Table 24c. Direct density measurements of Paradis et al. 2002 (1700-2180 K) are not related to a room temperature reference value and are therefore compared directly and are from 2.8% high at 1700 K trending to 0.9% high at 2180 K. Lattice parameter values of Henry et al. 1970 (293-1473 K) and dilatometric measurements of Nasekovskii 1969 (77-1200 K) were only shown graphically.

Table 23a. Lattice parameter values of vanadium at 293.15 K

References	Original Temperature K	*a* nm	Notes
Gurevič and Ormont 1957	298	0.30241	
Straumanis 1959	298	0.30236	
James and Straumanis 1960	298	0.30241	
James and Straumanis 1961	298	0.30241	
Bradford and Carlson 1962	RT	0.30261	a
Brauer and Schnell 1964	298	0.30231	
Schmitz-Pranghe and Dünner 1968	293	0.32073	
Finkel' et al. 1969	298	0.30294	b
Henry et al. 1970	293	0.30263	
Swanson et al. 1971	298	0.30273	c
Carlson et al. 1972	RT	0.30271	c
	Selected	0.30272 (2)	

Notes for Table 23a.

a. Extrapolated to zero oxygen content

b. Revised value as given by Westlake et al. 1972

c. Value included in the average

Group 5 metals are highly susceptible to expansion of the lattice by interstial elements and therefore the values of James and Straumanis 1960, 1961 would be considered as being the most likely values to select. However, the measurements of Swanson et al. 1971 and Carlson et al. 1972 on very high purity metal are notably higher and have been selected.

At 293.15 K: Density 6099 (1) kg m^{-3} Molar Volume 8.353 (1) m^3 mol^{-1}.

23.4 Deviations of other experimental values from the selected values

Table 23b. Lattice parameter values on the basis 100Δε

References	Temperature Range K	Deviations 100Δε
Smirnov and Finkel' 1965	112-398	99.74% purity sample bias only 0.001 low 99.20% purity sample bias only 0.006 high
Suzuki and Miyahara 1966	173-300	Above 240 K initially 0.046 low then trends towards selected values
Frantsevich et al. 1967	293, 1473	0.013 low at 1473 K
Schmitz-Pranghe and Dunner 1968	83-1708	Values in the low temperature region are initially 0.039 low then converge towards the selected values
Finkel et al. 1969	76-197	Values above 230 K bias 0.004 high

Table 23c. Dilatometric values on the basis 100Δε

References	Temperature Range K	Deviations 100Δε
Erfling 1942	58-313	Trends from an initial value of 0.016 high
Fieldhouse and Lang 1961	294-1797	Trends to 0.037 low at 713 K and to 1.14 high at 1797 K
Pridantseva and Solveva 1965	293, 1073	First sample 0.033 low at 1073 K
	293, 973	Second sample 0.040 high at 973 K
Yagee and Styles 1966	273-1273	First sample 0.011 high at 773 K and second sample 0.004 low at 1273 K
Yagee et al. 1969	294-1205	Average bias 0.013 high above 600 K
Bolef et al. 1971a	4-300	Average bias along the [100] crystal direction is 0.005 low while along the [110] crystal direction trends from initially 0.013 low
Bolef et al. 1971b	75-366	First sample: Trends fron initially 0.031high along the [100] crystal direction and trends 0.006 low to 0.004 high along the [110] crystal direction Second sample: Trends from initially 0.072 high along the [100] crystal direction and from initially 0.007 low along the [101] and [110] crystal directions.
Neimark et al. 1973	293-1573	Trends to 0.021 high
Stankus 1993	293-2172	Trends from 0.028 high at 800 K to 0.045 low at 2172 K
Hüpf and Pottlacher 2011	1200-2199	Trends from 0.024 high at 1200 K to 0.39 low at 2199 K

23.5 Comparison with previous evaluations in the high temperature region

Wang and Reeber 1998 appeared to be unaware of the measurements of Schmitz-Pranghe and Dünner 1968 but did include in their evaluation the dilatometric measurements of Yagee et al. 1969 and the direct density measurements of Stankus 1993. The differences from the present evaluation are a trend to 0.010 high at 700 K and then trending to 0.020 low at the melting point.

Table 23d. Low temperature crystallographic properties of vanadium

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	- 0.163	0.30223	0.26174	8.312	6129
10	0.045	- 0.163	0.30223	0.26174	8.312	6129
20	0.13	- 0.163	0.30223	0.26174	8.312	6128
30	0.35	- 0.163	0.30223	0.26174	8.312	6128
40	0.80	- 0.162	0.30223	0.26174	8.312	6128
50	1.39	- 0.161	0.30223	0.26174	8.313	6128
60	2.09	- 0.160	0.30224	0.26174	8.313	6128
70	2.85	- 0.157	0.30224	0.26175	8.314	6127
80	3.62	- 0.154	0.30225	0.26176	8.315	6127
90	4.34	- 0.150	0.30227	0.26177	8.316	6126
100	4.95	- 0.145	0.30228	0.26178	8.317	6125
110	5.46	- 0.140	0.30230	0.26180	8.318	6124
120	5.89	- 0.134	0.30231	0.26181	8.319	6123
130	6.25	- 0.128	0.30233	0.26183	8.321	6122
140	6.58	- 0.122	0.30235	0.26184	8.323	6121
150	6.86	- 0.115	0.30237	0.26186	8.324	6120
160	7.11	- 0.108	0.30239	0.26188	8.326	6118
170	7.34	- 0.101	0.30241	0.29190	8.328	6117
180	7.54	- 0.094	0.30244	0.26192	8.330	6116
190	7.72	- 0.086	0.30246	0.26194	8.312	6114
200	7.88	- 0.078	0.30248	0.26196	8.333	6113
210	8.02	- 0.070	0.30251	0.26198	8.335	6111
220	8.15	- 0.062	0.30253	0.26200	8.337	6110
230	8.26	- 0.054	0.30256	0.26202	8.340	6108
240	8.36	- 0.046	0.30258	0.26204	8.342	6107
250	8.45	- 0.037	0.30261	0.26207	8.344	6105
260	8.53	- 0.029	0.30263	0.26209	8.346	6104
270	8.61	- 0.020	0.30266	0.26211	8.348	6102
280	8.68	- 0.011	0.30269	0.26213	8.350	6101
290	8.74	- 0.003	0.30271	0.26216	8.352	6099
293.15	8.77	0	0.30272	0.26216	8.353	6099

Table 23e. High temperature crystallographic properties of vanadium

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
293.15	8.77	0	0.30272	0.26216	8.353	6099
300	8.79	0.006	0.30274	0.26218	8.355	6097
400	9.09	0.095	0.30301	0.26241	8.377	6081
500	9.42	0.188	0.30329	0.26260	8.400	6064
600	9.77	0.284	0.30358	0.26291	8.424	6047
700	10.14	0.384	0.30388	0.26317	8.450	6029
800	10.54	0.488	0.30420	0.26344	8.476	6010
900	10.97	0.596	0.30452	0.26373	8.503	5991
1000	11.42	0.709	0.30487	0.26402	8.532	5971
1100	11.89	0.826	0.30522	0.26433	8.562	5950
1200	12.39	0.949	0.30559	0.26465	8.593	5928
1300	12.92	1.076	0.30598	0.26499	8.626	5906
1400	13.47	1.210	0.30638	0.26533	8.660	5882
1500	14.04	1.350	0.30680	0.26570	8.696	5858
1600	14.63	1.494	0.30724	0.26608	8.733	5833
1700	15.25	1.646	0.30770	0.26648	8.772	5807
1800	15.89	1.805	0.30818	0.26685	8.813	5780
1900	16.56	1.970	0.30868	0.26733	8.856	5752
2000	17.24	2.142	0.30921	0.26778	8.901	5723
2100	17.95	2.322	0.30975	0.26825	8.949	5693
2200	18.68	2.510	0.31032	0.26874	8.998	5662
2201	18.69	2.512	0.31032	0.26875	8.998	5661

$$d = \sqrt{3}a/2$$

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24 CHROMIUM Cr

Atomic weight: 51.9961 (6) (Meija 2017)

Structure: Body-centered cubic (cI2)

Below the Néel temperature (T_N) selected as 311.4 K from the measurements of Polovov 1974, Benediktsson et al. 1975, and Williams et al. 1979, the antiferromagnetic ordering results in a transversely polarized spin density wave (SDW), while below the spin flip temperature (T_{SF}) of 123 K (White et al. 1986) the SDW is longitudinally polarized. Kondorsky et al. 1971 have suggested that the spin flip transition may be first order. A selected melting point of 2135 K on ITS-90 is based on a temperature scale correction to the value of Rudy and Windisch 1968 which is confirmed by more recent determinations of 2131 K by Stankus 1993 and 2130 K by Dubrovinskaia et al. 1997. The value of 2136 K selected by Neumann 1985 was probably also based on the value of Rudy and Windisch 1968.

24.1 Allotropy

The possibility of high temperature allotropic transformations in chromium culminated in the suggestion that there was five such phases (Grigor'ev and Sokolovskaya 1961, Grigor'ev et al. 1961 and Grigor'ev and Kuprina 1963). However, lattice parameter measurements by Vasuyutinskii et al. 1961, Wyder and Hoch 1963, Ross and Hume-Rothery 1963, Müller and Dünner 1965 and Dubrovinskaia et al. 1997 all showed that the structure remained body-centered cubic to within 15 K of the melting point. Even with this overwhelming evidence the existence of five allotropic modifications was still being suggested in 1966 by Grigor'ev et al. 1966 and Bezus et al. 1966.

24.2 Low temperature

Thermal expansion coefficients of White et al. 1978 (4-100, 283 K) and White et al. 1986 (2-600 K) were combined to represent the thermal expansion up to 600 K. From 125 K to 300 K the thermal expansion can be represented by the equation:

$$\alpha\ (K^{-1}) = -1.20203 \times 10^{-8}\, T + 2.37427 \times 10^{-9}\, T^{2} - 2.02322 \times 10^{-11}\, T^{3} + 6.65566 \times 10^{-14}\, T^{4} - 7.90415 \times 10^{-17}\, T^{5} - 6.41643 \times 10^{-6} \quad (24a)$$

Differences of other low temperature lattice parameter and dilatometric measurements from the selected values are given in Part 24.3. Of these, the dilatometric measurements of Fine et al. 1951 (98-673 K), Bolef and de Klerk 1963 (74-360 K) and Kondorsky et al. 1971 (86-334 K) were only shown graphically with actual data points given by Touloukian et al. 1975. Not included are the lattice parameter measurements of Smirnov and Finkel' 1964 (113-373 K) which were only shown graphically but a first order transition observed at 168 K was not confirmed by subsequent dilatometric measurements of thermal expansion.

24.3 High temperature

The Néel transition is weak first order with an enthalpy of transition of 1.2 J mol^{-1} (Benediktsson et al. 1975 and Williams et al. 1979) and a contraction estimated by Fawcett et al. 1986 to be $\varepsilon = 11 \times 10^{-6}$ although this estimate appears to be very tentative and is therefore not included in the evaluation. The thermal expansion coefficients up to 600 K as determined by White et al. 1986 (2-600 K) were accepted. These are considered to supersede earlier measurements in the region of the Néel temperature such as the lattice parameter measurements of Straumanis and Weng 1955 (283-333 K) and James et al. 1961-1962 (283-333 K) and the dilatometric measurements of White 1961 (308-315 K), Ishikawa et al. 1967 (245-323 K), Matsumoto and Mitsui 1969 (305-311 K) and Stebler et al. 1970 (298-324 K). Above 600 K a smooth continuity in the thermal expansion curve was obtained by deriving length change values from the lattice parameter measurements of Dubrovinskaia et al. 1997 (298-2120 K) and the direct density measurements of Stankus 1993 (293-2172 K) and fitting to polynomial equations which were then differentiated in order to obtain thermal expansion coefficients, α^*. These values were then combined with the thermal expansion coefficient at 600 K as a fixed point and the derived equation was integrated to obtain length change values which were then combined with length change values derived from integrating the thermal expansion coefficients of White et al. 1986:

$$\text{315-350 K:}\quad \varepsilon_T = -7.68326 \times 10^{-4}\, T + 3.35613 \times 10^{-6}\, T^2 - 6.46809 \times 10^{-9}\, T^3 + 4.68506 \times 10^{-12}\, T^4 + 6.51459 \times 10^{-2} \qquad (24b)$$

$$\text{350-600 K:}\quad \varepsilon_T = -8.18140 \times 10^{-6}\, T + 4.16000 \times 10^{-8}\, T^2 - 4.65667 \times 10^{-11}\, T^3 + 2.10218 \times 10^{-14}\, T^4 - 2.07895 \times 10^{-4} \qquad (24c)$$

$$\text{600-2135 K:}\quad \varepsilon_T = -1.40260 \times 10^{-6}\, T + 1.82581 \times 10^{-8}\, T^2 - 1.31694 \times 10^{-11}\, T^3 + 3.84863 \times 10^{-15}\, T^4 - 8.60264 \times 10^{-4} \qquad (24d)$$

Because of the very close agreement between these two sets of high temperature measurements then they were preferred to the dilatometric measurements of White and Andrikidis 1996, 1999 (400-1873 K) which, on the basis $100\Delta\varepsilon$, trend up to 0.13 high. The direct density measurements of Makeev and Popel 1990 (1000-2000 K) trend from 3.7% low to 2.4% low. Lattice parameter measurements of Vasuyutinskii et al. 1961 (973 – 1973 K), Ross and Hume-Rothery 1963 (1353-2073 K) and Smirnov and Finkel' 1963 (293-1013 K) were only shown in the form of small graphs. An equation given by the latter is not representative of the graphical data. Differences of other high temperature lattice parameter and dilatometric measurements from the selected values are given in Part 24.3.

Table 24a. Lattice parameter values of chromium at 293.15 K

References	Original Temperature K	*a* nm	Notes
Preston 1932	RT	0.28846	
Jette et al. 1934	RT	0.28847	
Wright et al. 1935	RT	0.28848	
Wood 1937	291	0.28856	
Van Arkel 1939	RT	0.28858	
Carlile et al. 1949-1950	298	0.28850	
Fine et al. 1951	293	0.28850	a
Taylor and Floyd 1951-1952	293	0.28844	
Pearson and Hume-Rothery 1952-1953	291	0.28847	
Sully et al. 1953	293	0.28850	b
Swanson et al. 1955	298	0.28840	
Straumanis and Weng 1955	293	0.28852	
Straumanis and Weng 1956	293	0.28851	
James et al. 1961-1962	293	0.28851	
Ageev and Model 1963	293	0.28853	b
Müller et al. 1967	294	0.28843	
Gordienko and Nikolaev 1971	293	0.28840	b
	Selected	0.28849 (5)	

Notes for Table 24a

a. Estimated from graph

b. Value given by Touloukian et al. 1975

At 293.15 K: Density 7192 (4) kg m^{-3} Molar Volume 7.230 (4) m^3 mol^{-1}.

24.4 Deviations of other experimental values from the selected values

Table 24b. Lattice parameter values on the basis 100Δε

References	Temperature Range K	Deviations 100Δε
Sully et al. 1953	293-493	Trends to 0.022 low
Wyder and Hoch 1963	298-1673	Trends 0.33 to 0.52 high
Ageev and Model 1963	282-893	Trends to 0.019 low
Müller and Dünner 1965	288-1761	Trends to 0.24 low
Müller et al. 1967	97-294	Initially scatter 0.026 low to 0.013 high but above 200 K bias 0.014 low
Gordienko and Nikolaev	80-299	Trends from 0.019 high initially to maximum low of 0.019 at 160 K

Table 24c. Dilatometric values on the basis 100Δε

References	Temperature Range K	Deviations 100Δε
Hidnert 1932	293-773	Trends to 0.008 low
Erfling 1939	57-273	First sample trends from initially 0.010 low and second Sample shows scatter 0.002 low to 0.004 high
Hidnert 1941a	293-973	99.3% purity: Scatters 0.005 low to 0.001 high
Hidnert 1941b	293-973	99.2% purity: Trends to 0.049 high
Fine et al. 1951	93-673	Initially trends to a maximum low of 0.010 at 223 K but above room temperature shows an average bias of 0.008 low
Shevlin and Hauck 1954	297-1589	Run 1: 297-1589 K: Trends from 0.037 low at 875 K to 0.25 high at 1589 K; Run 2: 300-1503 K: Trends to 0.15 high; Run 3: 300-1378 K: Trends from 0.012 low at 847 K to 0.099 high at 1378 K; Run 4: 300-1319 K: Trends From 0.016 low at 744 K to 0.068 high at 1319 K
Lucks and Deem 1956, 1958	293-1866	Trends to a maximum of 0.15 high at1589 K and then converges to only 0.073 high at 1866 K
Bolef and de Klerk 1963	74-360	Trends from initially 0.026 low but above room temperature Scatters 0.012 low to 0.010 high
Pridantseva and Solov'yeva 1965	297-973	Sample 1 trends to maximum 0.020 high and sample 2 trends to 0.032 high
Yagee and Styles 1966	273-1273	Sample 1: 0.052 low at 773 K and sample 2: 0.024 low at 1273 K
Yagee et al. 1969	273-1252	Trends to 0.052 low
Kondorsky et al. 1971	86-334	Trends from initially 0.077 low but above room temperature shows an average bias of 0.008 high

24.5 A comparison with other selected values in the high temperature region

Above 1300 K Touloukian et al. 1975 selected only tentative values as a compromise between the dilatometric measurements of Shevlin and Hauck 1954 and Lucks and Deem 1956, 1958 and on the divergent lattice parameter measurements of Müller and Dünner 1965. On the basis 100Δε the selected values trend to 0.037 high at 1400 K and then diverge significantly to 0.20 low at 1900 K. More recent measurements such as the dilatometric measurements of White and Andrikidis 1996, 1999, the lattice parameter measurements of Dubrovinskaia et al. 1997 and the direct density measurements of Stankus 1993 (293-2172 K) tend to agree with the earlier dilatometric measurements.

Table 24d. Low temperature crystallographic properties of chromium

T K	$\alpha \times 10^6$ K^{-1}	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	- 0.103	0.28819	0.24958	7.207	7214
5	- 0.016	- 0.103	0.28819	0.24958	7.207	7214
10	- 0.034	- 0.103	0.28819	0.24958	7.207	7214
15	- 0.049	- 0.103	0.28819	0.24958	7.207	7214
20	- 0.054	- 0.103	0.28819	0.24958	7.207	7214
25	- 0.053	- 0.103	0.28819	0.24958	7.207	7214
30	- 0.037	- 0.103	0.28819	0.24958	7.207	7214
40	0.050	- 0.103	0.28819	0.24958	7.207	7214
50	0.25	- 0.102	0.28819	0.24958	7.207	7214
60	0.71	- 0.102	0.28820	0.24958	7.207	7214
70	1.13	- 0.101	0.28820	0.24959	7.208	7214
80	1.58	- 0.100	0.28820	0.24959	7.208	7214
90	2.20	- 0.098	0.28821	0.24960	7.208	7213
100	2.70	- 0.095	0.28821	0.24960	7.209	7213
110	3.20	- 0.092	0.28822	0.24961	7.210	7212
120	3.70	- 0.089	0.28823	0.24962	7.210	7211
123	3.38	- 0.088	0.28824	0.24962	7.211	7211
125	3.50	- 0.087	0.28824	0.24962	7.211	7211
130	3.77	- 0.085	0.28824	0.24963	7.211	7211
140	4.24	- 0.081	0.28826	0.24964	7.212	7210
150	4.61	- 0.077	0.28827	0.24965	7.213	7209
160	4.90	- 0.072	0.28828	0.24966	7.214	7208
170	5.12	- 0.067	0.28830	0.24967	7.215	7207
180	5.29	- 0.062	0.28831	0.24968	7.216	7206
190	5.40	- 0.057	0.28833	0.24970	7.217	7204
200	5.49	- 0.051	0.28834	0.24971	7.218	7203
210	5.55	- 0.046	0.28836	0.24973	7.220	7202
220	5.60	- 0.040	0.28837	0.24974	7.221	7201
230	5.63	- 0.035	0.28839	0.24975	7.222	7200
240	5.65	- 0.029	0.28841	0.24977	7.223	7198
250	5.64	- 0.023	0.28842	0.24978	7.225	7197
260	5.59	- 0.018	0.28844	0.24980	7.226	7196
270	5.49	- 0.012	0.28846	0.24981	7.227	7195
280	5.28	- 0.007	0.28847	0.24982	7.228	7194
290	4.95	- 0.002	0.28849	0.24984	7.229	7192
293.15	4.81	0	0.28849	0.24984	7.230	7192

$$d = \sqrt{3}a/2$$

Table 24e. High temperature crystallographic properties of chromium

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
293.15	4.81	0	0.28849	0.24984	7.230	7192
300	4.43	0.0032	0.28850	0.24985	7.230	7191
305	4.12	0.0053	0.28851	0.24985	7.231	7191
310	3.93	0.0073	0.28851	0.24986	7.231	7191
311.4	3.92	0.0079	0.28851	0.24986	7.231	7190
312	3.93	0.0081	0.28851	0.24986	7.231	7190
313	4.39	0.0085	0.28851	0.24986	7.231	7190
314	6.30	0.0090	0.28852	0.24986	7.232	7190
315	6.39	0.0097	0.28852	0.24986	7.232	7190
316	6.45	0.010	0.28852	0.24987	7.232	7190
318	6.57	0.012	0.28852	0.24987	7.232	7190
320	6.68	0.013	0.28853	0.24987	7.232	7189
330	7.06	0.020	0.28855	0.24989	7.234	7188
340	7.28	0.027	0.28857	0.24991	7.235	7186
350	7.43	0.034	0.28859	0.24993	7.237	7185
360	7.59	0.042	0.28861	0.24994	7.239	7183
380	7.88	0.057	0.28866	0.24998	7.242	7180
400	8.12	0.733	0.28870	0.25002	7.245	7176
450	8.62	0.115	0.28882	0.25013	7.255	7167
500	8.99	0.159	0.28895	0.25024	7.264	7158
600	9.59	0.253	0.28922	0.25047	7.284	7138
700	10.01	0.351	0.28950	0.25072	7.306	7117
800	10.36	0.454	0.28980	0.25097	7.328	7095
900	10.62	0.559	0.29010	0.25124	7.352	7073
1000	10.93	0.667	0.29042	0.25151	7.375	7050
1100	11.36	0.780	0.29074	0.25179	7.400	7027
1200	12.02	0.897	0.29108	0.25208	7.426	7002
1300	12.99	1.023	0.29144	0.25240	7.454	6976
1400	14.36	1.161	0.29184	0.25274	7.484	6947
1500	16.22	1.315	0.29228	0.25313	7.519	6916
1600	18.66	1.492	0.29279	0.25357	7.558	6880
1700	21.76	1.696	0.29338	0.25408	7.604	6838
1800	25.60	1.937	0.29408	0.25468	7.658	6790
1900	30.27	2.221	0.29490	0.25538	7.722	6733
2000	35.84	2.559	0.29587	0.25623	7.799	6667
2100	42.36	2.960	0.29703	0.25723	7.891	6590
2135	44.89	3.117	0.29748	0.25763	7.927	6559

$$d = \sqrt{3}a/2$$

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25 MANGANESE Mn

Atomic weight: 54.938044 (2) (Meija 2017)

Structure: Alpha: Cubic (cI58)
Beta: Cubic (cP20)
Gamma: Face-centered cubic (cF4)
Delta: Body-centered cubic (cI2)

Petrenko et al. 1974 select 95.6 (1) for the Néel temperature of the alpha phase while the transition temperatures selected by Hultgren et al. 1973 correct to the following values on ITS-90: Alpha-Beta 980 (20) K Beta-Gamma 1361 (10) K Gamma-Delta 1411 (5) K Delta-Liquid 1518 (5) K.

25.1 Alpha Phase: Cubic (cI58): 0 K to 980 K.

Below the Néel temperature at 95.6 K length changes derived from the lattice parameter measurements of Marples 1967 (4-300 K) were selected and fitted to the equation:

$$\varepsilon_T = -1.60505 \times 10^{-8} T^2 - 3.18540 \times 10^{-3} \quad (25a)$$

From 165 K to 990 K length changes derived from the lattice parameter measurements of Schmitz-Pranghe and Dünner 1968 (85-990 K) were fitted to the equation:

$$\varepsilon_T = 8.02929 \times 10^{-6} T + 4.08987 \times 10^{-8} T^2 - 4.05380 \times 10^{-11} T^3 + 2.03368 \times 10^{-14} T^4 - 4.99744 \times 10^{-3} \quad (25b)$$

For the intermediate range the length change value derived from Equation 25a at 95.6 K was combined with the length change value and derived thermal expansion coefficient derived from Equation 25b at 170 K and fitted to the equation:

$$\varepsilon_T = -2.41596 \times 10^{-5} T + 1.26357 \times 10^{-7} T^2 - 2.17725 \times 10^{-3} \quad (25c)$$

Thermal expansion coefficients measured by White 1965 (4-85, 283 K) suggest that the Néel temperature is only about 70 K or about 25 K lower than the selected value and Therefore, these values are considered to be unsatisfactory above 30 K but below this temperature they show relatively good agreement with the thermal expansion coefficients derived from Equation 25a and differ by a trend of only 2×10^{-8} K^{-1} at 5 K to 8×10^{-8} K^{-1} at 30 K. On the basis $100\Delta\varepsilon$ dilatometric measurements of Erfling 1940 (77-293 K) above the Néel temperature on average show a bias of only 0.006 higher than selected values. Other lattice parameter and dilatometric measurements were only shown graphically with actual data points given by Touloukian et al. 1975. These include the lattice parameter measurements of Marples 1967 (4-300 K) which above the Néel temperature show a maximum deviation of 0.043 high at 164 K while the lattice parameter of Gazzara et al. 1967 (5-299 K) show an average deviation of 0.010 low. Dilatometric measurements of Masumoto et al. 1971, 1972 (115-673 K) show a major

trend from 0.095 low at 115 K to 0.21 high at 673 K. The length change values of Petrenko et al. 1974 (0-273 K) were only in the form of small graphs.

Table 25a. Lattice parameter values of alpha manganese at 293.15 K

References	Original Temperature K	*a* nm	Notes
Johannsen and Nitka 1938	293	0.89140	a
Carapella and Hultgren 1942	298	0.89134	a
Potter and Huber 1945	RT	0.89130	a
Marples 1967	299	0.89097	a, b
Gazzara et al. 1967	298	0.89121	
Swanson et al. 1969	298	0.89121	
Morris at al 1980	298	0.89111	
	Selected	0.89116 (5)	

Notes for Table 25a

a. Not included in the average

b. Value given by Touloukian et al. 1975

The distinct difference between values obtained for the older and newer measurements may be due to improvements in metal purity although a less accurate determination of 0.8912 nm determined by Carlisle et al. 1949-1950 would appear to confirm the later values as did 0.8911 (2) nm obtained by Oberteuffer and Ibers 1970.

At 293.15 K: Density 7476 (1) kg m^{-3} Molar Volume 7.348 (1) m^3 mol^{-1}.

Positional parameters in alpha manganese

The closely agreeing values obtained by Oberteuffer and Ibers 1970 and Yamada and Fujii 1970 were averaged:

Atom	Parameter	Value
II	x_{II}	0.31776
III	x_{III}	0.35708
III	z_{III}	0.03463
IV	x_{IV}	0.08963
IV	z_{IV}	0.28202

Calculation of interatomic distances in alpha manganese

MnI – MnIV: $d1 = a\,[\,2\,x_{IV}^{\,2} + z_{IV}^{\,2}\,]^{\,½}$

MnI – MnII: $d2 = \sqrt{3}\,a\,(0.5 - x_{II})$

MnII – MnIII: $d3 = a\,[\,2\,(x_{III} - x_{II})^{\,2} + (x_{II} - z_{III})^{\,2}\,]^{\,½}$

MnII – MnIV: $d4 = a\,[\,(x_{II} + z_{IV} - 0.5)^{\,2} + (0.5 + x_{IV} - x_{II})^{\,2} + (0.5 - x_{IV} - x_{II})^{\,2}\,]^{\,½}$

MnII - MnIV: $d5 = a\,[\,2\,(x_{II} - x_{IV})^{\,2} + (x_{II} - z_{IV})^{\,2}\,]^{\,½}$

MnII – MnIII: $d6 = a\,[\,(0.5 + z_{III} - x_{II})^{\,2} + (x_{II} + x_{III} - 0.5)^{\,2}\,]^{\,½}$

MnIII – MnIV: $d7 = a\,[2\,(0.5 - x_{IV} - x_{III})^{\,2} + (0.5 - z_{IV} + z_{III})^{\,2}\,]^{\,½}$

MnIII – MnIV: $d8 = a\,[\,(x_{III} - z_{IV})^{\,2} + (x_{III} - x_{IV})^{\,2} + (x_{IV} - z_{III})^{\,2}\,]^{\,½}$

MnIII – MnIII: $d9 = a\,[\,(1 - 2\,x_{III})^{\,2} + 4\,z_{III}^{\,2}\,]^{\,½}$

MnIII – MnIII: $d10 = a\,[\,(2\,x_{III} - 0.5)^{\,2} + (0.5 - x_{III} - z_{III})^{\,2} + (0.5 - x_{III} + z_{III})^{\,2}\,]^{\,½}$

MnII – MnIV: $d11 = a\,[\,(0.5 + x_{IV} - x_{III})^{\,2} + (0.5 - x_{IV} - x_{III})^{\,2} + (0.5 - z_{IV} - z_{III})^{\,2}\,]^{\,½}$

MnIV – MnIV: $d12 = \sqrt{8}\,a\,x_{IV}$

MnIV – MnIV: $d13 = \sqrt{2}\,a\,(z_{IV} - x_{IV})$

25.2 Beta phase: Cubic (cP20): 980 K to 1361 K.

The structure can be retained at very low temperatures and dilatometric measurements below room temperature have been given by Erfling 1939 (78-293 K) although the present evaluation on the metastable phase is only given from the reference temperature 293.15 K. Lattice parameter measurements by Basinski and Christian 1954 (298 K and 1023-1353 K) were only shown graphically with actual data as length change values being given by Touloukian et al. 1975 from which the original lattice parameter values could be estimated. Together with a lattice parameter value determined by Carlisle et al. 1949-1950 at 298 K these values less that at 1023 K were fitted to the following equations to represent the thermal expansion from 293.15 K to 1361 K:

$$a\ (\mathrm{nm}) = 1.93174 \times 10^{-5}\,T + 4.03092 \times 10^{-9}\,T^{\,2} + 0.625455 \qquad (25d)$$

$$\varepsilon_T = 3.09119 \times 10^{-5}\,T + 6.45032 \times 10^{-9}\,T^{\,2} - 8.59803 \times 10^{-4} \qquad (25e)$$

The values of ε_T were calculated by referring to the selected value for the alpha phase using the reduced lattice parameter $0.89116 / (58/20)^{\,⅓}$.

Table 25b. Lattice parameter values of beta manganese at 293.15 K

References	Original Temperature K	*a* nm	Notes
Johannsen and Nitka 1938	293	0.63041	a
Carlisle et al. 1949-1950	298	0.63138	
Basinski and Christian 1954	298	0.63155	
Morris et al. 1981	298	0.63105	a
	Selected	0.63146 (8)	

Notes for Table 25b

a. Not included in the average

At 293.15 K: Density 7246 (3) kg m^{-3} Molar Volume 7.582 (3) m^3 mol^{-1}.

The selected value represents a continuity with the high temperature data and was confirmed by a less accurate value of 0.6315 (2) nm obtained by Shoemaker et al. 1978. At the alpha-beta transition temperature the volume increase is 4.34%.

Lattice parameter values determined by Schmitz-Pranghe and Dünner 1968 (1008-1221 K) can be considered as being systematically 0.0001 nm lower then the selected values.

Positional parameters of beta manganese

Calculation of interatomic distances in beta manganese

MnI – MnI: $d1 = a\,[\,(0.25 - 2\,x_I)^2 + \tfrac{1}{8}\,]^{\frac{1}{2}}$

MnI – MnII: $d2 = a\,[\,(\tfrac{1}{8} + x_I)^2 + (0.5 + x_I - x_{II})^2 + (x_I + x_{II} - 0.25)^2\,]^{\frac{1}{2}}$

MnI – MnII: $d3 = a\,[\,(\tfrac{1}{8} - x_I)^2 + (x_{II} - x_I)^2 + (0.25 + x_{II} - x_I)^2\,]^{\frac{1}{2}}$

MnI - MnII: $d4 = a\,[\,(\tfrac{3}{8} - x_I)^2 + (x_I + x_{II})^2 + (0.25 - x_{II} + x_I)^2\,]^{\frac{1}{2}}$

MnII – MnII: $d5 = a\,[\,(\tfrac{1}{8} + x_{II})^2 + (x_{II} - \tfrac{1}{8})^2 + 0.25^2\,]^{\frac{1}{2}}$

MnII – MnII $d6 = a\,[\,2\,(\tfrac{3}{8} - x_{II})^2 + (\tfrac{3}{4} - 2\,x_{II})^2\,]^{\frac{1}{2}}$

MnII – MnII: $d7 = a\,[\,0.5^2 + 2\,(0.5 - 2\,x_{II})^2\,]^{\frac{1}{2}}$

Shoemaker et al. 1978 determined the positional parameters $x_I = 0.06361$ (10) and $x_{II} = 0.20224$ (11).

25.3 Gamma phase: Face-centered cubic (cF4): 1361 K to 1411 K.

Quenching into the room temperature region leads to a distortion of the structure to face-centered tetragonal which is also found in a number of manganese alloys. However, Basinski and Christian 1953 confirmed the true structure at high temperatures. Lattice parameter measurements of Basinski and Christian 1954 (1368-1405 K) were only shown graphically with actual lattice parameters values being deduced from length change values given by Touloukian et al. 1975 and which were fitted to the following equations:

$$a \text{ (nm)} = 1.84273 \times 10^{-5} T + 0.361032 \quad (25f)$$

$$\varepsilon_T = 5.04230 \times 10^{-5} T - 1.21010 \times 10^{-2} \quad (25g)$$

The values of ε_T were calculated by referring to the selected value for the alpha phase using the reduced lattice parameter $0.89116 / (58/4)^{1/3}$. The derived thermal expansion coefficient is $47.7 \times 10^{-6} K^{-1}$. At the beta-gamma transition the volume increase is 0.47 %.

25.4 Delta phase: Body-centered cubic (cI2): 1411K to 1518 K.

Lattice parameter measurements of Basinski and Christian 1954 (1406-1512 K) were only shown graphically with actual lattice parameters values being deduced from length change values given by Touloukian et al. 1975 and which were fitted to the following equations:

$$a \text{ (nm)} = 1.27678 \times 10^{-5} T + 0.290094 \quad (25h)$$

$$\varepsilon_T = 4.40176 \times 10^{-5} T + 1.12487 \times 10^{-4} \quad (25i)$$

The values of ε_T were calculated by referring to the selected value for the alpha phase using the reduced lattice parameter $0.89116 / (58/2)^{1/3}$. The derived thermal expansion coefficient is $41.3 \times 10^{-6} K^{-1}$. At the gamma-delta transition the volume increase is determined as 0.90 %.

Table 25c. Crystallographic properties of alpha manganese

T K	α x 10^6 K^{-1}	100 ε_T	*a* nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
0	0	- 0.319	0.88832	7.278	7548
10	- 0.32	- 0.319	0.88832	7.278	7548
20	- 0.64	- 0.319	0.88832	7.278	7548
30	- 0.97	- 0.320	0.88831	7.278	7548
40	- 1.29	- 0.321	0.88830	7.278	7549
50	- 1.61	- 0.323	0.88829	7.277	7549
60	- 1.93	- 0.324	0.88827	7.277	7549
70	- 2.25	- 0.326	0.88825	7.277	7550
80	- 2.58	- 0.329	0.88823	7.276	7550
90	- 2.90	- 0.332	0.88821	7.276	7551
95.6	- 3.08	- 0.333	0.88819	7.275	7551
100	1.12	- 0.333	0.88819	7.275	7551
110	3.65	- 0.331	0.88821	7.276	7551
120	6.19	- 0.326	0.88826	7.277	7550
130	8.72	- 0.318	0.88832	7.278	7548
140	11.26	- 0.308	0.88841	7.281	7546
150	13.79	- 0.296	0.88852	7.283	7543
160	16.32	- 0.281	0.88866	7.287	7540
170	18.86	- 0.263	0.88881	7.290	7536
180	19.33	- 0.244	0.88898	7.295	7531
190	19.78	- 0.225	0.88916	7.299	7527
200	20.22	- 0.204	0.88934	7.303	7522
210	20.63	- 0.184	0.88952	7.308	7518
220	21.04	- 0.163	0.88970	7.312	7513
230	21.43	- 0.142	0.88989	7.317	7508
240	21.81	- 0.121	0.89008	7.322	7503
250	22.17	- 0.099	0.89028	7.327	7498
260	22.52	- 0.076	0.89048	7.332	7493
270	22.86	- 0.054	0.89068	7.337	7488
280	23.19	- 0.031	0.89089	7.342	7483
290	23.51	- 0.007	0.89109	7.347	7478
293.15	23.61	0	0.89116	7.348	7476
300	23.82	0.016	0.89130	7.352	7473
400	26.43	0.268	0.89355	7.408	7416
500	28.54	0.545	0.89601	7.469	7355
600	30.64	0.842	0.89867	7.536	7290
700	33.21	1.164	0.90153	7.608	7221
800	36.73	1.518	0.90468	7.688	7146
900	41.64	1.915	0.90822	7.779	7063
980	46.89	2.275	0.91144	7.861	6988

Table 25d. Room temperature interatomic distances for alpha manganese

Atom Type	Neighbor	Number	Equation Number	*d* nm
I	IV	12	d1	0.2755
	II	4	d2	0.2813
II	III	3	d3	0.2571
	IV	6	d4	0.2710
	I	1	d2	0.2813
	IV	3	d5	0.2893
	III	3	d6	0.2931
III	IV	1	d7	0.2349
	IV	2	d8	0.2524
	II	1	d3	0.2571
	III	2	d9	0.2621
	III	4	d10	0.2660
	IV	2	d11	0.2681
	II	1	d6	0.2931
IV	IV	1	d12	0.2259
	III	1	d7	0.2349
	IV	2	d13	0.2425
	III	2	d8	0.2524
	III	2	d11	0.2681
	II	2	d4	0.2710
	I	1	d1	0.2755
	II	1	d5	0.2893

Table 25e. Crystallographic properties of beta manganese

T K	$\alpha \times 10^6$ K^{-1}	100 ε_T	*a* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
293.15	34.33	1.048	0.63146	7.582	7246
300	34.41	1.071	0.63161	7.587	7241
400	35.57	1.426	0.63383	7.667	7165
500	36.70	1.793	0.63612	7.751	7088
600	37.83	2.173	0.63850	7.838	7009
700	38.94	2.566	0.64095	7.929	6929
800	40.04	2.972	0.64349	8.023	6847
900	41.13	3.391	0.64611	8.121	6765
980	41.99	3.735	0.64826	8.203	6697
1000	42.20	3.822	0.64880	8.224	6681
1050	42.73	4.043	0.65018	8.276	6638
1100	43.26	4.267	0.65158	8.330	6595
1150	43.78	4.494	0.65380	8.384	6553
1200	44.38	4.724	0.65444	8.440	6509
1251	44.82	4.958	0.65590	8.496	6466
1300	45.33	5.195	0.65738	8.554	6422
1350	45.84	5.435	0.65888	8.613	6379
1361	45.95	5.488	0.65921	8.626	6369

Table 25f. Room temperature interatomic distances for beta manganese

Atom Type	Neighbor	Number	Equation Number	*d* nm
I	I	3	d1	0.2363
	II	3	d2	0.2576
	II	3	d3	0.2634
	II	3	d4	0.2679
II	I	2	d2	0.2576
	I	2	d3	0.2634
	I	2	d4	0.2679
	II	4	d5	0.2646
	II	2	d6	0.2672
	II	2	d7	0.3271

Table 25g. Crystallographic properties of gamma manganese

T K	$100\varepsilon_T$	*a* nm	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1361	5.652	0.38611	0.27302	8.666	6339
1370	5.698	0.38628	0.27314	8.677	6331
1380	5.748	0.38646	0.27327	8.690	6322
1390	5.799	0.38665	0.27340	8.702	6313
1400	5.849	0.38683	0.27353	8.715	6304
1410	5.900	0.38701	0.27366	8.727	6295
1411	5.905	0.38703	0.27367	8.728	6294

$$d1 = a/\sqrt{2} \quad d2 = a$$

Table 25h: Crystallographic properties of delta manganese

T K	$100\ \varepsilon_T$	*a* nm	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1411	6.222	0.30811	0.26683	8.807	6238
1420	6.262	0.30822	0.26693	8.817	6231
1430	6.306	0.30835	0.26704	8.828	6223
1440	6.350	0.30848	0.26715	8.839	6215
1450	6.394	0.30861	0.26726	8.850	6208
1460	6.438	0.30873	0.26737	8.861	6200
1470	6.482	0.30886	0.26748	8.872	6192
1480	6.526	0.30899	0.26759	8.883	6185
1490	6.570	0.30912	0.26770	8.894	6177
1500	6.614	0.30925	0.26781	8.905	6169
1510	6.658	0.30937	0.26793	8.916	6162
1518	6.693	0.30948	0.26801	8.925	6156

$$d1 = \sqrt{3}a/2 \quad d2 = a$$

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26 IRON Fe

Atomic weight: 55.845 (2) (Meija 2017)

Structure: Alpha, Beta, Delta: Body-centered cubic (cI2)
Gamma: Face-centered cubic (cF4)

Desai 1986 selects 1043 K for the alpha – beta Curie transition temperature (T_C), 1185 K for the beta – gamma transition temperature, 1667 K for the gamma – delta transition temperature and 1811 K for the melting point which is identical to the freezing point value of 1811 (3) K as a secondary fixed point on ITS-90 (Bedford et al. 1996).

26.1 Alpha Phase - Low temperature: Body-centered cubic (cI2): 0 K to 1185 K.

Thermal expansion coefficients of White 1965 (3-85, 283 K) were selected and above 57.5 K were combined with the specific heat (C_p) values selected by Desai 1986 and fitted to Equation A with an overall accuracy as a standard deviation of ± 6 x 10^{-8} K^{-1}:

$$\alpha\ (K^{-1}) = C_p\ (3.36853 \times 10^{-7} + 4.09667 \times 10^{-10}\ T + 7.83291 \times 10^{-6}/\ T) \qquad (26a)$$

This equation is considered to be confirmed by the fact that on the basis 100Δε the dilatometric measurements of Dorsey 1907 (93-293 K) give values agreeing to within 0.001 while the derived thermal expansion coefficient of 12.07 x 10^{-6} K^{-1} at 293.15 K is very similar to the values of 12.1 x 10^{-6} K^{-1} as a mean value over the range 288 to 329 K obtained by Straumanis and Kim 1969 from lattice parameter measurements, and 12.01 x 10^{-6} K^{-1} at 293.15 K derived from the equations given by Touloukian et al. 1975, although they give a tabulated value of 11.8 x 10^{-6} K^{-1}. Dilatometric measurements of Nix and MacNair 1941 (92-958 K) lead to a higher value of 12.5 x 10^{-6} K^{-1} over the narrow range 287 to 295 K while those of Esser and Eusterbrock 1941 (291-1273 K) lead to a lower mean value of 11.8 x 10^{-6} K^{-1} between 291 and 323 K. Thermal expansion coefficients determined by Krishnan 1966 (5-39 K) on pure iron show a trend to be 1.2 x 10^{-7} K^{-1} high on a first sample and 2.4 x 10^{-7} K^{-1} high on a second sample. The lattice parameter values of Shah 1971 (40-180 K) were not evaluated because they are not connected to room temperature values. The graphical representation of the dilatometric measurements of Lysak and Andrushchik 1969 (93-293 K) appears to be incorrect. Other length change values derived from lattice parameter and dilatometric measurements in the low temperature region are compared with selected values in Part 26.3.

26.2 Alpha and Beta Phases – High temperature

Although it can be considered that the beta and delta phases may form a continuous thermal expansion curve, considered in isolation the delta phase can be more simply represented by a linear relationship within the range of stability. Athough specific heat values as selected by Desai 1986 showed a marked second order lambda peak centering on the Curie transition point, initially lattice parameter and dilatometric measurements

generally showed little evidence of the transition and therefore Tououkian et al. 1975 appeared not to consider the anomalies in evaluating the thermal expansion. In view of the large number of measurements for the alpha phase and the spread in the values, the equation given by Touloukian et al. 1975 was accepted after correction to the selected thermal expansion coefficient at 293.15 K and was initially used to represent the high thermal expansion up to 1185 K:

$$\varepsilon_T = 7.55577 \times 10^{-6} T + 9.01828 \times 10^{-9} T^2 - 2.99886 \times 10^{-12} T^3 - 2.91442 \times 10^{-3} \quad (26b)$$

However, using sensitive differential dilatometry Liu et al. 2004 (300-1185 K) obtained definate evidence of the thermal expansion coefficient behavior in the region of the Curie temperature and the following equations were used to represent the thermal expansion from 960 K to 1185 K with equation 26b now representing the thermal expansion only up to 930 K, while values in the region 930 K to 960 K were obtained by interpolation:

$$960 - 1043 \text{ K}: \quad \alpha (K^{-1}) = -4.125 \times 10^{-9} + 2.100 \times 10^{-8} T - 1.587 \times 10^{-11} T^2 + 1.399 \times 10^{-5} \exp(-1.131\, t^*) (t^*)^{0.066} \quad (26c)$$

$$1043 - 1185 \text{ K}: \quad \alpha (K^{-1}) = -4.125 \times 10^{-9} + 2.100 \times 10^{-8} T - 1.587 \times 10^{-11} T^2 + 1.210 \times 10^{-5} \exp(1.920\, t^*) (t^*)^{0.033} \quad (26d)$$

Where $t^* = \left| (T - T_C) / T_C \right|$

The deviations of other length change values derived from lattice parameter and dilatometric measurements in the high temperature region are compared with selected values in Part 26.3.

Table 26a. Lattice parameter of alpha iron at 293.15 K

References	Original Temperature K	*a* nm
Mayer 1929	295	0.28669
Owen and Yates 1933	291	0.28668
Esser and Müller 1933	293	0.28670
Jette and Foote 1935	298	0.28662
Straumanis and Ievinš 1936	295	0.28664
Jette and Foote 1936	298	0.28865
Owen and Yates 1937	293	0.28666
Owen et al. 1937	288	0.28666
Van Bergen 1941	293	0.28667
Lu and Chang 1941	293	0.28664
Troiano and McGuire 1943	RT	0.28667
Thomas 1948	293	0.28666
Van Horn 1949	293	0.28663
Kochanovska 1949	295	0.28668
Zhmudskii 1949	292, 300	0.28664
Owen and Williams 1954	291	0.28664
Von Batchelder and Raeuchle 1954	298	0.28665
Grønvold et al. 1954	293	0.28665
Swanson et al. 1955	298	0.28664
Basinski et al. 1955	293	0.28663
Sutton and Hume-Rothery 1955	293	0.28663
Taylor and Jones 1958	298	0.28664
Gale 1959	298	0.28665
Lihl and Ebel 1961	293	0.28661
Cotta and Gazzara 1962	310	0.28665
Goldschmidt 1962	293	0.28663
Cockett and Davis 1963	293	0.28664
Chessin et al. 1963	298	0.28663
Hanneman and Mariano 1964	RT	0.28663
Gorton et al. 1965	295	0.28664
Abrahamson and Lopata 1966	295	0.28663
Stuart and Ridley 1966	293	0.28663
Kohlhaas et al. 1967	293	0.28667
Straumanis and Kim 1969	298	0.28662
Polcarová et al. 1988	295	0.28665
Wokulska et al. 1990	293	0.28662
	Selected	0.28665 (2)

At 293.15 K: Density 7874 (1) kg m^{-3} Molar volume 7.092 (1) cm^3 mol^{-1}.

26.3 Deviations of experimental values for alpha – beta iron from the selected values

Table 26b. Lattice parameter values

References	Temperature Range K	Deviations 100Δε
Owen and Yates 1937	287-913	Trends 0.006 low to 0.010 high at 849 K and 0.047 high at 913 K
Owen et al. 1937	288-873	Average bias 0.008 low to 773 K then 0.014 high at 873 K
Kochanovska 1949	295-639	Trends to average of 0.045 high for two runs
Owen and Williams 1954	79-291	Scatters 0.004 low to 0.008 high
Von Batchelder and Raeuchle 1954	298-636	Scatters 0.017 low to 0.003 high but with average bias 0.005 low
Basinski et al. 1955	293-1807	In alpha range trends 0.014 high to 0.037 low
Lihl and Ebel 1961	293-1070	Trends 0.030 high to 0.001 low
Goldschmidt 1962	293-1528	In alpha range trends 0.013 high maximum at 636 K to 0.035 low at 1172 K to 0.020 low at 1180 K
Cockett and Davis 1963	293-1423	In alpha range trends to average 0.036 high above 873 K
Gorton et al. 1965	295-1343	In alpha range trends to average bias of 0.037 high above 500 K
Stuart and Ridley 1966	348-1148	Average bias 0.017 low above 600 K
Fassiska and Zwell 1967	296-951	0.007 high at 687 K and 0.018 low at 951 K
Kohlhaas et al. 1967	93-1781	In alpha range below room temperature initially 0.005 high to maximum deviation of 0.024 low at 193 K. Above room temperature trends to 0.16 low above 1037 K
Gen and Petrov 1968	293-1019	Scatters 0.007 low to 0.091 low
Ridley and Stuart 1968	298-1172	Trend to 0.051 low at 1106 K then average 0.031 low above
Straumanis and Kim 1969	280-1423	In alpha range first sample (523-1173 K) scatters 0.035 low to 0.033 low. Second sample (282-1097 K) trends from 0.047 high at 713 K to 0.033 low. Third sample (280-1116 K) trends from 0.081 high at 814 K to 0.014 high. Fourth sample thermal expansion measured in hydrogen atmosphere
Onink et al. 1993	800-1250	In alpha range trends from initially 0.045 low to 0.008 high

Table 26c. Dilatometric values

References	Temperature Range K	Deviations 100Δε
Holborn and Day 1901	273-1023	Average bias 0.005 low
Souder and Hidnert 1922	298-973	Average bias 0.008 low to 873 K then 0.004 high at 973 K
Masumoto and Nara 1927	303, 373	0.015 low at 373 K
Masumoto 1931	303, 373	Average bias for two samples 0.004 low at 373 K
Austin and Pierce 1933	373-1073	First sample average bias 0.007 low below 700 K the 0.007 high to 1010 K and agreement with selected values at 1070 K and 1125 K. Second sample trends to 0.027 low
Austin and Pierce 1934	273-1230	Average of ten samples averages to 0.009 low .Transition effects in the region 1123 to 1230 K
Jaeger et al. 1938	273-1073	Average bias 0.004 low to 1005 K then maximum deviation 0.035 low at 1011 K trending to 0.005 low at 1073 K
Esser and Eusterbrock 1941	291-1273	Average of three samples trends to 0.065 low at 1190 K . Transition effects in the region 1191 to 1273 K
Nix and MacNair 1941	92-958	In the low temperature region shows average bias of 0.001 low. Above room temperature trends 0.011 low to 0.009 high
Fine and Ellis 1948	303-1073	Trends to 0.014 low
Miller 1958	310-1123	Trends to maximum 0.032 low at 473 K then to 0.043 high at 817 K then to average 0.006 high
Allen 1959	293-922	Trends 0.022 low to 0.018 high
Arbuzov and Zelenko 1964	374-1069	Average bias 0.005 low to 770 K then average bias 0.004 high to 1004 K then trends to 0.014 low at 1069 K
Andreeva and Gel'd 1965	293-1206	Trends to 0.086 low at 1138 K
Fraser and Hollis Hallet 1965	20-121	Average bias 0.003 low
Masumoto and Kobayashi 1965	273-313	0.001 low at 313 K
Richter and Lotter 1969	831-1115	Trends 0.019 low to 0.045 low
Ryabov et al. 1969	293-773	Scatters 0.007 low to 0.004 high
Yagee and Styles 1969	273-1173	Scatters 0.016 low to 0.006 high
Richter 1970	81-1673	Above room temperature: First sample trends to average 0.13 low and second sample to average 0.064 low. Measurements 1173 to 1250 K in the transition zone
Sinha and Balasundaram 1970	273-673	Trends to 0.054 low
Miiller and Cezairliyan 1984	1130-1330	In the alpha region trends 0.025 high to 0.013 high

26.4 Gamma phase: Face-centered cubic (cF4) 1185 K to 1667 K.

In this region lattice parameter measurements of Basinski et al. 1955 (1189-1661 K), Goldschmidt 1962 (1185-1528 K), Cockett and Davis 1963 (1173-1423 K), Gorton et al. 1965 (1193-1343 K), Kohlhaas et al. 1967 (1223-1634 K), Straumanis and Kim 1969 (1173-1423 K), and Onink et al. 1993 (1180-1250 K), as well as dilatometric measurements of Miiller and Cezairliyan 1984 (1200-1330 K) (converted to equivalent lattice parameter values), show marked scatter. This was overcome by separately fitting all sets of measurements to linear equations and extrapolating or interpolating to 1185 K.

After rejection of the values of Cockett and Davis 1963 and Onink 1993 as being too high the remainder were averaged to 0.36743 (6) nm and combined with a value of 0.35731 nm at room temperature (presumed to be 293 K) determined by Li et al. 2002 by extrapolating lattice parameters of Fe-Mn austenitic alloys to pure iron. The latter value exactly confirms previous determinations by Ridley et al. 1969 on equilibrium austenite and by Liu et al. 1990 by extrapolating Fe-Mn alloys. This combination leads to the following equations:

$$a \text{ (nm)} = 8.31978 \times 10^{-6} T + 0.354871 \quad (26e)$$

$$\varepsilon_T = 2.30365 \times 10^{-5} T - 1.74035 \times 10^{-2} \quad (27f)$$

The derived thermal expansion coefficient is 22.7×10^{-6} K^{-1} and the volume change at the beta – gamma transition is a contraction of 1.11% compared to a value of 0.94% determined by Watanabe et al. 1981 (673-1923 K) from direct density measurements. The equations are considered to be satisfactory because they agree closely with the lattice parameters determined by Basinski et al. 1955 above 1400 K. On the basis $100\Delta\varepsilon$ the deviations of the various sets of measurements from the selected values are as follows:

Table 26d. Deviations of experimental values for gamma iron from the selected values

References	Temperature Range K	Deviations $100\Delta\varepsilon$
Basinski et al. 1955	1189-1661	Trends 0.019 low to 0.007 high
Goldschmidt 1962	1185-1528	Trends 0.015 low to 0.050 low
Cockett and Davis 1963	1173-1423	Average bias 0.054 high
Gorton et al. 1965	1193-1343	Trends 0.002 low to 0.062 low
Kohlhaas et al. 1967	1223-1634	Trends 0.015 high to 0.095 low
Straumanis and Kim 1969	1173-1423	Trends 0.014 high to 0.019 low
Onink et al. 1993	1180-1250	Average bias 0.043 high
Miiller and Cezailiyan 1984	1200-1330	Trends 0.017 high to 0.036 high

26.5 Delta phase : Body-centered cubic (cI2): 1167 K to 1811 K.

Lattice parameter measurements of Basinski et al. 1955 (1662-1807 K) and Kohlhaas et al. 1967 (1663-1781 K) were related directly to the selected values for the alpha phase and derived length change values were fitted to the following equations:

$$a \text{ (nm)} = 6.68682 \times 10^{-6} T + 0.282064 \quad (26g)$$

$$\varepsilon_T = 2.33275 \times 10^{-5} T - 1.59986 \times 10^{-2} \quad (26h)$$

The derived thermal expansion coefficient is 22.8×10^{-6} K^{-1}. The molar volume change at the gamma – delta transition is an expansion of 0.56% in exact agreement with the value determined by Watanabe et al. 1981 from direct density measurements.

Table 26e. Low temperature crystallographic properties of alpha iron

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	- 0.202	0.28607	0.24775	7.049	7922
10	0.040	- 0.202	0.28607	0.24775	7.049	7922
20	0.12	- 0.201	0.28607	0.24775	7.049	7922
30	0.31	- 0.201	0.28607	0.24775	7.049	7922
40	0.75	- 0.201	0.28607	0.24775	7.050	7922
50	1.29	- 0.200	0.28608	0.24775	7.050	7922
60	2.21	- 0.198	0.28608	0.24775	7.050	7921
70	3.12	- 0.195	0.28609	0.24776	7.051	7921
80	3.98	- 0.192	0.28610	0.24777	7.052	7920
90	4.76	- 0.187	0.28611	0.24778	7.052	7919
100	5.50	- 0.182	0.28613	0.24779	7.053	7917
110	6.14	- 0.176	0.28614	0.24781	7.055	7916
120	6.71	- 0.170	0.28616	0.24782	7.056	7915
130	7.24	- 0.163	0.28618	0.24784	7.058	7913
140	7.71	- 0.156	0.28620	0.24786	7.059	7911
150	8.15	- 0.148	0.28623	0.24788	7.061	7909
160	8.53	- 0.139	0.28625	0.24790	7.063	7907
170	8.89	- 0.131	0.28628	0.24792	7.064	7905
180	9.23	- 0.122	0.28630	0.24794	7.066	7903
190	9.55	- 0.112	0.28633	0.24797	7.068	7901
200	9.85	- 0.102	0.28636	0.24799	7.070	7898
210	10.12	- 0.092	0.28638	0.24802	7.072	7896
220	10.37	- 0.082	0.28641	0.24804	7.075	7894
230	10.63	- 0.072	0.28644	0.24807	7.077	7891
240	10.87	- 0.061	0.28648	0.24809	7.079	7889
250	11.11	- 0.050	0.28651	0.24812	7.081	7886
260	11.35	- 0.039	0.28654	0.24815	7.084	7883
270	11.57	- 0.027	0.28657	0.24818	7.086	7881
280	11.79	- 0.016	0.28661	0.24821	7.089	7878
290	12.00	- 0.004	0.28664	0.24824	7.091	7875
293.15	12.07	0	0.28665	0.24825	7.092	7874

$$d = \sqrt{3}a/2$$

Table 26f. High temperature crystallographic properties of alpha - beta iron

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
293.15	12.07	0	0.28665	0.24825	7.092	7874
300	12.16	0.008	0.28667	0.24827	7.094	7872
350	12.76	0.071	0.28685	0.24842	7.107	7858
400	13.31	0.136	0.28704	0.24858	7.121	7842
450	13.82	0.204	0.28723	0.24875	7.136	7826
500	14.29	0.274	0.28744	0.24893	7.151	7810
550	14.70	0.347	0.28764	0.24911	7.166	7793
600	15.08	0.422	0.28786	0.24929	7.182	7775
650	15.40	0.498	0.28808	0.24948	7.199	7758
700	15.68	0.576	0.28830	0.24968	7.215	7740
750	15.92	0.656	0.28853	0.24987	7.233	7721
800	16.11	0.737	0.28876	0.25007	7.250	7703
850	19.25	0.818	0.28900	0.25028	7.268	7684
900	16.35	0.900	0.28923	0.25048	7.285	7665
950	16.37	0.983	0.28947	0.25069	7.303	7646
1000	15.94	1.065	0.28970	0.25089	7.321	7628
1010	15.76	1.081	0.28975	0.25093	7.325	7624
1020	15.51	1.097	0.28979	0.25097	7.328	7621
1030	15.12	1.112	0.28984	0.25101	7.331	7617
1035	14.79	1.120	0.28986	0.25103	7.333	7615
1040	14.15	1.127	0.28988	0.25104	7.335	7614
1041	13.90	1.129	0.28989	0.25105	7.335	7613
1042	13.48	1.130	0.28989	0.25105	7.335	7613
1042.5	13.08	1.131	0.28989	0.25105	7.335	7613
1042.7	12.80	1.131	0.28989	0.25105	7.336	7613
1042.9	12.23	1.131	0.28989	0.25105	7.336	7613
1043.1	13.55	1.132	0.28989	0.25106	7.336	7613
1043.3	13.88	1.132	0.28989	0.25106	7.336	7613
1043.5	14.04	1.132	0.28990	0.25106	7.336	7613
1044	14.26	1.133	0.28990	0.25106	7.336	7613
1045	14.49	1.134	0.28990	0.25106	7.336	7612
1050	14.94	1.142	0.28992	0.25108	7.338	7611
1060	15.23	1.157	0.28997	0.25112	7.341	7607
1070	15.57	1.173	0.29001	0.25116	7.345	7604
1080	15.77	1.188	0.29006	0.25120	7.348	7600
1090	15.94	1.205	0.29010	0.25124	7.352	7596
1100	16.10	1.221	0.29015	0.25128	7.355	7593
1120	16.40	1.254	0.29024	0.25136	7.362	7585
1140	16.68	1.287	0.29034	0.25144	7.370	7578
1150	16.83	1.304	0.29039	0.25148	7.373	7574
1160	16.96	1.321	0.29044	0.25153	7.377	7570
1180	17.24	1.356	0.29054	0.25161	7.385	7562
1185	17.31	1.365	0.29056	0.25163	7.386	7560

$$d = \sqrt{3}a/2$$

Table 26g. Crystallographic properties of gamma iron

T K	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1185	0.989	0.36473	0.25790	7.305	7645
1200	1.024	0.36485	0.25799	7.312	7637
1250	1.139	0.36527	0.25829	7.337	7611
1300	1.254	0.36569	0.25858	7.362	7585
1350	1.370	0.36610	0.25887	7.388	7559
1400	1.485	0.36652	0.25917	7.413	7534
1450	1.600	0.36693	0.25946	7.438	7508
1500	1.715	0.36735	0.25976	7.463	7483
1550	1.830	0.36777	0.26005	7.489	7457
1600	1.945	0.36818	0.26034	7.514	7432
1650	2.061	0.36860	0.26064	7.540	7407
1667	2.100	0.36874	0.26074	7.548	7398

$$d = a/\sqrt{2}$$

Table 26h. Crystallographic properties of delta iron

T K	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1667	2.289	0.29321	0.25393	7.590	7357
1680	2.319	0.29330	0.25400	7.597	7351
1700	2.366	0.29343	0.25412	7.607	7341
1720	2.413	0.29357	0.25424	7.618	7331
1740	2.459	0.29370	0.25435	7.628	7321
1750	2.483	0.29377	0.25441	7.634	7316
1760	2.506	0.29383	0.25447	7.639	7311
1780	2.553	0.29397	0.25458	7.649	7301
1800	2.599	0.29410	0.25470	7.660	7291
1811	2.625	0.29417	0.25476	7.665	7285

$$d = \sqrt{3}a/2$$

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27 COBALT Co

Atomic weight: 58.933194 (3) (Meija 2017))

Allotropy: Epsilon phase: Hexagonal close-packed (hP2)
Alpha phase: Face-centered cubic (cF4)

The phase designations are that given by Nishizawa and Ishida 1983. The freezing point is a secondary fixed point on ITS-90 at 1768 (3) K (Bedford et al. 1996). The epsilon – alpha transformation is martensitic and in agreement with Nishizawa and Ishida 1983 and Fernández Guillermet 1987 an equilibrium transition temperature of 695 K is selected. The alpha phase can easily be retained at room temperature. For the Curie temperature specific heat values (Braun and Kohlhaas 1964, Ray et al. 1973, Normanton 1975 and Dobrosavljević et al. 1989) suggest a value in the range 1367 to 1380 K while magnetic measurements (Myers and Sucksmith 1951, Colvin and Arajs 1965, Richter and Lotter 1969, Peletskii and Zaretskii 1981 and Maglić et al. 1983) suggest a value in the range 1388 K to 1396 K, averaging at 1394 K on ITS-90. In agreement with Fernández Guillermet 1987 the higher temperature value is accepted.

27.1 Epsilon Phase: Hexagonal close-packed (hP2): 0 K to 695 K.

In the low temperature region lattice parameter measurements of Ono and Maeta 1988 (4.2-300 K) were shown only graphically except for reported values at 4.2 K. Length change values estimated from these graphs at 10 K and 293 K and at 25 K intervals from 75 K to 275 K were fitted to Equation B using the values of enthalpy given in Part 27.3. On the basis $100\varepsilon_T$ it was found that the estimated values and the smooth values overall agreed to within 0.001:

$$\mathrm{Ln}(L_a) = (H_T - H_0)\,(2.52177 \times 10^{-7} + 3.80260 \times 10^{-10}\,T + 2.84737 \times 10^{-6} / T) - 1.73823 \times 10^{-3} \quad (27a)$$

$$\mathrm{Ln}(L_c) = (H_T - H_0)\,(4.42553 \times 10^{-7} + 4.90783 \times 10^{-10}\,T + 5.08718 \times 10^{-6} / T) - 2.81095 \times 10^{-3} \quad (27b)$$

Dilatometric thermal expansion coefficient measurements of White 1965 (4-85, 283 K) could be subject to preferred orientation effects but the agreement with selected values is to within 1×10^{-7} K^{-1} at 283 K, although at 65 to 85 K the difference averages to 7×10^{-7} K^{-1} high. On the basis $100\Delta\varepsilon$ length changes derived from the lattice parameter measurements of Müller et al. 1967 (97-296 K) scatter 0.046 low to 0.010 high for the *a*-axis but for the *c*-axis trend from 0.041 low to then agree with the selected values.

In the high temperature region length change values derived for both axes from the thermal expansion coefficients of Bibring and Sebilleau 1955 (293-690 K) and the lattice parameter measurements of Bolgov et al. 1964 (293-675 K) and additionally for the *c*-axis from lattice parameter measurements of Kulesco and Seryugin 1968 (293-673 K) were fitted to the following equations which, on the basis $\pm\ 100\varepsilon_T$, have relatively low accuracies of ± 0.034 and ± 0.024 respectively:

$$\varepsilon_T a = 6.31383 \times 10^{-6} T + 8.99802 \times 10^{-9} T^2 - 2.79031 \times 10^{-12} T^3 - 2.55387 \times 10^{-3} \quad (27c)$$

$$\varepsilon_T c = 1.62358 \times 10^{-5} T + 1.09785 \times 10^{-10} T^2 + 2.59829 \times 10^{-12} T^3 - 4.83441 \times 10^{-3} \quad (27d)$$

In order to ensure a smooth continuity between the high and low derived thermal expansion coefficients, experimental values for the *a*-axis only at 600 K and above and for the *c*-axis at 500 K and above were used in the evaluation. The measurements of both Bolgov et al. 1964 and Kulesco and Seryugin 1968 were only shown graphically with actual data points given by Touloukian et al. 1975. Dilatometric measurements on high purity single crystals by Kasamatsu et al. 1981 (77-900 K) were unfortunately shown only in the form of small graphs although the quoted thermal expansion coefficients at 300 K at 12.5 x 10^{-6} K^{-1} along the *a*-axis and 17.8 x 10^{-6} K^{-1} along the *c*-axis differ markedly from the presently accepted values. On the basis $100\Delta\varepsilon$ the *a*-axis lattice parameter values of Kulescu and Seryugen 1968 (293-696 K) trend to 0.13 high while the values of Marick 1936 (293-693 K) trend to 0.15 high along the *a*-axis and 0.38 high along the *c*-axis. The values of Shinoda 1934 (306, 373 K) are 0.010 high and 0.008 low respectively along the *a* and *c* axes at 373 K. Dilatometric measurements of Masumoto et al. 1967 (173-623 K) at 173 K and 623 K are respectively 0.019 low and 0.053 low along the a-axis, and 0.005 high and 0.096 low along the c-axis. Other dilatometric values determined in the epsilon region were not considered because of possible preferred orientation effects.

Table 27a. Lattice parameter of epsilon cobalt at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Notes
Hofer and Peebles 1947	RT	0.25069	0.40713	
Taylor and Floyd 1950	293	0.25075	0.40701	
Taylor 1950	293	0.25068	0.40700	
Morral 1958	RT	0.25060	0.40697	a
Anatharaman 1958	293	0.25072	0.40688	
Vincent and Figlarz 1967	RT	0.25072	0.40697	
	Selected	0.25071 (3)	0.40700 (8)	

Notes to Table 27a

a. *a* axis value not included in the average

At 293.15 K: Density 8834 (3) kg m^{-3} Molar volume 6.671 (2) cm^3 mol^{-1}.

27.2 Alpha Phase: Face-centered cubic (cF4): 695 K to 1768 K.

Dilatometric measurements of Brenner et al. 1947, Fine and Ellis 1948, Arbuzov and Zelenkov 1964, Krajewski et al. 1970, and Richter and Lotter 1969 and lattice parameter measurements of Bolgov et al. 1964 were only shown graphically with actual data points given by Touloukian et al. 1975. Of measurements which are not directly related to room temperature those of Bolgov et al. 1964 (677-1593 K) and Arbuzov and Zelenkov 1964 (423-1024 K) were related by using measurements of Owen and Madoc Jones 1954 at

these temperatures while the lattice parameter measurements of Kohlhaas et al. 1967 (793-1671 K) were related by using a room temperature value of 3.5445 Å. By ratioing the molar volumes of the epsilon and alpha phases at 293.15 K the difference is equivalent to the length change value of the alpha phase being equivalent to 1.72 x 10^{-3} higher than the reference value. On this basis length changes derived from the lattice parameter measurements of Owen and Madoc Jones 1954 (323-823 K), Bolgov et al. 1964 (677-1593 K) and Müller and Scholten 1966 (293-1623 K), and dilatometric measurements of Brenner et al. 1947 (293-1217 K) and Fine and Ellis 1948 (293-1152 K) were combined. The dilatometric measurements were only used directly in the alpha range, 865 to 1217 K in the heating range, and 718 to 1217 K in the cooling range in the case of Brenner et al. 1947, and 823 to 1152 K and 823 to 1152 K in the case of Fine and Ellis 1948. The measurements of Bolgov et al. 1964 were only considered to 1277 K. On the basis ± 100ε_T the accuracy of the equations are ± 0.017:

$$\varepsilon_{T\ REF} = 1.34368 \times 10^{-5}\, T - 1.93034 \times 10^{-9}\, T^{2} + 2.07476 \times 10^{-12}\, T^{3} - 2.10538 \times 10^{-3} \quad (27e)$$

$$\varepsilon_{T\ FCC} = 1.34368 \times 10^{-5}\, T - 1.93034 \times 10^{-9}\, T^{2} + 2.07476 \times 10^{-12}\, T^{3} - 3.82538 \times 10^{-3} \quad (27f)$$

These equations, which do not suggest anomalous behavior in the region of the Curie transition, were extrapolated to the freezing point. At 695 K the molar volume difference between the epsilon and alpha phases is an expansion of 0.31%. Fernández Guillermet 1987 suggested on theoretical grounds that in the region of the Curie transition the thermal expansion behavior showed a large lambda peak leading to a maximum value of 83 x 10^{-6} K^{-1} at the Curie temperature. Although also appearing to suggest an increase in the thermal expansion coefficient in the region of the Curie transition, the measurements of Richter and Lotter 1969 (1173-1486 K) as given by Touloukian et al. 1975 showed a considerable scatter but did suggest a much lower peak value of about 23 x 10^{-6} K^{-1}. The measurements of Bolgov et al. 1964 above 1300 K show a broad peak leading to a maximum deviation 0.26 high at 1354 K and decreasing to 0.15 high at 1593 K. Therefore, until more accurate measurements are available in the Curie transition region the anomalous behavior in this region is not considered. Other deviations of experimental measurements from equations 27e and 27f are considered in Table 27c.

Table 27b. Lattice parameter of alpha cobalt at 293.15 K

References	Original Temperature K	*a* nm	Note
Taylor and Floyd 1950	293	0.35444	
Taylor 1950	293	0.35444	
Owen and Madoc Jones 1954	291	0.35444	
Luo and Duwez 1963	RT	0.35454	a
Swanson et al. 1966, p.10	298	0.35447	
Vincent and Figlarz 1967	RT	0.35448	
	Selected	0.35447 (4)	

Notes for Table 27b

a. Although appearing to be discrepant, in agreement with Donohue 1974 this value is included

At 293.15 K: Density 8789 (3) kg m^{-3} Molar volume 6.705 (2) cm^3 mol^{-1}.

Table 27c. Deviations of experimental values from the selected values for alpha cobalt

References	Temperature Range K	Deviations 100Δε
Marick 1936	293-1460	Trends to 0.66 high
Newkirk and Geisler 1953	293-1496	Trends to 0.58 high at 1420 K and 1496 K
Arbuzov and Zelenkov 1964	423-1023	Trends to 0.059 high
Kohlhaas et al. 1967	793-1671	Trends to 0.19 low at 1400 K and then to 0.12 low at 1671 K
Petrov 1966	293-1103	Trends to 0.18 high
Kulesco and Seryugin 1968	293-701	Trends to an average bias of 0.053 high above 600 K

27.3 Low temperature thermodynamic properties of epsilon cobalt

The specific heat value at 10 K is that selected by Hultgren et al. 1973 and the value at 298.15 K from JANAF (Chase 1998). Intermediate specific heat values are from the smooth values selected by Clusius and Schachinger 1952 (14-270 K) over the range 20 K to 273.2 K after correcting for atomic weight 58.933194/58.94. Enthalpy values were derived by integration. C_p values are given in J mol^{-1} K^{-1} and $H_T - H_0$ values in J mol^{-1}

Table 27d. Low temperature specific heat and enthalpy values

T K	10	20	30	40	50	60	65	70	75
C_p	0.072	0.284	1.092	2.380	4.301	6.501	7.621	8.729	9.815
$H_T - H_0$	0.243	1.527	8.007	24.84	58.01	112.0	147.3	188.3	234.7
T K	80	85	90	100	110	120	130	140	150
C_p	10.831	11.704	12.496	13.952	15.348	16.609	17.702	18.654	19.477
$H_T - H_0$	286.4	342.7	403.2	535.5	682.1	842.1	1013.7	1195.6	1386.4
T K	160	170	180	190	200	210	220	230	240
C_p	20.190	20.810	21.353	21.835	22.277	22.715	23.122	23.483	23.796
$H_T - H_0$	1584.8	1789.8	2000.7	2216.7	2437.2	2662.2	2891.4	3124.5	3361.0
T K	250	260	270	280	290	293.15	298.15		
C_p	24.041	24.252	24.456	24.626	24.748	24.774	24.802		
$H_T - H_0$	3600.2	3841.6	4085.2	4330.7	4577.6	4655.6	4779.5		

Table 27e. Crystallographic properties of epsilon cobalt

Values below 293.15 K are considered to be tentative.

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
0	0	0	0	- 0.174	- 0.281	- 0.209
10	0.03	0.06	0.04	- 0.174	- 0.281	-0.209
20	0.10	0.18	0.13	- 0.174	- 0.281	- 0.209
30	0.37	0.64	0.46	- 0.173	- 0.280	- 0.209
40	0.77	1.34	0.96	- 0.173	- 0.279	- 0.208
50	1.37	2.36	1.70	- 0.172	- 0.277	- 0.207
60	2.05	3.52	2.54	- 0.170	- 0.274	- 0.205
70	2.75	4.69	3.40	- 0.168	- 0.270	- 0.202
80	3.43	5.82	4.23	- 0.165	- 0.265	- 0.198
90	3.99	6.73	4.90	- 0.161	- 0.259	- 0.194
100	4.50	7.56	5.52	- 0.157	- 0.252	- 0.188
110	5.01	8.38	6.13	- 0.152	- 0.244	- 0.183
120	5.49	9.15	6.71	- 0.147	- 0.235	- 0.176
130	5.94	9.85	7.24	- 0.141	- 0.226	- 0.169
140	6.36	10.5	7.74	- 0.135	- 0.215	- 0.162
150	6.74	11.1	8.19	- 0.128	- 0.205	- 0.154
160	7.11	11.6	8.62	- 0.121	- 0.193	- 0.145
170	7.45	12.1	9.01	- 0.114	- 0.181	- 0.137
180	7.77	12.6	9.38	- 0.106	- 0.169	- 0.127
190	8.08	13.1	9.74	- 0.099	- 0.156	- 0.118
200	8.38	13.5	10.1	- 0.090	- 0.143	- 0.108
210	8.69	13.9	10.4	- 0.082	- 0.129	- 0.098
220	8.99	14.4	10.8	- 0.073	- 0.115	- 0.087
230	9.29	14.8	11.1	- 0.064	- 0.101	- 0.076
240	9.57	15.2	11.4	- 0.054	- 0.086	- 0.065
250	9.83	15.6	11.7	- 0.045	- 0.070	- 0.053
260	10.1	15.9	12.0	- 0.035	- 0.055	- 0.041
270	10.3	16.2	12.3	- 0.025	- 0.038	- 0.029
280	10.6	16.6	12.6	- 0.014	- 0.022	- 0.017
290	10.8	16.9	12.8	- 0.003	- 0.005	- 0.004
293.15	10.9	17.0	12.9	0	0	0
300	11.0	17.0	13.0	0.007	0.012	0.009
350	11.6	17.3	13.5	0.064	0.097	0.075
400	12.2	17.5	14.0	0.123	0.184	0.144
450	12.7	17.9	14.4	0.186	0.273	0.215
500	13.2	18.2	14.9	0.250	0.364	0.288
550	13.6	18.6	15.3	0.318	0.456	0.364
600	14.0	19.1	15.7	0.387	0.551	0.442
650	14.4	19.5	16.1	0.459	0.648	0.522
695	14.7	20.0	16.5	0.524	0.737	0.595

Table 27f. Crystallographic properties of epsilon cobalt (Continued)

Values below 293.15 K are considered to be tentative.

T K	*a* nm	*c* nm	*c*/*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.25027	0.40586	1.6216	0.24912	6.629	8890
10	0.25027	0.40586	1.6216	0.24912	6.629	8890
20	0.25027	0.40586	1.6216	0.24912	6.629	8890
30	0.25028	0.40586	1.6217	0.24912	6.629	8890
40	0.25028	0.40586	1.6217	0.24912	6.629	8890
50	0.25028	0.40587	1.6217	0.24912	6.630	8889
60	0.25028	0.40588	1.6217	0.24913	6.630	8889
70	0.25029	0.40590	1.6217	0.24914	6.631	8888
80	0.25030	0.40592	1.6218	0.24915	6.631	8887
90	0.25031	0.40595	1.6218	0.24916	6.632	8886
100	0.25032	0.40598	1.6218	0.24918	6.633	8884
110	0.25033	0.40601	1.6219	0.24920	6.635	8883
120	0.25034	0.40604	1.6220	0.24922	6.636	8881
130	0.25036	0.40608	1.6220	0.24924	6.637	8879
140	0.25037	0.40612	1.6221	0.24926	6.639	8877
150	0.25039	0.40617	1.6221	0.24928	6.640	8875
160	025041	0.40621	1.6222	0.24931	6.642	8873
170	0.25042	0.40626	1.6223	0.24933	6.644	8871
180	0.25044	0.40631	1.6224	0.24936	6.646	8868
190	0.25046	0.40636	1.6225	0.24939	6.647	8866
200	0.25048	0.40642	1.6225	0.24942	6.649	8863
210	0.25050	0.40647	1.6226	0.24944	6.651	8860
220	0.25053	0.40653	1.6227	0.24948	6.654	8857
230	0.25055	0.40659	1.6228	0.24951	6.656	8854
240	0.25057	0.40665	1.6229	0.24954	6.658	8851
250	0.25060	0.40671	1.6230	0.24957	6.660	8848
260	0.25062	0.40678	1.6231	0.24961	6.663	8845
270	0.25065	0.40684	1.6232	0.24964	6.665	8842
280	0.25067	0.40691	1.6233	0.24968	6.667	8839
290	0.25070	0.40698	1.6234	0.24972	6.670	8835
293.15	0.25071	0.40700	1.6234	0.24973	6.671	8834
300	0.25073	0.40705	1.6235	0.24975	6.673	8832
350	0.25087	0.40740	1.6239	0.24994	6.686	8814
400	0.25102	0.40775	1.6244	0.25014	6.700	8796
450	0.25118	0.40811	1.6248	0.25034	6.714	8778
500	0.25134	0.40848	1.6252	0.25054	6.729	8758
550	0.25151	0.40886	1.6256	0.25075	6.744	8739
600	0.25168	0.40924	1.6260	0.25097	6.760	8718
650	0.25186	0.40964	1.6265	0.25119	6.776	8697
695	0.25202	0.41000	1.6268	0.25139	6.790	8678

$$d1 = (a^2/3 + c^2/4)^{½} \quad d2 = a$$

Table 27g. Crystallographic properties of alpha cobalt

T K	$\alpha \times 10^6$ K^{-1}	100 ε_T	100 ε_T fcc base	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
293.15	12.82	0.172	0	0.35447	0.25065	6.705	8789
300	12.82	0.181	0.009	0.35450	0.25067	6.707	8787
350	12.82	0.245	0.073	0.35473	0.25083	6.720	8770
400	12.85	0.309	0.137	0.35496	0.25099	6.733	8753
450	12.91	0.374	0.202	0.35519	0.25115	6.746	8736
500	13.01	0.439	0.267	0.35542	0.25132	6.759	8719
550	13.13	0.505	0.333	0.35565	0.25148	6.773	8702
600	13.29	0.571	0.399	0.35588	0.25165	6.786	8684
650	13.47	0.638	0.466	0.35612	0.25182	6.800	8667
695	13.66	0.700	0.528	0.35634	0.25197	6.812	8651
700	13.69	0.707	0.535	0.35636	0.25199	6.814	8649
800	14.21	0.847	0.675	0.35686	0.25234	6.842	8613
900	14.86	0.994	0.822	0.35738	0.25271	6.872	8576
1000	15.62	1.148	0.976	0.35793	0.25309	6.904	8537
1100	16.51	1.310	1.138	0.35850	0.25350	6.937	8495
1200	17.51	1.482	1.310	0.35911	0.25393	6.973	8452
1300	18.63	1.666	1.494	0.35977	0.25439	7.010	8404
1400	19.86	1.862	1.690	0.36046	0.25488	7.051	8358
1500	21.21	2.071	1.899	0.36120	0.25542	7.095	8307
1600	22.67	2.295	2.123	0.36200	0.25597	7.142	8252
1700	24.25	2.535	2.363	0.36285	0.25657	7.192	8194
1768	25.38	2.708	2.536	0.36346	0.25701	7.229	8153

$$d = a/\sqrt{2}$$

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28 NICKEL Ni

Atomic weight: 58.6934 (4) (Meija 2017)

Structure: Face-centered cubic (cF4)

The freezing point is a secondary fixed point on ITS-90 at 1728 (1) K (Bedford et al. 1996). A Curie temperature of 628.2 K was selected to be consistent with the thermal expansion coefficients of Kollie 1977.

28.1 Low temperature

Thermal expansion coefficients of White 1965 (4-85, 283 K), and those of Altman et al. 1954 (20-300 K) as given by Touloukian et al. 1975, were combined with the specific heat (C_p) values selected by Desai 1987 and fitted to Equation A. Because of their close agreement the values at 300 K of 12.9 x 10^{-6} K^{-1} as determined by Altman et al. 1954, and 12.89 x 10^{-6} K^{-1} as determined by Kollie 1977, were selected in preference to the value of 12.9 x 10^{-6} K^{-1} at 283 K as determined by White 1965. The overall accuracy of the equation is ± 3 x 10^{-8} K^{-1}:

$$\alpha\ (K^{-1}) = C_p\,(5.64826 \times 10^{-7} - 1.64718 \times 10^{-10}\ T - 5.98824 \times 10^{-6}/T) \qquad (28a)$$

On the basis 100Δε dilatometric measurements of Fraser and Hollis Hallet 1965 (29-84 K) show an average bias of 0.003 high while those of Clark 1968 (20-300 K) trend from initially 0.004 high to agree with the selected values. In the region below room temperature the dilatometric measurements of Nix and MacNair 1941 (81-762 K) trend from initially 0.007 high to agree with the selected values while the values of Abdullaev et al. 2015 (145 to 1650 K) agree to within 0.001. Length change values from the lattice parameter values of Kohlhaas et al. 1967 (85-1665 K) trend from initially 0.056 low.

28.2 High Temperature

Precision thermal expansion coefficients of Kollie 1977 (300-973 K) were accepted up to 863 K. In the ranges 293.15 to 600 K and 668 to 863 K the data was represented by equivalent length change analytical equations 28b and 28c while in the intermediate region 600 to 668 K values were already given at very close intervals and length change values were determined by three point integration:

$$293.15 - 600\ K: \varepsilon_T = 4.14456 \times 10^{-6}\,T + 2.56959 \times 10^{-8}\,T^2 - 3.24460 \times 10^{-11}\,T^3 + 1.96969 \times 10^{-14}\,T - 2.75128 \times 10^{-3} \qquad (28b)$$

$$668 - 863\ K: \varepsilon_T = 3.88361 \times 10^{-6}\,T + 3.16859 \times 10^{-8}\,T^2 - 3.51510 \times 10^{-11}\,T^3 + 1.45178 \times 10^{-14}\,T^4 - 3.45598 \times 10^{-3} \qquad (28c)$$

The selection of the values of Kollie 1977 were particularly confirmed by the dilatometric measurements of Rosenbohm 1938 (373-793 K) which, on the basis 100Δε, although differing by 0.004 low at 613 K agree exactly with the selected values above 633 K while above room temperature the measurements of Nix and MacNair 1941 (81-

762 K) show an average bias of only 0.001 low. Additional measurements of the magnetic contribution to the thermal expansion coefficient in the critical region were given by Major et al. 1971, Yousef et al. 1986 and Faisst 1988. As indicated in Table 28c, at 863 K the dilatometric measurements in the high temperature region such as those of Holborn and Day 1901 (273-1273 K), Jordan and Swanger 1930 (298-1173 K), Totskii 1964 (273-1373 K), Drotning 1982 (297-1728 K) and Suh et al. 1988 (293-1600 K) give length change values which are systematically lower than the selected values at this temperature and it was found that a smooth thermal expansion curve above this temperature could only be achieved by using the values of Drotning 1982 at 1300 K and above, which were then combined with the selected values at 863 K to cover the range from 863 K to 1728 K:

$$\varepsilon_T = 4.12769 \times 10^{-5} T - 3.53552 \times 10^{-8} T^2 + 2.13907 \times 10^{-11} T^3 - 4.15694 \times 10^{-15} T^4 - 1.17791 \times 10^{-2} \quad (28d)$$

Compared to the selected values, thermal expansion coefficients of Glazkov 1987 (900-1400 K) trend from initially 4.1 x 10^{-7} K^{-1} high to a maximum low of 8.0 x 10^{-7} K^{-1} at 1250 K while direct density measurements of Makeev and Popel' 1990 (710-1700 K) trend from 1.0% low to 1.0% high. Lattice parameter measurements of Esser et al. 1938 (273-1373 K) were only shown graphically. The deviations of other high temperature dilatometric and lattice parameter measurements from the selected values are given in Part 28.3.

Table 28a. Lattice parameter of nickel at 293.15 K

References	Original Temperature K	*a* nm	Note
Phragmén 1931	291	0.35253	a
Owen and Iball 1932	289.7	0.35254	a
Owen and Pickup 1934	291	0.35249	
Jette and Foote 1935	298	0.35239	
Owen and Yates 1936	291	0.35246	
Owen et al. 1937	288	0.35247	
Lu and Chang 1941	294	0.35247	
Fricke 1941	RT	0.35241	
Esch and Schneidner 1944	RT	0.35242	
Taylor 1950	293	0.35242	
Taylor and Floyd 1951-1952	293	0.35241	
Ellwood and Bagley 1951-1952	298	0.35240	
Swanson and Tatge 1953	298	0.35238	
Von Baltchelder and Raeuchle 1954	298	0.35238	
Coles 1955-1956	291	0.35240	
Diament 1956	290	0.35256	a
Day 1961	RT	0.35242	
Casselton and Hume-Rothery 1964	RT	0.35240	
Bidwell and Speiser 1964	298	0.35235	
Rao 1965	RT	0.35242	
Kantola and Tokola 1967	298	0.35236	
Kohlhaas et al. 1967	293	0.35234	
Zwell et al. 1968	296	0.35239	
	Selected	0.35241 (4)	

Note for Table 28a

a. Not included in the average

At 293.15 K for Ni: Density 8907 (3) kg m^{-3} Molar volume 6.589 (2) cm^3 mol^{-1}.

28.3 Deviations of experimental values from the selected values

Table 28b. Dilatometric values

References	Temperature Range K	Deviations 100Δε
Holborn and Day 1901	273-1273	Average bias 0.013 low
Masumoto and Nara 1927	303, 373	0.002 high at 373 K
Jordan and Swanger 1930	298-1173	Trends to 0.031 low
Uffelmann 1930	361-941	Heating: Trends to 0.082 low. Cooling: Trends To 0.061 low
Masumoto 1931	303, 373	Average of two samples 0.004 low at 373 K
Nakamura 1936	288-678	Trends to 0.044 low
Trombe and Foex 1953	273-773	Average bias 0.001 low
Davis et al. 1955	293, 593	0.042 low at 593 K
Fieldhouse et al. 1956	386-1658	Trends to 0.12 low at 1394 K and then average bias 0.074 low below 1400 K
Saur and Wenkowitsch 1958	291-745	Trends to 0.035 low
Allen 1959	293-1033	Initially 0.043 low then trends to selected values
Totskii 1964	273-1373	Trends to average bias 0.040 low above 650 K
Arbuzov and Zelenkov 1964	295-974	Average bias 0.007 low
Masumoto et al. 1968	273-780	Trends to average 0.045 high
Richter and Lotter 1969	373-773	Average bias 0.028 low
Masumoto et al. 1969a	273-773	Trends to average 0.083 low above 600 K
Masumoto et al. 1969b	273, 313	0.001 high at 313 K
Masumoto and Sawaya 1970	293-773	Trends to 0.095 low
Gurevich and Larikov 1970	293-841	Average bias 0.003 low
Tanji 1971	273-1073	Average bias 0.031 low
Drotning 1982	297-1728	Trends to 0.031 low at 750 K and then trends to be representative values above 1300 K
Suh et al. 1988	293-1600	Trends to 0.053 low
Abdullaev et al. 2015	145-1650	Above room temperature averages 0.009 high between 600 K and 1100 K then trends to 0.030 low at 1650 K

Table 28c. Lattice parameter values

References	Temperature Range K	Deviations 100Δε
Owen and Yates 1936	291-873	Trends to 0.041 high
Owen et al. 1937	288-873	Trends to 0.040 high
Eisenstein 1946	293, 1148	0.26 high at 1148 K
Diament 1956	290-1160	Scatter 0.003 high to 0.032 high but average bias 0.017 high
Shevlin et al. 1956	302-1366	Trends to maximum of 0.11 high at 994 K then trends to 0.048 high
Saur and Wenkowitsch 1958	291-753	Sample 1: trends to 0.039 high at 456 K then trends to 0.013 low. Sample 2: average bias 0.011 high below 650 K then trends to 0.006 low
Kagan 1964	295, 473	Sample 1: 0.003 high at 473 K. Sample 2: 0.010 low at 473 K
Kohlhaas et al. 1967	85-1665	Above room temperature trends to 0.043 low at 991 K and then trends to 0.11 high at 1665 K
Kantola and Tokola 1967	298-1063	Initially 0.028 high trending to average bias 0.002 low above 650 K
Suh et al. 1988	293-1676	Scatter 0.040 low to 0.006 high but average bias 0.024 low

Table 28d. Low temperature crystallographic properties of nickel

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	- 0.231	0.35160	0.24862	6.544	8969
10	0.050	- 0.231	0.35160	0.24862	6.544	8969
20	0.16	- 0.231	0.35160	0.24862	6.544	8969
30	0.35	- 0.230	0.35160	0.24862	6.544	8969
40	0.90	- 0.230	0.35160	0.24862	6.544	8969
50	1.78	- 0.228	0.35161	0.24862	6.544	8969
60	2.77	- 0.226	0.35161	0.24863	6.545	8968
70	3.81	- 0.223	0.35162	0.24864	6.545	8967
80	4.85	- 0.219	0.35164	0.24865	6.546	8966
90	5.80	- 0.213	0.35166	0.24866	6.547	8965
100	6.64	- 0.207	0.35168	0.24868	6.548	8963
110	7.40	- 0.200	0.35171	0.24869	6.550	8961
120	8.08	- 0.192	0.35173	0.24871	6.551	8959
130	8.67	- 0.184	0.35176	0.24813	6.553	8957
140	9.20	- 0.175	0.35179	0.24876	6.555	8954
150	9.66	- 0.166	0.35183	0.24818	6.557	8952
160	10.08	- 0.156	0.35186	0.24880	6.559	8949
170	10.44	- 0.145	0.35190	0.24883	6.561	8946
180	10.76	- 0.135	0.35193	0.24886	6.563	8944
190	11.03	- 0.124	0.35197	0.24888	6.565	8941
200	11.27	- 0.113	0.35201	0.24891	6.567	8938
210	11.49	- 0.101	0.35205	0.24894	6.569	8935
220	11.68	- 0.090	0.35209	0.24897	6.571	8932
230	11.87	- 0.078	0.35213	0.24900	6.574	8928
240	12.05	- 0.066	0.35218	0.24903	6.576	8925
250	12.21	- 0.054	0.35222	0.24906	6.579	8922
260	12.37	- 0.042	0.35226	0.24909	6.581	8919
270	12.52	- 0.029	0.35231	0.24912	6.583	8915
280	12.66	- 0.017	0.35235	0.24915	6.586	8912
290	12.79	- 0.004	0.35240	0.24918	6.588	8909
293.15	12.83	0	0.35241	0.24919	6.589	8907

$$d = a/\sqrt{2}$$

Table 28e. High temperature crystallographic properties of nickel

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
298.15	12.83	0	0.35241	0.24919	6.589	8907
300	12.93	0.009	0.35244	0.24921	6.591	8905
400	14.15	0.145	0.35292	0.24955	6.618	8869
500	15.31	0.292	0.35344	0.24992	6.647	8830
550	16.01	0.371	0.35372	0.25051	6.663	8809
600	16.88	0.453	0.35401	0.25032	6.679	8787
610	17.14	0.470	0.35407	0.25036	6.683	8783
620	17.57	0.487	0.35413	0.25041	6.686	8778
625	17.95	0.496	0.35416	0.25043	6.688	8776
626	18.07	0.498	0.35417	0.25043	6.688	8776
627	18.28	0.500	0.35417	0.25044	6.689	8775
628	18.70	0.502	0.35418	0.25044	6.689	8775
628.2	18.86	0.502	0.35418	0.25044	6.689	8775
629	18.00	0.504	0.35419	0.25045	6.689	8774
630	17.62	0.506	0.35419	0.25045	6.690	8774
631	17.39	0.507	0.35420	0.25046	6.690	8773
632	17.22	0.509	0.35420	0.25046	6.690	8773
633	17.11	0.511	0.35421	0.25046	6.691	8772
635	16.97	0.514	0.35422	0.25047	6.691	8771
640	16.73	0.523	0.35425	0.25049	6.693	8769
645	16.56	0.531	0.35428	0.25051	6.695	8767
650	16.44	0.539	0.35431	0.25054	6.696	8765
660	16.40	0.556	0.35437	0.25058	6.700	8761
670	16.38	0.572	0.35443	0.25062	6.703	8756
680	16.38	0.589	0.35448	0.25066	6.706	8752
690	16.38	0.605	0.35454	0.25070	6.710	8748
700	16.39	0.622	0.35460	0.25074	6.713	8743
750	16.48	0.704	0.35489	0.25095	6.729	8722
800	16.69	0.788	0.35519	0.25115	6.746	8700
900	17.33	0.960	0.35579	0.25158	6.780	8656
1000	17.91	1.138	0.35642	0.25203	6.817	8610
1100	18.76	1.323	0.35707	0.25249	6.854	8563
1200	19.80	1.518	0.35776	0.25298	6.894	8516
1300	20.91	1.725	0.35849	0.25349	6.936	8462
1400	22.01	1.944	0.35926	0.25404	6.981	8408
1500	22.98	2.174	0.36007	0.25461	7.028	8351
1600	23.74	2.413	0.36091	0.25520	7.078	8293
1700	24.19	2.659	0.36178	0.25582	7.129	8233
1728	24.25	2.728	0.36203	0.25599	7.143	8216

$$d = a/\sqrt{2}$$

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29 COPPER Cu

Atomic weight: 63.546 (3) (Meija 2017)

Structure: Face-centered cubic (cF4)

The freezing point is a primary fixed point on ITS-90 at 1357.77 K (Preston-Thomas 1990).

29.1 Low temperature

Up to 293.15 K the thermal expansion equations of Kroeger and Swenson 1977 (0-320 K) were accepted. Thermal expansion values derived from these equations were also fitted to Equation A and given in Appendix A.

The differences between other experimental low temperature thermal expansion coefficients and the selected values are given in Part 29.6. The differences between length change values in the low temperature region and the selected values are also given in Part 29.6, except for the lattice parameter measurements of Simmons and Balluffi 1957 (8-103 K) and Shah 1971 (40-180 K) and the dilatometric measurements of Kasai 1968 (0-60 K) which cannot be directly connected to room temperature values.

29.2 High temperature

Lattice parameter and dilatometric measurements of Simmons and Balluffi 1963 (293-1323 K) were combined with dilatometric measurements of Pathak and Vasavada 1970 (300-1300 K), Pojor and Yates 1973 (325-763 K), Kollie et al. 1974 (300-1000 K and 300-840 K), Bennett 1978 (327-675 K) and Kirby and Hahn 1975, 1990 (20-800 K). All values were initially reduced to thermal expansion coefficients as α^* and the various weightings attached to these values are considered in Part 29.3. By not including dilatometric measurements above 1023 K to avoid the inclusion of values affected by thermal vacancy effects, then the derived equation was considered as representing the "crystallographic" properties and was integrated in order to obtain a length change equation covering the range from 293.15 K to the freezing point:

$$\varepsilon_T = 1.34504 \times 10^{-5} T + 6.76395 \times 10^{-9} T^2 - 3.60162 \times 10^{-12} T^3 + 1.51287 \times 10^{-15} T^4 - 4.44470 \times 10^{-3} \quad (29a)$$

Lattice parameter measurements of Esser et al. 1938 (293-1273 K) and dilatometric measurements of Nasekovskii 1967 (31-985 K) were only shown graphically but the latter values were given by Touloukian et al. 1975. The deviations of other high temperature lattice and dilatometric measurements from the selected values are given in Part 29.6, except for the lattice parameter measurements of Straumanis and Yu 1969 (288-328 K) because they were determined over a very narrow temperature range, but also led to a discrepant value of the thermal expansion coefficient at 14.87×10^{-6} K^{-1}.

Table 29a. Lattice parameter of copper at 293.15 K

References	Original Temperature K	*a* nm	Note
Owen and Iball 1932	289.7	0.36153	
Obinata and Wasserman 1933	291	0.36155	
Owen and Pickup 1933	291	0.36154	
Owen and Yates 1933	291	0.36154	
Owen and Pickup 1934	291	0.36155	
Vegard and Kloster 1934	RT	0.36156	
Owen and Rogers 1935	291	0.36154	
Hume-Rothery et al. 1936	296	0.36147	
Van Bergen 1937.1938	293	0.36150	
Owen and Roberts 1939	291	0.36150	
Foote and Jette 1940	298	0.36150	
Felipe 1940	291	0.36149	
Owen and Rowlands 1940	291	0.36151	
Carapella and Hultgren 1941	298	0.36145	
Lu and Chang 1941	292	0.36148	
Hume-Rothery and Andrews 1942	291	0.36150	
Anderson and Kingbury 1943	298	0.36149	
Rose 1946	294	0.36147	
Crussard and Aubertin 1949	RT	0.36146	
Frohnmeyer and Glocker 1953	293	0.36149	
Swanson and Tatge 1953	298	0.36149	
Jones and Owen 1954	291	0.36151	
Graf 1954	293.2	0.36153	
Coles 1955-1956	297	0.36150	
Otte 1961	297	0.36150	
Calvert and Henry 1962	294	0.36150	
Mitra and Mitra 1963	300	0.36145	
Rao 1965	297	0.36151	
Batchelder and Simmons 1965	298	0.36151	
Ullrich 1967	286.8	0.36160	a
Kantola and Tokola 1967	296, 298	0.36145	
Straumanis and Yu 1969	298	0.36148	
Krull and Newman 1970	300	0.36148	
Peljo et al. 1974	294.4	0.36153	
Seshadri and Downie 1979	294	0.36155	
	Selected	0.36150 (3)	

Note for Table 29a

a. Not included in the average

At 293.15 K: Density 8935 (2) kg m^{-3} Molar volume 7.112(2) cm^3 mol^{-1}.

29.3 Weighting of the high temperature input values for equation 29b

Simmons and Balluffi 1963: Both lattice and dilatometric length change values from 323 K to 1323 K and the extrapolated values at 1356 K were separately fitted to equations and differentiated in order to obtain values of α* at 50 K intervals from 523 K to 1323 K and

at 1356 K in the case of the lattice parameter values and up to 1023 K in the case of the dilatometric values.

Pathak and Vasavada 1970: Values of α* at 100 K intervals from 400 K to 1000 K.

Pojur and Yates 1973: Thirty three values of α* were fitted to an equation and derived values at 50 K intervals from 350 K to 600 K.

Kollie et al. 1974: Thermal expansion equations of α* for copper standard SRM 736 and for OFHC copper separately evaluated at 50 K intervals from 350 to 850 K.

Bennett 1978: The equation in α* was evaluated at 25 K intervals from 350 to 650 K

Kirby and Hahn 1975, 1990: Published values of α* at 20 K intervals from 320 K to 800 K.

29.4 Bulk properties of copper

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High precision measurements of both lattice and dilatometric length change values over the range from 500 K to close to the freezing point by Hehenkamp et al. 1992 lead to the values $C_V = 7.6\ (3) \times 10^{-4}$, $H_V = 1.19\ (3)$ eV and $S_V = 3.0\ (3)\ k$ which were accepted and compared directly to the selected crystallographic properties. Henenkamp et al. 1992 explained that the much lower value of $C_V = 2.0\ (5) \times 10^{-4}$ at the freezing point obtained by Simmons and Balluffi 1963 as being due to temperature homogeneity problems which could explain the scatter obtained for these measurements and lead to incorrect values. An apparent agreeing value of $C_V = 2.1\ (1) \times 10^{-4}$ obtained by Trost et al. 1986 using neutron diffraction was considered by Henenkamp et al. 1992 to be highly preliminary. The net result of selecting the values of Henenkamp et al. 1992 is that on the basis $100\Delta\varepsilon$ the actual dilatometric measurements of Simmons and Balluffi 1963 trend to 0.015 low at 1323 K.

29.5 A comparison with previous evaluations

The three principal reviews by Touloukian et al. 1975, White and Roberts 1980 and Wang and Reeber 1996 did not distinguish between lattice and dilatometric measurements of thermal expansion. Therefore, comparisons are compared to the selected crystallographic values below 950 K and to an average of the crystallographic and dilatometric values above. Touloukian et al. 1975 had to rely on the earlier measurements of Kirby and Hahn 1969 and Hahn 1970 instead of the later corrected measurements of Kirby and Hahn 1975, 1990. However, on the basis $100\Delta\varepsilon$ the difference from the presently selected values is a maximum deviation of only 0.004 low at 900 K. White and Roberts 1980 used the same input values as considered here but with a different weighting procedure and this leads to a trend of 0.007 low at 1250 K. Wang and Reeber 1996 used a complex function to calculate the thermal expansion coefficient. However, on a length change basis, while their values showed an average bias of only

0.002 high below 1000 K above this temperature then trend to 0.037 low at 1350 K which would of course also represent a significant departure from the selected values of White and Roberts.

29.6 Deviations of experimental values from the selected values

Table 29b. Low temperature thermal expansion coefficients

References	Temperature Range K	Deviations $\delta\alpha$ K^{-1}
Novikova and Strelkov 1959	30 – 105	Average bias of 2.3 x 10^{-7} K^{-1} low
Shapiro et al. 1964	8 – 54	Trends to 1.2 x 10^{-7} K^{-1} high for a first sample and to 2.6 x 10^{-7} K^{-1} high for a second sample
Channing and Weintroub 1965	20 – 270	Average bias of 6 x 10^{-8} K^{-1} low above 35 K
Bunton and Weintroub 1968	10 – 200	Sinusoidal trend of 2.8 x 10^{-7} K^{-1} low at 40 K increasing to 1.3 x 10^{-7} K^{-1} high at 130 K and then to 9 x 10^{-8} K^{-1} low at 200 K
Kos and Lamarche 1969	5 – 15	Agrees to within 1 x 10^{-8} K^{-1}
Awad and Gugan 1971	10 – 80	Average bias of 8 x 10^{-8} K^{-1} high between 30 and 70 K but 1.0 x 10^{-7} K^{-1} low at 80 K
White and Collins 1972	2 – 85, 283	Trends to 2 x 10^{-8} K^{-1} low at 85 K and then to 1.0 x 10^{-7} K^{-1} low at 283 K
McLean et al. 1972	1 – 26	Agrees to within 1 x 10^{-8} K^{-1}
Okaji et al. 1997	20 – 300	Average bias of 3 x 10^{-8} K^{-1} low above 50 K

Table 29c. Lattice parameter values

References	Temperature Range K	Deviations $100\Delta\varepsilon$
Vegard and Kloster 1934	293, 748	0.37 high at 748 K
Eisenstein 1946	293, 1148	0.33 low at 1148 K
Hume-Rothery and Andrews 1942	291 – 1144	Trends from 0.012 high to 0.013 low
Eppelsheimer and Penman 1950	291 – 1043	Two samples trend to average 0.23 low
Mitra and Mitra 1963	303 – 803	Average bias 0.004 high
Kantola and Tokola 1967	296 – 843	Trends to a maximum of 0.050 high at 649 K then decreases to 0.036 high at 843 K
Ullrich 1967	83 – 363	Average bias 0.005 high
Gehlen 1969	100 – 1183	Trends from 0.019 low to 0.067 high
Peljo et al. 1974	294 – 800	Trends to 0.012 low
Seshadri and Downie 1979	294-917	Trends from 0.021 high at 535 K to 0.029 low at 917 K
Suh et al. 1988	293-1343	Average of two samples trends from 0.13 low at 1179 K to 0.013 high at 1340 K
Vesnin and Shubin 1988	293-1358	Trends to 0.23 high

Table 29d. Dilatometric values

References	Temperature Range K	Deviations 100Δε
Dorsey 1907	93 – 293	Average bias 0.001 high
Buffington and Latimer 1926	109 – 312	Maximum deviations 0.012 high at 171 K and 0.022 low at 224 K
Keesom et al. 1926	20 – 374	Trends 0.003 high to 0.006 low
Uffelman 1930	383-573	Trends to 0.023 low
Kurnakow and Ageew 1931	293-873	Heating run trends from 0.024 high at 373 K to 0.094 low at 873 K and cooling run trends from 0.014 high at 373 K to 0.047 low at 773 K
Burger 1934	298-544	Trends to 0.035 low
Rosenbohm 1938	273-633	Trends initially 0.030 high to fall to 0.004 low
Aoyama and Ito 1939	77 – 273	Average bias 0.002 high
Esser and Eusterbrock 1941	273-1273	Trends to 0.039 low
Nix and Macnair 1941	88 – 773	Average bias 0.002 low below 293.15 K and 0.004 low above
Richards 1942	83, 301 – 1207	Trends to 0.16 high above 293.15 K
Rubin et al. 1954	15-300	Agrees to better than 0.001
Bijl and Pullan 1955	20 – 273	Trends from 0.002 high to exactly agree with selected values at 90 K and above
Beenakker and Swenson 1955	4 – 300	Average bias 0.001 low
Fieldhouse et al. 1956	352-1257	Trends to maximum deviation of 0.037 high at 1000 K and then falls to 0.016 low
Lucks and Deem 1956	293-1255	Trends from initially 0.021 low to 0.13 high
Strelkov and Novikova 1957	100-345	Trends from 0.006 low to agree with selected values above 260 K
Lucks and Deem 1958	293-1255	Trends from 0.024 low at 477 K to 0.12 high at 1255 K
Paine et al. 1959	290-1256	Trends to maximum of 0.061 high at 813 K then falls to 0.041 low at 1256 K
Sandenaw 1960	4 – 300	Trends from 0.010 low to maximum 0.010 high at 165 K
Rhodes et al. 1963	18 – 573	Average bias 0.005 low below 293.15 K trending to 0.014 high above
Leksina and Novikova 1963	90 – 1323	Agrees to within 0.001 below 293.15 K trending to 0.12 low at 1323 K
Fraser and Hollis Hallet 1965	17 – 100	Average bias 0.003 low
Nasekovskii 1967	31 – 985	Trends from 0.041 high to average 0.073 low above 800 K
Lifanov and Sherstyukov 1968	88 – 573	Agrees to within 0.001 below 293.15 K trending to 0.008 low above
Pavese et al. 1970	293-873	Trends to 0.004 high
Fitzer 1971	293-1273	Average of seven participants. Average bias 0.028 low above 573 K
Masumoto et al. 1972	115 – 673	Trends from 0.047 low to 0.23 high
Kirby and Hahn 1975, 1990	20 – 800	Agrees to better than 0.001 below 293.15 K and used in the evaluation above this temperature
Suh et al. 1988	293-1100	Scatters 0.038 to 0.008 low below 1000 K then 0.082 high at 1100 K
Astrov et al. 1989	93 – 373	Trends from initially 0.003 high
Astrov et al. 1995-1996	77 – 291	Agrees to better than 0.001
Valdiviez et al. 2003	293-1324	Trends from maximum 0.027 low at 800 K to 0.009 high at 1324 K

Table 29e. Low temperature crystallographic properties of copper

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	- 0.326	0.36032	0.25479	7.043	9022
10	0.03	- 0.326	0.36032	0.25479	7.043	9022
20	0.26	- 0.326	0.36032	0.25479	7.043	9022
30	1.00	- 0.325	0.36033	0.25479	7.043	9022
40	2.28	- 0.323	0.36033	0.25479	7.044	9022
50	3.85	- 0.320	0.36034	0.25480	7.044	9021
60	5.48	- 0.316	0.36036	0.25481	7.045	9020
70	7.00	- 0.309	0.36038	0.25483	7.047	9018
80	8.35	- 0.302	0.36041	0.25485	7.048	9016
90	9.52	- 0.293	0.36044	0.25487	7.050	9014
100	10.52	- 0.283	0.36048	0.25490	7.052	9011
110	11.36	- 0.272	0.36052	0.25492	7.055	9008
120	12.08	- 0.260	0.36056	0.25495	7.057	9005
130	12.69	- 0.248	0.36060	0.25497	7.060	9001
140	13.22	- 0.235	0.36065	0.25502	7.062	8998
150	13.67	- 0.222	0.36070	0.25505	7.065	8994
160	14.06	- 0.208	0.36075	0.25509	7.068	8990
170	14.40	- 0.193	0.36080	0.25512	7.071	8987
180	14.70	- 0.179	0.36085	0.25516	7.074	8983
190	14.97	- 0.164	0.36091	0.25520	7.077	8979
200	15.21	- 0.149	0.36096	0.25524	7.081	8975
210	15.42	- 0.134	0.36102	0.25528	7.084	8991
220	15.62	- 0.118	0.36107	0.25532	7.087	8966
230	15.80	- 0.103	0.36113	0.25536	7.091	8962
240	15.96	- 0.087	0.36119	0.25540	7.094	8958
250	16.11	- 0.071	0.36124	0.25544	7.097	8954
260	16.25	- 0.055	0.36130	0.25548	7.101	8949
270	16.38	- 0.038	0.36136	0.25552	7.104	8945
280	16.50	- 0.022	0.36142	0.25556	7.108	8940
290	16.61	- 0.005	0.36148	0.25561	7.111	8936
293.15	16.64	0	0.36150	0.25562	7.112	8935

$$d = a/\sqrt{2}$$

Table 29f. High temperature crystallographic properties of copper

T K	α x 10^6 K^{-1}	100 ε_T	*a* nm	*d* nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
293.15	16.64	0	0.36150	0.25562	7.112	8935
300	16.70	0.011	0.36154	0.25565	7.115	8931
350	17.10	0.096	0.36185	0.25586	7.133	8909
400	17.49	0.183	0.36216	0.25609	7.151	8886
450	17.85	0.271	0.36248	0.25631	7.170	8862
500	18.20	0.362	0.36281	0.25654	7.190	8838
550	18.54	0.454	0.36314	0.25678	7.210	8814
600	18.88	0.548	0.36348	0.25702	7.230	8789
650	19.22	0.644	0.36383	0.25726	7.251	8764
700	19.56	0.741	0.36418	0.25751	7.272	8739
750	19.90	0.841	0.36454	0.25777	7.293	8713
800	20.27	0.942	0.36491	0.25803	7.315	8687
850	20.64	1.045	0.36528	0.25829	7.338	8660
900	21.04	1.151	0.36566	0.25856	7.361	8673
950	21.47	1.258	0.36605	0.25884	7.384	8606
1000	21.92	1.368	0.36645	0.25912	7.408	8578
1050	22.42	1.481	0.3668/5	0.25940	7.433	8549
1100	22.95	1.596	0.36727	0.25970	7.458	8520
1150	23.52	1.714	0.36770	0.26000	7.484	8491
1200	24.14	1.835	0.36813	0.26031	7.511	8460
1250	24.81	1.960	0.36858	0.26063	7.539	8429
1300	25.54	2.088	0.36905	0.26096	7.567	8397
1350	26.32	2.220	0.36953	0.26129	7.597	8365
1357.77	26.45	2.241	0.36960	0.26135	7.601	8360

$$d = a/\sqrt{2}$$

Table 29g. Bulk properties of copper

$3\,(\varepsilon_T L - \varepsilon_T a) = \exp(3.0 - 13809/T)$ $\quad \alpha_L - \alpha_a = (4603/T^2)\exp(3.0 - 13809/T)$

T K	α x 10^6 K^{-1}	100 ε_T	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
950	21.47	1.258	7.384	8606
1000	22.01	1.369	7.408	8578
1050	22.58	1.482	7.433	8549
1100	23.22	1.598	7.459	8519
1150	23.95	1.718	7.485	8489
1200	24.79	1.842	7.513	8459
1250	25.75	1.971	7.541	8426
1300	26.87	2.104	7.571	8393
1350	28.15	2.244	7.602	8359
1357.77	28.37	2.266	7.607	8354

This Table is considered to be identical to Table 29f below 950 K.

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30 ZINC Zn

Atomic weight: 65.38 (2) (Meija 2017)

Structure: Hexagonal close packed (hP2)

The freezing point is a primary fixed point on ITS-90 at 692.677 K (Preston Thomas 1990)

30.1 Crystallographic properties

Above 293.15 K for the *a* axis length change, values derived from the lattice parameter measurements of Apostolu 1970 (319-684 K) are combined with dilatometric measurements of Gilder and Wallmark 1969 (319-683 K) where the latter are only included up to 518 K to avoid the inclusion of values affected by thermal vacancy effects, while for the *c* axis length change values derived from the lattice parameter values of Current and Gilder 1977 (293-687 K) are combined with the dilatometric measurements of Gilder and Wallmark 1969 (321-672 K) which again were limited to 518 K. On the basis $\pm 100\varepsilon_T$ the overall accuracies were ± 0.001 for the *a* axis and ± 0.004 for the *c* axis:

$$\varepsilon_T a = 1.45017 \times 10^{-5} T - 1.16837 \times 10^{-8} T^2 + 2.09734 \times 10^{-11} T^3 - 3.77548 \times 10^{-3} \quad (30a)$$

$$\varepsilon_T c = 9.20080 \times 10^{-5} T - 1.04142 \times 10^{-7} T^2 + 1.71821 \times 10^{-10} T^3 - 1.10419 \times 10^{-13} T^4 - 2.15356 \times 10^{-2} \quad (30b)$$

Below 190 K the thermal expansion coefficients of McCammon and White 1965 (4-85, 283 K), which are considered as superseding earlier measurements of White 1964, were combined with the values of Channing and Weintroub 1965b (15-270 K) with preference given to the latter measurements above 30 K. Between 190 K and 293.15 K for the *a* axis and 170 K to 293.15 K for the *c* axis, the measurements of Channing and Weintroub 1965b were adjusted in order to coincide with the selected thermal expansion values at 293.15 K derived from Equations 30a and 30b. The adjusted values were then fitted to the following equations over temperature range 15 K to 293.15 K:

$$\alpha_a (K^{-1}) = 1.17784 \times 10^{-7} T + 1.41706 \times 10^{-10} T^2 - 1.98817 \times 10^{-12} T^3 + 3.33709 \times 10^{-15} T^4 - 8.20701 \times 10^{-6} \quad (30c)$$

$$\alpha_c (K^{-1}) = 1.31065 \times 10^{-8} T - 1.62597 \times 10^{-12} T^2 - 3.87491 \times 10^{-13} T^3 + 6.95215 \times 10^{-16} T^4 + 6.50422 \times 10^{-5} \quad (30d)$$

Experimental values determined by McCammon and White 1965 at 283 K as $\alpha_a = 12.9 \times 10^{-6} K^{-1}$ and $\alpha_c = 64.5 \times 10^{-6} K^{-1}$ agree with the selected values.

On the basis $100\Delta\varepsilon$, in the low temperature region dilatometric measurements of Grüneisen and Goens 1924 (58-373 K) show a bias of only 0.001 high along the *a* axis and an initial value of 0.012 high along the *c* axis then trending to agree with the selected values while the dilatometric measurements of Meyerhoff and Smith 1962 (0-273 K) are initially 0.010 high along the *a* axis reaching a maximum of 0.017 high at 65 K while for

the *c* axis the initial value is 0.081 high and reaches a maximum of 0.094 high at 30 K. In the high temperature region length changes derived from the lattice parameter measurements of Owen and Yates 1934 (290-688 K) trend to 0.016 high along the *a* axis and 0.071 low along the *c* axis while values derived from the equations of Pathak and Desai 1980 (273-688 K) trend to only 0.010 high along the *a* axis and with a maximum deviation of only 0.010 low at 623 K along the *c* axis. Along the *a* axis at low temperatures, measurements of Nuss et al. 2010 (40-500 K) are initially 0.022 high then generally trend to agree with the selected values while in the high temperature region the trend is to 0.058 low. For the *c* axis the values show scatter from 0.055 low to 0.065 high in the low temperature region and from 0.062 low to 0.029 high in the high temperature region.

Table 30a. Lattice parameter values of zinc at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Notes
Boas 1932	293	0.26639	0.49456	a
Stenzel and Weerts 1932	293	0.26645	0.49454	b
Owen and Yates 1934	293	0.26644	0.49452	c
Jette and Foote 1935	298	0.26648	0.49455	
Owen et al. 1935	291	0.26647	0.49462	
Ancker 1953	295.2	0.26648	0.49458	
Brown 1954-1955	298	0.26647	0.49456	
Current and Gilder 1977	319.4, 321.1	0.26644	0.49453	
Balzer and Sigvaldason 1979	296.3	0.26648	0.49449	
Pathak and Desai 1980	293	0.26644	0.49453	d
Nuss et al. 2010	293	0.26634	0.49435	e ,f
	Selected	0.26646 (2)	0.49455 (4)	

Notes for Table 30a

a. *a* axis value not included in the average

b. Also Hansen and Stenzel 1933

c. From fit 290 - 296 K

d. Calculated from equations

e. From fit 260 – 300 K

f. Not included in the average

At 293.15 K: Density 7140 (3) kg m^{-3} Molar volume 9.156 (2) cm^3 mol^{-1}

30.2 Bulk properties of zinc

The following values have been determined for the vacancy concentration parameter (c_V), the enthalpy of vacancy formation (H_V) and the entropy of vacancy formation (S_V/k). The value of McKee et al. 1972 was obtained by positron annihilation and the other two values by equating dilatometric and lattice parameter length change values.

Table 30b. Thermal vacancy parameters for zinc

References	c_V	H_V eV	S_V/k
McKee et al. 1972	-	0.54 (2)	-
Current and Guilder 1977	3.0 (1.0) x 10^{-4}	0.52 (5)	0.5 (3)
Balzer and Sigvaldason 1979	4.9 (3) x 10^{-4}	0.53 (7)	1.1 (1.0)
Selected	3.0 x 10^{-4}	0.52	0.6

After adjustment the measurements of Current and Gilder 1977 were selected to be consistent with values selected for the crystallographic values.

Table 30c. Bulk properties of zinc

3 ($\varepsilon_T L - \varepsilon_T$ avr) = exp (0.6 - 6034/ T) $\alpha_L - \alpha_{avr} = (2011.3/ T^2) \exp (0.6 - 6034/ T)$

T K	α x 10^6 K^{-1}	$100\varepsilon_T$	Molar Volume $cm^3\ mol^{-1}$	Density kg m^{-3}
500	32.57	0.645	9.335	7004
525	33.13	0.729	9.358	6986
550	33.59	0.813	9.382	6969
575	34.05	0.899	9.405	6951
600	34.49	0.985	9.430	6933
625	34.90	1.073	9.454	6915
650	35.29	1.162	9.479	6897
675	35.62	1.252	9.505	6879
692.677	35.83	1.316	9.523	6866

This Table is assumed to be identical to Tables 30d and 30e below 500 K

Table 30d. Crystallographic properties of zinc

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
0	0	0	0	- 0.180	- 1.680	- 0.680
5	0	0.05	0.02	- 0.180	- 1.680	- 0.680
10	-0.06	0.76	0.21	- 0.180	- 1.679	- 0.680
15	-0.73	5.00	1.18	- 0.180	- 1.678	- 0.680
20	-1.98	13.50	3.18	- 0.181	- 1.674	- 0.679
25	-3.38	23.10	5.45	- 0.182	- 1.665	- 0.677
30	- 4.45	32.90	8.00	- 0.184	- 1.651	- 0.673
40	- 4.20	45.40	12.33	- 0.189	- 1.612	- 0.663
50	- 3.00	54.10	16.03	- 0.193	- 1.563	- 0.649
60	- 1.50	59.60	18.87	- 0.195	- 1.506	- 0.632
70	0	62.60	20.86	- 0.196	- 1.446	- 0.612
80	1.60	64.10	22.43	- 0.195	- 1.383	- 0.591
90	2.90	64.90	23.57	- 0.193	- 1.320	- 0.568
100	4.10	65.40	24.53	- 0.189	- 1.255	- 0.544
110	5.10	65.70	25.30	- 0.184	- 1.191	- 0.520
120	6.00	65.90	25.97	- 0.179	- 1.125	- 0.494
130	6.80	66.00	26.53	- 0.172	- 1.060	- 0.468
140	7.49	66.03	27.00	- 0.165	- 0.995	- 0.442
150	8.10	66.00	27.40	- 0.158	- 0.930	- 0.414
160	8.68	65.96	27.77	- 0.149	- 0.864	- 0.388
170	9.20	65.90	28.10	- 0.140	- 0.799	- 0.360
180	9.62	65.82	28.35	- 0.131	- 0.733	- 0.332
190	10.00	65.72	28.57	- 0.121	- 0.668	- 0.303
200	10.45	65.61	28.84	- 0.111	- 0.603	- 0.274
210	10.85	65.49	29.06	- 0.100	- 0.538	- 0.246
220	11.21	65.35	29.26	- 0.089	- 0.473	- 0.217
230	11.53	65.20	29.42	- 0.077	- 0.408	- 0.188
240	11.81	65.04	29.55	- 0.066	- 0.343	- 0.158
250	12.07	64.88	29.67	- 0.054	- 0.278	- 0.129
260	12.30	64.71	29.77	- 0.042	- 0.213	- 0.099
270	12.53	64.53	29.86	- 0.030	- 0.149	- 0.069
280	12.75	64.35	29.95	- 0.017	- 0.084	- 0.039
290	12.98	64.17	30.04	- 0.004	- 0.020	- 0.009
293.15	13.06	64.12	30.08	0	0	0
300	13.15	63.96	30.09	0.009	0.044	0.021
325	13.55	63.47	30.19	0.042	0.203	0.096
350	14.02	63.09	30.38	0.077	0.362	0.172
375	14.57	62.77	30.64	0.113	0.520	0.248
400	15.20	62.48	30.96	0.150	0.677	0.326
425	15.91	62.17	31.33	0.189	0.834	0.404
450	16.69	61.80	31.73	0.230	0.991	0.483
475	17.55	61.34	32.15	0.272	1.146	0.564
500	18.49	60.73	32.57	0.318	1.301	0.645
525	19.50	59.95	32.99	0.365	1.454	0.728
550	20.60	58.95	33.38	0.416	1.605	0.812
575	21.77	57.69	33.74	0.469	1.753	0.897
600	23.01	56.14	34.05	0.525	1.898	0.983
625	24.33	54.25	34.30	0.584	2.039	1.069
650	25.73	51.98	34.48	0.647	2.175	1.156
675	27.20	49.30	34.57	0.714	2.304	1.244
692.677	28.29	47.14	34.57	0.763	2.391	1.306

Table 30e. Crystallographic properties of zinc

T K	*a* nm	*c* nm	*c*/*a*	*d*2 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.26598	0.48624	1.8281	0.28756	8.970	7288
5	0.26598	0.48624	1.8281	0.28756	8.970	7288
10	0.26598	0.48624	1.8281	0.28756	8.970	7288
15	0.26598	0.48625	1.8281	0.28756	8.970	7288
20	0.26598	0.48627	1.8282	0.28757	8.971	7288
25	0.26597	0.48631	1.8284	0.28759	8.971	7288
30	0.26597	0.48638	1.8287	0.28762	8.972	7287
40	0.26596	0.48658	1.8295	0.28769	8.975	7285
50	0.26595	0.48682	1.8305	0.28779	8.979	7282
60	0.26594	0.48710	1.8316	0.28791	8.984	7278
70	0.26594	0.48740	1.8327	0.28804	8.989	7273
80	0.26594	0.48771	1.8339	0.28817	8.995	7269
90	0.26595	0.48802	1.8350	0.28830	9.001	7264
100	0.26596	0.48834	1.8362	0.28844	9.007	7258
110	0.26597	0.48866	1.8373	0.28858	9.014	7253
120	0.26598	0.48898	1.8384	0.28872	9.021	7247
130	0.26600	0.48931	1.8395	0.28886	9.028	7242
140	0.26602	0.48963	1.8406	0.28900	9.035	7236
150	0.26604	0.48995	1.8416	0.28915	9.043	7230
160	0.26606	0.49028	1.8427	0.28929	9.050	7224
170	0.26609	0.49060	1.8438	0.28944	9.058	7218
180	0.26611	0.49092	1.8448	0.28958	9.066	7212
190	0.26614	0.49125	1.8458	0.28972	9.073	7206
200	0.26616	0.49157	1.8469	0.28987	9.081	7200
210	0.26619	0.49189	1.8479	0.29002	9.089	7193
220	0.26622	0.49221	1.8489	0.29016	9.097	7187
230	0.26625	0.49253	1.8499	0.29031	9.105	7181
240	0.26628	0.49286	1.8509	0.29045	9.113	7174
250	0.26632	0.49318	1.8518	0.29060	9.121	7168
260	0.26635	0.49350	1.8528	0.29074	9.129	7162
270	0.26638	0.49381	1.8538	0.29089	9.137	7155
280	0.26641	0.49413	1.8547	0.29103	9.146	7149
290	0.26645	0.49445	1.8557	0.29118	9.154	7142
293.15	0.26646	0.49455	1.8560	0.29122	9.156	7140
300	0.26648	0.49477	1.8566	0.29132	9.162	7136
325	0.26657	0.49556	1.8590	0.29169	9.183	7120
350	0.26666	0.49634	1.8613	0.29205	9.204	7104
375	0.26676	0.49712	1.8636	0.29241	9.225	7087
400	0.26686	0.49790	1.8658	0.29277	9.246	7071
425	0.26696	0.49868	1.8680	0.29313	9.268	7055
450	0.26707	0.49945	1.8701	0.29349	9.290	7038
475	0.26719	0.50022	1.8722	0.29386	9.312	7021
500	0.26731	0.50098	1.8742	0.29422	9.335	7004
525	0.26743	0.50174	1.8761	0.29458	9.358	6987
550	0.26757	0.50249	1.8780	0.29494	9.381	6970
575	0.26771	0.50322	1.8797	0.29529	9.404	6952
600	0.26786	0.50394	1.8814	0.29564	9.428	6934
625	0.26802	0.50463	1.8828	0.29599	9.453	6917
650	0.26819	0.50530	1.8842	0.29632	9.477	6899
675	0.26836	0.50594	1.8853	0.29665	9.502	6881
692.677	0.26849	0.50638	1.8860	0.29687	9.519	6868

Interatomic distance calculations for Table 30e: $d1 = a$ $d2 = (a^2/3 + c^2/4)^{1/2}$

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31 GALLIUM Ga

Atomic Weight: 69.723 (1) (Meija 2017)

Structure: Orthorhombic (oS8)

The melting point is a primary fixed point on ITS-90 at 302.9146 K (Preston-Thomas 1990) and the triple point is a secondary fixed point at 302.9166 (1) K (Bedford et al. 1996).

31.1 Higher temperature crystallographic properties of gallium

Much confusion exists in the literature as to the lattice parameter sequencing but Donohue 1974 has shown that for the correct space group D^{18}_{2h} Cmca that the sequence is $a < c < b$ and all values have been adjusted on this basis including the room temperature value for the thermal expansion coefficients determined either dilatometrically (D) or by X-ray diffraction (X). The measurements of Geshko et al. 1972 were only shown graphically with values being estimated by Mair et al. 1976.

Table 31a. Thermal expansion coefficients of gallium in the room temperature region

References	Method	Temperature Range K	$\alpha_a \times 10^6$ K^{-1}	$\alpha_b \times 10^6$ K^{-1}	$\alpha_c \times 10^6$ K^{-1}
Powell 1951	D	273-293	31.5	16.5	11.5
Geshko et al. 1972	D	RT	34.5	17.8	9.3
Mair et al. 1976	D	283-302.9	33.8	18.5	11.2
	X	283-302.9	31.9	16.2	13.3

Above 100 K length change values of Powell 1951 (93-293 K) were adjusted to correspond to the X-ray diffraction thermal expansion coefficients of Mair et al. 1976. The corrected values can be represented by the following equations. Because of the relatively low accuracies of the measurements of Powell 1951 then the derived thermal expansion coefficients are considered to be only of nominal quality:

$$\varepsilon_T a = -4.42133 \times 10^{-5} T + 4.64333 \times 10^{-7} T^2 - 1.25507 \times 10^{-9} T^3 + 1.26718 \times 10^{-12} T^4 - 4.68236 \times 10^{-3} \quad (31a)$$

$$\varepsilon_T b = 5.90588 \times 10^{-6} T + 2.60371 \times 10^{-8} T^2 + 1.99573 \times 10^{-11} T^3 - 1.02511 \times 10^{-13} T^4 - 3.71457 \times 10^{-3} \quad (31b)$$

$$\varepsilon_T c = 1.68057 \times 10^{-5} T - 9.55523 \times 10^{-8} T^2 + 4.00455 \times 10^{-10} T^3 - 5.02683 \times 10^{-13} T^4 - 3.09115 \times 10^{-3} \quad (31c)$$

Above 210 K for the *a* axis, 240 K for the *b* axis and 280 K for the *c* axis thermal expansion coefficients are considered to be constant at 31.9×10^{-6} K^{-1}, 16.2×10^{-6} K^{-1} and 13.3×10^{-6} K^{-1} respectively.

Table 31b. Lattice parameters of gallium at 293.15 K

References	Original Temperature K	*a* nm	*b* nm	*c* nm	Note
Bradley 1935	RT	0.45201	0.76607	0.45261	
Swanson and Fuyat 1953	298	0.45223	0.76609	0.45232	a
Barrett 1962	297	0.45194	0.76633	0.45260	
Barrett and Spooner 1965	297	0.45183	0.76570	0.45258	
Haemmerle and Lastovka 1977	298.0	0.452052	0.766251	0.452664	
	Selected	0.45205	0.76625	0.45266	

Note for Table 31b

a. As recalculated by Barrett 1962 from 19 lines.

At 293.15 K: Density 5907 (1) kg m^{-3} Molar volume 11.803(1) cm^3 mol^{-1}

The very high precision values of Haemmerle and Lastovka 1977 are selected with assigned accuracies of ± 0.0001 nm and takes into account the inaccuracies in the thermal expansion coefficients and the fact that no calibrating wavelength standards were reported. However, because of the large spread in the lattice parameter values then the selected values of density and molar volume at 293.15 K are given a nominal accuracy.

Donohue 1974 selected the room temperature positional parameters $y = 0.1539$ (13) and $z = 0.0798$ (11). Based on the equations for calculating inter atomic distances as given below then a gallium atom at (0yz) has one neighbor at 0.2467 (20) nm (d1), two at 0.2700 (10) nm (d2), two at 0.2736 (5) nm (d3) and one at 0.2793 (11) nm (d4)

Calculation of interatomic distance in gallium

$$d1 = [\,(2yb)^2 + (2zc)^2\,]^{½} \qquad d2 = [\,(½ - 2y)^2 b^2 + c^2/4\,]^{½}$$

$$d3 = [\,a^2/4 + (½ - 2z)^2 c^2\,]^{½} \qquad d4 = [\,a^2/4 + (½ - 2y)^2 b^2 + (2zc)^2\,]^{½}$$

31.2 Low temperature crystallographic properties of gallium

Lattice parameter values determined by Barrett 1962 at 2.35 K and 4.2 K do not agree with each other but based on a preliminary evaluation then the values at 4.2 K are preferred. In order to preserve the integrity in these values they were compared directly with the selected values at 293.15 K and on the basis of $100\varepsilon_T$ lead to – 0.661 along the a axis, – 0.382 along the b axis and – 0.238 along the c axis. In the absence of other criteria these values were combined with selected values 100 K to 150 K and fitted to the following equations using the smooth enthalpy values of Amitin et al. 1984 (5-320 K). However, it was found for the b axis that spurious values were obtained for the derived thermal expansion coefficients and therefore a value of – 0.348 was chosen instead

because this gave a minimum in the standard deviation of the fit. All values below 100 K are therefore considered to be highly tentative, especially the derived thermal expansion coefficients:

$$\ln(L_a) = (H_T - H_0)\,(-4.12538 \times 10^{-7} + 6.12119 \times 10^{-9}\,T + 8.62890 \times 10^{-5}/\,T) - 6.63128 \times 10^{-3} \quad (31d)$$

$$\ln(L_b) = (H_T - H_0)\,(4.52135 \times 10^{-7} + 5.10621 \times 10^{-10}\,T + 1.48939 \times 10^{-5}/\,T) - 3.48615 \times 10^{-3} \quad (31e)$$

$$\ln(L_c) = (H_T - H_0)\,(4.94171 \times 10^{-7} - 4.72303 \times 10^{-10}\,T - 6.52377 \times 10^{-6}/\,T) - 2.38483 \times 10^{-3} \quad (31f)$$

31.3 The orthorhombic asymmetry of gallium

The close agreement between the *a* and *c* lattice parameter values led Barrett 1962 to confuse the lattice parameter sequences at low temperature and at 297 K. However, Haemmerle and Lastovka 1977 carried out precision strain-gauge measurements over the temperature range 190 K to 300 K which distinguished the lattice parameter difference as given in the present format as $\varepsilon_{ca} = 2\,[c\,(T) - a\,(T)] / [c\,(T) + a\,(T)]$. At 293.15 K the difference is 1.353×10^{-3} which is in excellent agreement with a value of 1.357×10^{-3} as an average of values derived from equations (7) and (8) of Haemmerle and Lastovka 1977, while extrapolated to 0 K the difference is 5.60×10^{-3} whereas based on unpublished measurements and literature values Haemmerle and Lastovka 1977 select 5.75×10^{-3}.

31.4 The quality of the selected lattice parameter values at 293.15 K

Table 31b shows marked differences between the various determinations of the lattice parameters, and the values selected are based entirely on the high precision values obtained by Haemmerle and Lastovka 1977. An independent check on the quality of these measurements can be obtained from precision determinations of the density of liquid gallium and an estimate of the volume change on transition from the Clausius-Clapeyron equation. Liquid density values of Basin and Solev'ev 1967 and Mathiak et al. 1983 agree closely and can be averaged to a molar volume of 11.438 (1) $cm^3\,mol^{-1}$ at the melting point. Magnum and Thornton 1979 determined the initial slope of the melting curve to be – 0.01985 (1) K MPa^{-1}, while Archer 2002 determined the enthalpy of fusion to be 5585 (2) J mol^{-1}, which leads to a molar volume change at the melting point of 0.3660 (2) $cm^3\,mol^{-1}$ and a molar volume for the solid at the melting point of 11.804 (1) $cm^3\,mol^{-1}$. Mair et al. 1976 showed that thermal vacancy effects were negligible so the above value could be applied equally to both crystallographic and bulk properties. Extrapolation to 293.15 K leads to 11.797 (1) $cm^3\,mol^{-1}$ which compares favorably to the selected value of 11.803 (1) $cm^3\,mol^{-1}$, obtained from the measurements of Haemmerle and Lastovka 1977.

Table 31c. Crystallographic properties of gallium

All values below 100 K are considered to be tentative.

T K	α_a x 10^6 K^{-1}	α_b x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 ε_T *a*	100 ε_T *b*	100 ε_T *c*	100 ε_T avr
0	0	0	0	0	- 0.661	- 0.348	- 0.238	- 0.416
10	1.5	0.4	0	0.2	- 0.661	- 0.348	- 0.238	- 0.416
20	6.5	2.2	0.5	3.1	- 0.656	- 0.347	- 0.238	- 0.414
30	9.0	4.1	1.6	4.9	- 0.648	- 0.343	- 0.237	- 0.410
40	10.2	5.6	2.9	6.2	- 0.639	- 0.339	- 0.235	- 0.404
50	11.1	7.0	4.0	7.3	- 0.628	- 0.332	- 0.231	- 0.397
60	11.9	8.1	5.0	8.3	- 0.617	- 0.325	- 0.227	- 0.390
70	13.0	9.1	5.8	9.3	- 0.604	- 0.316	- 0.221	- 0.381
80	14.2	9.9	6.4	10.2	- 0.591	- 0.307	- 0.215	- 0.371
90	15.7	10.6	6.9	11.1	- 0.576	- 0.296	- 0.209	- 0.360
100	17.5	11.3	7.3	12.0	- 0.559	- 0.285	- 0.202	- 0.349
110	19.4	11.8	7.6	12.9	- 0.541	- 0.274	- 0.194	- 0.336
120	21.9	12.3	7.7	14.0	- 0.521	- 0.262	- 0.186	- 0.323
130	24.1	12.8	7.9	14.9	- 0.498	- 0.249	- 0.179	- 0.309
140	26.0	13.3	8.1	15.8	- 0.473	- 0.236	- 0.171	- 0.293
150	27.6	13.7	8.4	16.6	- 0.446	- 0.223	- 0.162	- 0.277
160	28.9	14.1	8.8	17.3	- 0.418	- 0.209	- 0.154	- 0.260
170	29.9	14.5	9.2	17.8	- 0.389	- 0.195	- 0.145	- 0.243
180	30.6	14.9	9.6	18.4	- 0.359	- 0.180	- 0.135	- 0.225
190	31.2	15.2	10.1	19.1	- 0.328	- 0.165	- 0.126	- 0.196
200	31.6	15.5	10.6	19.3	- 0.296	- 0.150	- 0.115	- 0.187
210	31.8	15.7	11.0	19.5	- 0.265	- 0.134	- 0.104	- 0.168
220	31.9	15.9	11.5	19.8	- 0.233	- 0.118	- 0.093	- 0.148
230	31.9	16.1	11.9	20.0	- 0.201	- 0.102	- 0.081	- 0.128
240	31.9	16.2	12.4	20.2	- 0.169	- 0.086	- 0.069	- 0.108
250	31.9	16.2	12.7	20.3	- 0.138	- 0.070	- 0.057	- 0.088
260	31.9	16.2	13.0	20.4	- 0.106	- 0.054	- 0.044	- 0.068
270	31.9	16.2	13.2	20.4	- 0.074	- 0.037	- 0.031	- 0.047
280	31.9	16.2	13.3	20.5	- 0.042	- 0.021	- 0.018	- 0.027
290	31.9	16.2	13.3	20.5	- 0.010	- 0.005	- 0.004	- 0.006
293.15	31.9	16.2	13.3	20.5	0	0	0	0
300	31.9	16.2	13.3	20.5	0.022	0.011	0.009	0.014
302.915	31.9	16.2	13.3	20.5	0.031	0.016	0.013	0.020

Table 31d. Crystallographic properties of gallium

All values below 100 K are considered to be tentative.

T K	*a* nm	*b* nm	*c* nm	$10^3 \varepsilon_{ca}$	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.44906	0.76358	0.45159	5.60	11.656	5981
10	0.44907	0.76359	0.45159	5.59	11.657	5981
20	0.44908	0.76360	0.45159	5.56	11.657	5981
30	0.44912	0.76362	0.45159	5.49	11.659	5980
40	0.44916	0.76366	0.45160	5.41	11.661	5979
50	0.44921	0.76371	0.45162	5.34	11.663	5978
60	0.44926	0.76376	0.45164	5.27	11.666	5977
70	0.44932	0.76383	0.45166	5.20	11.669	5975
80	0.44938	0.76390	0.45169	5.12	11.672	5973
90	0.44945	0.76398	0.45172	5.04	11.676	5971
100	0.44952	0.76406	0.45175	4.94	11.680	5969
110	0.44961	0.76415	0.45179	4.83	11.684	5967
120	0.44970	0.76424	0.45182	4.71	11.689	5965
130	0.44980	0.76434	0.45186	4.56	11.694	5962
140	0.44991	0.76444	0.45189	4.39	11.700	5959
150	0.45004	0.76454	0.45193	4.20	11.705	5957
160	0.45016	0.76465	0.45197	4.00	11.711	5954
170	0.45029	0.76476	0.45201	3.80	11.717	5950
180	0.45043	0.76487	0.45205	3.59	11.724	5947
190	0.45057	0.76499	0.45210	3.38	11.730	5944
200	0.45071	0.76510	0.45214	3.17	11.737	5940
210	0.45085	0.76522	0.45219	2.96	11.744	5937
220	0.45100	0.76534	0.45224	2.75	11.751	5934
230	0.45114	0.76547	0.45230	2.55	11.758	5930
240	0.45129	0.76559	0.45235	2.36	11.765	5926
250	0.45143	0.76572	0.45241	2.16	11.772	5923
260	0.45157	0.76584	0.45246	1.97	11.779	5919
270	0.45172	0.76596	0.45252	1.78	11.786	5916
280	0.45186	0.76609	0.45258	1.60	11.794	5912
290	0.45201	0.76621	0.45264	1.41	11.801	5908
293.15	0.45205	0.76625	0.45266	1.35	11.803	5907
300	0.45215	0.76634	0.45271	1.22	11.808	5905
302.9146	0.45219	0.76637	0.45272	1.17	11.810	5904

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32 GERMANIUM Ge

Atomic weight: 72.630 (8) (Meija 2017)

Selecting a lattice parameter of 0.565790 (2) at 298.15 from the present evaluation and a density value of 5326.73 (5) kg m^{-3} as determined by Smakula et al. 1955 and Smakula and Kalnajs 1957 leads to an atomic weight of 72.625 (1), which is used as a "working value" for calculating density values in Tables 32d and 32e.

Structure: Cubic (cF8)

The melting point selected by Gurvich et al. 1991 corrects to 1211.4 K on ITS-90.

32.1 Low temperature

Up to 130 K thermal expansion coefficient measurements of Carr et al. 1965 (8-130 K), Sparks and Swenson 1967 (2-34 K), White 1974 (3-34 K) and Smith and White 1975 (4-30, 283 K) were combined. These suggested a maximum negative value in the thermal expansion coefficient of -6.7×10^{-8} K^{-1} at 31 K and also suggested that the two values selected by Touloukian et al. at 25 K and 50 K were incorrect. Above 130 K the thermal expansion coefficients of Novikova 1960 (25-349 K), Zhdanova 1963 (85-337 K), and Zhdanova and Kontorova 1965 (81-341 K) were only shown graphically with actual data points given by Touloukian et al. 1975. These showed marked scatter and therefore the equation given by Touloukian et al. 1975 to represent thermal expansion from 100 K to 293 K was accepted because it gave derived thermal expansion coefficients which showed a smooth continuity with the values selected at 130 K and below. Lattice parameter measurements of Bhalla and White 1971 (298-314 K) lead to a thermal expansion coefficient of 5.72×10^{-6} K^{-1} in reasonable agreement with the selected values. Thermal expansion coefficients of Novikova 1960 and Browder and Ballard 1977 (80-300 K) were integrated and the derived length change values and other values obtained in the low temperature region are compared with selected values in Part 32.4.

32.2 High temperature

Dilatometric measurements of Zhdanova et al. 1967 (289-1067 K), Janot et al. 1968 (323-1198 K) and Feder and Light (3-634 K) were combined which on the basis $\pm 100\varepsilon_T$ give an equation accurate to ± 0.001:

$$\varepsilon_T = 4.47951 \times 10^{-6} T + 2.50782 \times 10^{-9} T^2 - 6.20017 \times 10^{-13} T^3 - 1.51306 \times 10^{-3} \quad (32a)$$

The measurements of Zhdanova 1967 were only shown graphically with actual data points given by Touloukian et al. 1975. For statistical reasons the value at 1067 K was not included in the evaluation. Lattice parameter measurements of Dimukes et al. 1964 (293-973 K) and dilatometric measurements of Dolivo-Dobrovol'skaya et al. 1973 (293-1023 K) were only shown graphically. Dilatometric measurements of Fine 1953 (98-548

K) were also only shown graphically with actual data points given by Touloukian et al. 1975. These and other values in the high temperature region are compared with selected values in Part 32.4.

32.3 Lattice parameter value of germanium

Table 32a. Medium and high precision lattice parameter of germanium at 293.15 K

References	Original Temperature K	*a* nm
Straumanis and Aka 1950	RT	0.565775
Straumanis and Aka 1952	293	0.565775
Greiner 1952	298	0.56577
Swanson and Tatge 1953	298	0.56578
Smakula and Kalnajs 1955, 1957	298	0.565768
Mack 1958	293	0.565767
Potts et al. 1963	298	0.565782
Dismukes et al. 1964	298	0.56577
Batchelder and Simmons 1965	298	0.565785
Kiendl and Witt 1966, Witt 1967	296	0.565742
Holloway et al. 1991	298	0.565768
	Average	0.56577 (1)

Table 32b. Ultra high precision lattice parameter of germanium at 293.15 K

References	Original Temperature K	*a* nm
Cooper 1962	297.8	0.5657727
Baker and Hart 1975	295.7, 298.2	0.5657718
Hom et al. 1975	298.2	0.5657770
Deslattes et al. 1980	295.7	0.5657740
	Selected	0.565774 (2)

At 293.15 K: Density 5327.2 (1) kg m^{-3} ; Molar volume 13.6330 (1) cm^3 mol^{-1}

32.4 Deviations of experimental values from the selected values

Table 32c. Dilatometric values

References	Temperature Range K	Deviations $100\Delta\varepsilon$
Fine 1953	98-548	Average bias 0.003 low below room temperature then trending to 0.010 low above room temperature
Gibbons 1958	40-300	Trends from initially 0.003 low to converge to the selected values
Novikova 1960	25-349	Agrees with selected values to within 0.001 over the whole temperature range
Nasekovskii 1967	71-700	Trends 0.011 high to 0.006 low
Browder and Ballard 1977	80-300	Initially 0.002 low then agrees to better than 0.001 above 160 K

Table 32d. Lattice parameter values

References	Temperature Range K	Deviations 100Δε
Nitka 1937	20-1113	Above room temperature trends 0.022 low to 0.012 high
Shaw and Liu 1964	291-1163	Trends from 0.013 low to 0.054 high
Singh 1968	293-1085	Trends to 0.039 high

32.5 A comparision with previous evaluations in the high temperature region

Although Touloukian et al. 1975 used the same data sources as used here they misinterpreted the measurements of Janot et al. 1968 in that the zero baseline was 298.15 K so that on the basis 100Δε the correction to the tabulated values should have been an increase of 0.003 and not a decrease of 0.005. As a result the selected values differ by up to 0.004 low above 800 K compared to the present values. Reeber and Wang 1996b appear to have not included the important measurements of Janot et al. 1968 and relied only on the measurements of Zhdanova et al. 1967 in the very high temperature region. As a result, their values differ as 0.003 high at 700 K trending to 0.007 low at 1200 K.

Table 32e. Low temperature crystallographic properties of germanium

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d*1 nm	*d*2 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	- 0.0946	0.56524	0.24476	0.39968	13.594	5342
5	0.0010	- 0.0946	0.56524	0.24476	0.39968	13.594	5342
10	0.0050	- 0.0946	0.56524	0.24476	0.39968	13.594	5342
15	- 0.0003	- 0.0946	0.56524	0.24476	0.39968	13.594	5342
20	- 0.023	- 0.0946	0.56524	0.24476	0.39968	13.594	5342
25	- 0.050	- 0.0946	0.56524	0.24476	0.39968	13.594	5342
30	- 0.066	- 0.0946	0.56524	0.24476	0.39968	13.594	5342
35	- 0.060	- 0.0946	0.56524	0.24476	0.39968	13.594	5342
40	- 0.023	- 0.0947	0.56524	0.24476	0.39968	13.594	5342
50	0.165	- 0.0946	0.56524	0.24476	0.39968	13.594	5342
60	0.51	- 0.0943	0.56524	0.24476	0.39969	13.594	5342
70	0.93	- 0.0936	0.56524	0.24476	0.39969	13.595	5342
80	1.38	- 0.0924	0.56525	0.24476	0.39969	13.595	5342
90	1.84	- 0.0908	0.56526	0.24476	0.39970	13.596	5342
100	2.28	- 0.0888	0.56527	0.24477	0.39971	13.597	5341
110	2.69	- 0.0863	0.56529	0.24478	0.39972	13.598	5341
120	3.07	- 0.0834	0.56530	0.24478	0.39973	13.599	5341
130	3.41	- 0.0801	0.56532	0.24479	0.39974	13.600	5340
140	3.69	- 0.0766	0.56534	0.24480	0.39976	13.602	5339
150	3.93	- 0.0728	0.56536	0.24481	0.39977	13.603	5339
160	4.14	- 0.0688	0.56538	0.24482	0.39979	13.605	5338
170	4.35	- 0.0645	0.56541	0.24483	0.39980	13.607	5337
180	4.54	- 0.0601	0.56543	0.24484	0.39982	13.608	5337
190	4.72	- 0.0554	0.56546	0.24485	0.39984	13.610	5336
200	4.89	- 0.0506	0.56549	0.24486	0.39986	13.612	5335
210	5.04	- 0.0457	0.56551	0.24488	0.39988	13.614	5334
220	5.18	- 0.0406	0.56554	0.24489	0.39990	13.616	5334
230	5.31	- 0.0353	0.56557	0.24490	0.39992	13.619	5333
240	5.42	- 0.0300	0.56560	0.24491	0.39994	13.621	5332
250	5.52	- 0.0245	0.56564	0.24493	0.39996	13.623	5331
260	5.60	- 0.0189	0.56567	0.24494	0.39999	13.625	5330
270	5.68	- 0.0133	0.56570	0.24495	0.40001	13.628	5329
280	5.73	- 0.0076	0.56573	0.24497	0.40003	13.630	5328
290	5.78	- 0.0018	0.56576	0.24498	0.40006	13.632	5327
293.15	5.79	0	0.56577	0.24499	0.40006	13.633	5327

$$d1 = \sqrt{3}a/4 \qquad d2 = a/\sqrt{2}$$

Table 32f. High temperature crystallographic properties of germanium

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d*1 nm	*d*2 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
293.15	5.79	0	0.56577	0.24499	0.40006	13.633	5327
300	5.82	0.004	0.56580	0.24500	0.40008	13.635	5327
350	6.01	0.034	0.56596	0.24507	0.40020	13.647	5322
400	6.18	0.064	0.56614	0.24514	0.40032	13.659	5317
450	6.35	0.095	0.56631	0.24522	0.40044	13.672	5312
500	6.51	0.128	0.56650	0.24530	0.40057	13.685	5307
550	6.66	0.161	0.56668	0.24538	0.40071	13.699	5302
600	6.81	0.194	0.56687	0.24546	0.40084	13.713	5296
650	6.94	0.229	0.56707	0.24555	0.40098	13.727	5291
700	7.06	0.264	0.56727	0.24563	0.40112	13.741	5285
750	7.17	0.300	0.56747	0.24572	0.40126	13.756	5280
800	7.28	0.336	0.56767	0.24581	0.40141	13.771	5274
850	7.37	0.373	0.56788	0.24590	0.40155	13.786	5268
900	7.46	0.410	0.56809	0.24599	0.40170	13.801	5262
950	7.53	0.447	0.56831	0.24608	0.40185	13.817	5256
1000	7.60	0.485	0.56852	0.24618	0.40200	13.832	5250
1050	7.66	0.524	0.56874	0.24627	0.40216	13.848	5244
1100	7.70	0.562	0.56896	0.24637	0.40231	13.864	5238
1150	7.74	0.601	0.56918	0.24646	0.40247	13.880	5232
1200	7.77	0.640	0.56940	0.24656	0.40262	13.896	5226
1211.4	7.78	0.649	0.56945	0.24658	0.40266	13.900	5225

$$d1 = \sqrt{3}a/4 \qquad d2 = a/\sqrt{2}$$

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33 ARSENIC As

Atomic weight: 74.921595 (6) (Meija 2017)

Structure: Rhombohedral (hR2)

Gocken 1989 selects 887 (1) K for the sublimation temperature and 1090 (1) K for the melting point at a pressure of 36.3 bar. It is noted that Brebrick 1999 suggests a much higher melting point pressure at 39.42 bar.

Thermal expansion coefficients of White 1972 (2-85, 283 K) were accepted up to 85 K. Above 293.15 K lattice parameter measurements were determined by Taylor et al. 1965 (296-677 K), Pawar and Deshpande 1970 (301-559 K) and Klemm et al. 1960 (273-750 K) where the latter measurements were only shown graphically with actual values given by Touloukian et al. 1977. Derived length change values show marked scatter and on these grounds the equations given by Touloukian et al. 1977, to represent thermal expansion above 293.15 K, were accepted except for an adjustment to pass through zero at this temperature:

$$\varepsilon_T\, a = 1.22000 \times 10^{-5}\, T - 1.93000 \times 10^{-8}\, T^2 + 8.50800 \times 10^{-12}\, T^3 - 2.13218 \times 10^{-3} \quad (33a)$$

$$\varepsilon_T\, c = 4.60100 \times 10^{-5}\, T - 1.22700 \times 10^{-8}\, T^2 + 1.87000 \times 10^{-11}\, T^3 - 1.28615 \times 10^{-2} \quad (33b)$$

Equation 33a shows a minimum in the derived *a* axis thermal expansion coefficient at 756 K. This was considered to be an artifact of the fitting process and therefore, above this temperature, the value was assumed to be constant at $-2.4 \times 10^{-6}\ K^{-1}$.

For the *a* axis in the temperature interval 90 to 293.15 K values of White 1972 over the range 57 to 85 K were combined with the thermal expansion coefficient at 293.15 K derived from equation Equation 33a and fitted to Equation A using the specific heat (C_p) values selected by Paukov et al. 1969, after correction from cal $mol^{-1}\ K^{-1}$ to J $mol^{-1}\ K^{-1}$:

$$\alpha_a\,(K^{-1}) = C_p\,(\,2.87708 \times 10^{-7} - 1.84145 \times 10^{-10}\, T - 3.16370 \times 10^{-5}/\, T) \quad (33c)$$

For the *c* axis it was found that the same procedure did not give a satisfactory fit and therefore values were estimated graphically between 85 and 293.15 K and then refined using the following equation:

$$\alpha_c\,(K^{-1}) = 2.47904 \times 10^{-7}\, T - 1.16617 \times 10^{-9}\, T^2 + 2.85361 \times 10^{-12}\, T^3 - 2.84506 \times 10^{-15}\, T^4 + 2.00119 \times 10^{-5} \quad (33d)$$

On the basis $100\Delta\varepsilon$, in the low temperature region length change values derived from the lattice parameter values of Schiferl and Barrett 1969 (4.2-298 K) average 0.021 high along both axes. The scatter in the high temperature data is indicated by the fact that for the measurements of Klemm et al. 1960 the *a* axis value reaches a maximum deviation of 0.082 high at 513 K before trending to agree with the selected values, while for the *c* axis the maximum deviation is 0.15 high at 501 K before again trending to agree with the

selected values. For the measurements of Pawar and Deshpande 1970 the *a* axis averages to 0.011 high while the *c* axis values show scatter with a maximum deviation of 0.11 low at 428 K. The measurements of Taylor et al. 1965 show better agreement with the *a* axis values averaging 0.013 low and the *c* axis value averaging 0.014 high. Lattice parameter measurements of Fischer et al. 1978 (5-820 K) were only shown in the form of small graphs.

The positional parameter z

Values of *z* determined by Fischer et al. 1978 (5-820 K) were selected because they virtually covered the whole temperature range. They can be represented by the equation: $z = 0.22853 - 2.157 \times 10^{-6} T$. Values over the range 4.2 to 298 K as determined by Schiferl and Barrett 1969 average 0.0008 lower than the selected values.

Table 33a. Lattice parameter measurements of arsenic at 293.15 K

References	Original Temperature K	Hexagonal		Note
		a_h nm	c_h nm	
Taylor et al. 1965	295.6	0.37600	1.05465	
Schiferl and Barrett 1969	299	0.37598	1.05451	
Pawar and Deshpande 1970	301	0.37586	1.05533	a
	Selected	0.37599 (1)	1.05458 (7)	

Note for Table 33a

a. Not included in the average

The selected equivalent rhombohedral cell is a_r 0.41315 (2) nm α 54.133 (4) °

At 293.15: Density 5782 (1) kg m^{-3} Molar volume 12.959 (1) cm^3 mol^{-1}.

Table 33b. Crystallographic properties of arsenic

T K	α_{ah} x 10^6 K^{-1}	α_{ch} x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 ε_T *a*	100 ε_T *c*	100 ε_T avr	*z*
0	0	0	0	- 0.017	- 0.998	- 0.344	0.2266
5	- 0.02	0.11	0.02	- 0.017	- 0.998	- 0.344	0.2285
10	- 0.12	0.75	0.17	- 0.017	- 0.998	- 0.344	0.2285
15	- 0.41	2.80	0.66	- 0.017	- 0.997	- 0.344	0.2285
20	- 0.90	6.20	1.47	- 0.018	- 0.995	- 0.343	0.2285
25	- 1.49	10.56	2.53	- 0.018	- 0.991	- 0.342	0.2285
30	- 2.00	14.70	3.57	- 0.019	- 0.985	- 0.341	0.2285
40	- 2.63	21.54	5.43	- 0.021	- 0.966	- 0.336	0.2285
50	- 2.78	20.59	7.01	- 0.024	- 0.943	- 0.330	0.2284
60	- 2.57	30.12	8.33	- 0.027	- 0.914	- 0.323	0.2284
70	- 2.15	32.41	9.37	- 0.029	- 0.883	- 0.314	0.2284
80	- 1.68	33.79	10.14	- 0.031	- 0.850	- 0.304	0.2284
90	- 1.23	34.77	10.77	- 0.033	- 0.816	- 0.294	0.2284
100	- 0.78	35.71	11.38	- 0.034	- 0.781	- 0.283	0.2283
110	- 0.36	36.56	11.95	- 0.034	- 0.746	- 0.271	0.2283
120	0.04	37.31	12.46	- 0.034	- 0.709	- 0.259	0.2283
130	0.40	37.99	12.93	- 0.034	- 0.672	- 0.247	0.2283
140	0.72	38.60	13.35	- 0.034	- 0.633	- 0.234	0.2282
150	1.01	39.15	13.72	- 0.033	- 0.595	- 0.220	0.2282
160	1.28	39.65	14.07	- 0.031	- 0.556	- 0.206	0.2282
170	1.51	40.10	14.37	- 0.030	- 0.516	- 0.192	0.2282
180	1.72	40.51	14.65	- 0.028	- 0.476	- 0.178	0.2282
190	1.91	40.88	14.90	- 0.027	- 0.435	- 0.163	0.2281
200	2.08	41.23	15.13	- 0.025	- 0.394	- 0.148	0.2281
210	2.23	41.54	15.33	- 0.023	- 0.353	- 0.133	0.2281
220	2.37	41.83	15.52	- 0.020	- 0.312	- 0.117	0.2281
230	2.49	42.10	15.69	- 0.018	- 0.270	- 0.102	0.2281
240	2.61	42.35	15.86	- 0.015	- 0.228	- 0.086	0.2280
250	2.72	42.58	16.01	- 0.013	- 0.185	- 0.070	0.2280
260	2.81	42.79	16.14	- 0.010	- 0.143	- 0.054	0.2280
270	2.91	42.98	16.27	- 0.007	- 0.100	- 0.038	0.2280
280	2.99	43.16	16.38	- 0.004	- 0.057	- 0.022	0.2279
290	3.05	43.31	16.47	- 0.001	- 0.014	- 0.005	0.2279
293.15	3.08	43.34	16.50	0	0	0	0.2279
300	2.91	43.38	16.40	0.002	0.030	0.011	0.2279
350	1.82	43.83	15.82	0.014	0.248	0.092	0.2279
400	0.84	44.56	15.41	0.020	0.470	0.170	0.2278
450	0	45.56	15.19	0.022	0.696	0.247	0.2277
500	- 0.72	46.83	15.13	0.021	0.929	0.323	0.2276
550	- 1.31	48.37	15.25	0.016	1.169	0.400	0.2275
600	- 1.77	50.17	15.54	0.008	1.419	0.478	0.2273
650	- 2.11	52.23	16.00	- 0.002	1.679	0.558	0.2272
700	- 2.31	54.56	16.65	- 0.013	1.950	0.641	0.2271
750	- 2.39	57.13	17.45	- 0.025	2.235	0.728	0.2270
800	- 2.40	59.96	18.39	- 0.037	2.535	0.820	0.2269
850	- 2.40	63.04	19.41	- 0.049	2.850	0.918	0.2268
887	- 2.40	65.47	20.22	- 0.058	3.095	0.993	0.2267

Table 33c. Crystallographic properties of arsenic

T K	a_h nm	c_h nm	a_r nm	α°	$d1$ nm	$d2$ nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.37593	1.04405	0.41015	54.552	0.2526	0.3082	12.825	5842
5	0.37593	1.04405	0.41015	54.552	0.2526	0.3082	12.825	5842
10	0.37593	1.04405	0.41015	54.552	0.2526	0.3082	12.825	5842
15	0.37593	1.04406	0.41015	54.552	0.2525	0.3083	12.825	5842
20	0.37592	1.04409	0.41016	54.551	0.2525	0.3083	12.825	5842
25	0.37592	1.04413	0.41017	54.549	0.2525	0.3083	12.826	5842
30	0.37592	1.04420	0.41019	54.546	0.2525	0.3083	12.826	5841
40	0.37591	1.04439	0.41024	54.537	0.2525	0.3084	12.828	5840
50	0.37590	1.04464	0.41031	54.525	0.2525	0.3085	12.830	5839
60	0.37589	1.04494	0.41039	54.512	0.2525	0.3085	12.833	5838
70	0.37588	1.04526	0.41048	54.498	0.2525	0.3086	12.837	5836
80	0.37587	1.04561	0.41057	54.483	0.2525	0.3087	12.841	5835
90	0.37587	1.04597	0.41067	54.468	0.2525	0.3088	12.845	5833
100	0.37586	1.04634	0.41078	54.452	0.2525	0.3089	12.849	5831
110	0.37586	1.04672	0.41088	54.437	0.2525	0.3089	12.853	5829
120	0.37586	1.04710	0.41099	54.424	0.2525	0.3090	12.858	5827
130	0.37586	1.04750	0.41111	54.405	0.2525	0.3091	12.863	5825
140	0.37586	1.04790	0.41122	54.389	0.2525	0.3092	12.868	5822
150	0.37587	1.04831	0.41134	54.373	0.2525	0.3093	12.873	5820
160	0.37587	1.04872	0.41145	54.356	0.2525	0.3094	12.879	5818
170	0.37588	1.04914	0.41157	54.340	0.2525	0.3095	12.884	5815
180	0.37588	1.04956	0.41170	54.324	0.2525	0.3096	12.890	5813
190	0.37589	1.04999	0.41182	54.307	0.2525	0.3097	12.895	5810
200	0.37590	1.05042	0.41194	54.291	0.2525	0.3098	12.901	5807
210	0.37591	1.05085	0.41207	54.274	0.2525	0.3099	12.907	5805
220	0.37591	1.05129	0.41220	54.257	0.2525	0.3100	12.913	5802
230	0.37592	1.05173	0.41232	54.240	0.2525	0.3101	12.919	5799
240	0.37593	1.05218	0.41245	54.224	0.2525	0.3102	12.925	5797
250	0.37594	1.05262	0.41258	54.207	0.2525	0.3103	12.931	5794
260	0.37595	1.05308	0.41271	54.190	0.2526	0.3104	12.938	5791
270	0.37596	1.05353	0.41284	54.173	0.2526	0.3105	12.944	5788
280	0.37597	1.05398	0.41298	54.156	0.2526	0.3106	12.950	5785
290	0.37599	1.05444	0.41311	54.139	0.2526	0.3107	12.957	5782
293.15	0.37599	1.05458	0.41315	54.133	0.2526	0.3108	12.959	5782
300	0.37600	1.05489	0.41324	54.122	0.2526	0.3108	12.963	5780
350	0.37604	1.05719	0.41391	54.034	0.2526	0.3114	12.994	5766
400	0.37607	1.05953	0.41458	53.944	0.2527	0.3119	13.025	5752
450	0.37607	1.06192	0.41526	53.849	0.2527	0.3124	13.055	5739
500	0.37607	1.06438	0.41596	53.751	0.2528	0.3130	13.084	5726
550	0.37605	1.06691	0.41667	53.648	0.2528	0.3135	13.114	5713
600	0.37602	1.06954	0.41741	53.541	0.2528	0.3141	13.145	5700
650	0.37598	1.07228	0.41818	53.428	0.2529	0.3146	13.176	5686
700	0.37594	1.07515	0.41898	53.312	0.2529	0.3152	13.208	5672
750	0.37590	1.07815	0.41983	53.190	0.2529	0.3158	13.242	5658
800	0.37585	1.08131	0.42072	53.062	0.2530	0.3165	12.377	5643
850	0.37581	1.08464	0.42165	52.928	0.2531	0.3172	13.315	5627
887	0.37577	1.08722	0.42238	52.824	0.2531	0.3177	13.344	5614

$$d1 = [\ a_h{}^2/\ 3 + c_h{}^2 (2z - ⅓)^2\ ]^{½} \qquad d2 = [\ a_h{}^2/\ 3 + c_h{}^2 (2z - ⅔)^2\ ]^{½}$$

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34 SELENIUM Se

Atomic weight: 78.971 (8) (Meija 2017)

Allotropy Trigonal: Hexagonal (hP3)
Alpha monoclinic: Monoclinic (mP32)
Beta monoclinic: Monoclinic (mP32)
Rhombohedral: Rhombohedral (hR6)

The trigonal phase is in the form of helical chains and is the thermodynamically stable phase with the melting point determined by Grønvold 1973 correcting to 494.29 (2) K on ITS-90. Both monoclinic forms exist as Se_8 rings with the melting point of alpha determined to be 413 K by Murphy et al. 1977. The rhombohedral phase which exists as Se_6 rings converts to the trigonal phase above 378 K (Miyamoto 1980). The possible existence of additional allotropic modifications have been summarized by Minaev et al. 2005.

PART 34A. TRIGONAL SELENIUM

Structure: Hexagonal (hP3): 0 – 494.29 K

Up to 293.15 K the thermal expansion coefficients determined by Grosse et al. 1978 (10-300 K) were selected while in the high temperature region length change values selected from the lattice parameter measurements of Bonnier et al. 1964 (298-486 K) were used to produce the following equations, which are considered to be representative from 293.15 K to the melting point:

$$\varepsilon_T a = 6.90853 \times 10^{-5} T - 3.95435 \times 10^{-8} T^2 + 8.96356 \times 10^{-11} T^3 - 1.91122 \times 10^{-2} \quad (34a)$$

$$\varepsilon_T c = -6.64023 \times 10^{-6} T - 1.19372 \times 10^{-9} T^2 - 2.35440 \times 10^{-11} T^3 + 2.64230 \times 10^{-3} \quad (34b)$$

On the basis $100\Delta\varepsilon$ length change values derived from the lattice parameter measurements of Hamilton et al. 1974 (77 and 298 K) show very poor agreement with selected values at 77 K being 0.37 low along the *a* axis and 0.29 high along the *c* axis while lattice parameter measurements of Grosse et al. 1975 (85-380 K), given in the form of equations, initially show poor agreement along the *a* axis trending initially from 0.26 low but above 293.15 K biasing on average only 0.008 high. The *c* axis shows satisfactory agreement averaging as a bias of only 0.006 high along the whole temperature range. Length change values derived from the lattice parameter measurements of Deshpande and Pawar (1964) (303-435 K) scatter 0.012 low to 0.087 high along the *a* axis and 0.012 to 0.060 high along the *c* axis. Lattice parameter measurements of Klemm et al. 1960 (293-473 K) were only shown in the form of small graphs.

Calculation of interatomic distances in trigonal selenium

$d1 = [\,(c/3)^2 + 3\,(ua)^2\,]^{1/2}$ $\quad d2 = [\,(c/3)^2 + 3\,(ua)^2 - a^2(3u-1)\,]^{1/2}$

$d3 = [\,(2c/3)^2 + 3\,(ua)^2\,]^{1/2}$ $\quad d4 = a$ $\quad d5 = [\,(2c/3)^2 + 3\,(ua)^2 - a^2(3u-1)\,]^{1/2}$

arc cos (bond angle) $= 1 - d3^2 / (\sqrt{2}\, d1)^2$

where u is the positional parameter, $d1$ is the bond length, $d2$ is the interatomic distance between chains and the bond angle is equal to Se-Se-Se

Cherin and Unger 1967b determined $u = 0.2254$ (10) and Goodman 1968 as $u = 0.2240$ (17) from which a weighted average of 0.2250 (6) is used to calculated the above values in the room temperature region: $d1 = 0.2372$ nm; $d2 = 0.3437$ nm; $d3 = 0.3717$ nm; $d4 = 0.4365$ nm; $d5 = 0.4473$ nm and bond angle = 103.2°.

Table 34a. Lattice parameters of trigonal selenium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Notes
Straumanis 1940	293	0.43642	0.49597	a
Krebs 1949	293	0.43718	0.49589	a
Straumanis 1949	293	0.43626	0.49597	b
Addink 1951	298	0.43644	0.49597	
Swanson et al. 1955	299	0.43646	0.49543	
Deshpande and Pawar 1964	303	0.43655	0.49557	
Bonnier et al. 1964	298	0.43593	0.49610	a
Goodman 1968	295	0.43657	0.49590	
	Selected	0.43646 (12)	0.49577 (25)	

Notes for Table 34a

a. Not included in the average

b. Corrected for refraction

At 293.15 K: Density 4810 (4) kg m^{-3} Molar Volume 16.418 (12) $cm^3\ mol^{-1}$.

Table 34b. Crystallographic properties of trigonal selenium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
0	0	0	0	- 1.540	0.399	- 0.893
5	0.30	- 0.22	0.13	- 1.539	0.399	- 0.893
10	2.4	- 1.75	1.02	- 1.539	0.399	- 0.893
15	8.1	- 5.7	3.5	- 1.536	0.397	- 0.892
20	15.2	- 10.0	6.8	- 1.531	0.393	- 0.890
25	23.8	- 14.2	10.5	- 1.521	0.387	- 0.885
30	29.7	- 16.1	14.4	- 1.508	0.379	- 0.879
40	36.8	- 19.3	18.1	- 1.475	0.362	- 0.863
50	42.0	- 19.9	21.4	- 1.436	0.342	- 0.843
60	46.9	- 19.0	24.9	- 1.392	0.322	- 0.821
70	49.5	- 18.2	26.9	- 1.344	0.303	- 0.795
80	50.4	- 17.0	27.9	- 1.295	0.286	- 0.768
90	52.0	- 14.5	29.8	- 1.245	0.270	- 0.740
100	53.5	- 13.8	31.1	- 1.192	0.256	- 0.710
110	55.2	- 13.6	32.3	- 1.139	0.242	- 0.678
120	56.7	- 13.4	33.3	- 1.083	0.229	- 0.646
130	57.9	- 13.2	34.2	- 1.027	0.215	- 0.613
140	58.9	- 13.1	34.9	- 0.969	0.202	- 0.579
150	59.7	- 13.0	35.5	- 0.910	0.189	- 0.544
160	60.5	- 13.0	36.0	- 0.851	0.176	- 0.508
170	61.1	- 13.0	36.4	- 0.790	0.163	- 0.472
180	61.6	- 13.1	36.7	- 0.729	0.150	- 0.436
190	62.1	- 13.1	37.0	- 0.668	0.137	- 0.400
200	62.6	- 13.1	37.3	- 0.606	0.124	- 0.363
210	63.0	- 13.2	37.6	- 0.544	0.111	- 0.326
220	63.5	- 13.2	37.9	- 0.481	0.097	- 0.288
230	64.0	- 13.2	38.3	- 0.417	0.084	- 0.250
240	64.6	- 13.2	38.6	- 0.353	0.071	- 0.212
250	65.2	- 13.3	39.0	- 0.288	0.058	- 0.173
260	65.9	- 13.3	39.5	- 0.223	0.044	- 0.134
270	66.7	- 13.3	40.0	- 0.157	0.031	- 0.094
280	67.6	- 13.4	40.6	- 0.090	0.018	- 0.054
290	68.7	- 13.4	41.3	- 0.022	0.004	- 0.013
293.15	69.0	- 13.4	41.5	0	0	0
300	69.5	- 13.7	41.8	0.047	- 0.009	0.029
320	71.2	- 14.6	42.6	0.188	- 0.038	0.113
340	73.0	- 15.6	43.5	0.333	- 0.068	0.199
350	74.0	- 16.1	44.0	0.407	- 0.084	0.243
360	75.1	- 16.7	44.5	0.482	- 0.100	0.288
380	77.4	- 17.8	45.7	0.635	- 0.135	0.378
400	79.8	- 18.9	46.9	0.793	- 0.171	0.472
420	82.5	- 20.1	48.3	0.957	- 0.210	0.568
440	85.4	- 21.4	49.8	1.127	- 0.252	0.667
450	86.9	- 22.1	50.6	1.214	- 0.273	0.718
460	88.5	- 22.8	51.4	1.302	- 0.296	0.770
480	91.7	- 24.1	53.1	1.485	- 0.342	0.876
494.29	94.2	- 25.2	54.4	1.620	- 0.377	0.954

Table 34c. Crystallographic properties of trigonal selenium

T K	*a* nm	*c* nm	*c*/*a*	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.42974	0.49775	1.1583	15.980	4942
5	0.42974	0.49775	1.1583	15.980	4942
10	0.42974	0.49775	1.1582	15.980	4942
15	0.42975	0.49774	1.1582	15.981	4942
20	0.42978	0.49772	1.1581	15.982	4941
25	0.42982	0.49769	1.1579	15.984	4941
30	0.42988	0.49765	1.1577	15.987	4940
40	0.43002	0.49756	1.1571	15.995	4937
50	0.43019	0.49746	1.1564	16.005	4934
60	0.43038	0.49737	1.1556	16.016	4931
70	0.43059	0.49727	1.1549	16.028	4927
80	0.43081	0.49719	1.1541	16.042	4923
90	0.43103	0.49711	1.1533	16.055	4919
100	0.43126	0.49704	1.1525	16.070	4914
110	0.43149	0.49697	1.1518	16.085	4909
120	0.43173	0.49690	1.1510	16.101	4905
130	0.43198	0.49684	1.1501	16.118	4900
140	0.43223	0.49677	1.1493	16.134	4895
150	0.43249	0.49671	1.1485	15.151	4889
160	0.43275	0.49664	1.1476	16.169	4884
170	0.43301	0.49658	1.1468	16.186	4879
180	0.43328	0.49651	1.1459	16.204	4874
190	0.43354	0.49645	1.1451	16.222	4868
200	0.43382	0.49638	1.1442	16.240	4863
210	0.43409	0.49632	1.1434	16.258	4857
220	0.43436	0.49625	1.1425	16.277	4852
230	0.43464	0.49619	1.1416	16.295	4846
240	0.43492	0.49612	1.1407	16.314	4841
250	0.43520	0.49606	1.1398	16.333	4835
260	0.43549	0.49599	1.1389	16.352	4829
270	0.43578	0.49592	1.1380	16.372	4823
280	0.43607	0.49586	1.1371	16.392	4818
290	0.43633	0.49579	1.1362	16.412	4813
293.15	0.43646	0.49577	1.1359	16.418	4810
300	0.43667	0.49572	1.1352	16.432	4806
320	0.43728	0.49558	1.1333	16.474	4794
340	0.43791	0.49543	1.1314	16.517	4781
350	0.43823	0.49535	1.1303	16.538	4775
360	0.43856	0.49527	1.1293	16.560	4769
380	0.43923	0.49510	1.1272	16.605	4756
400	0.43992	0.49492	1.1250	16.651	4743
420	0.44064	0.49473	1.1228	16.699	4729
440	0.44138	0.49452	1.1204	16.748	4715
450	0.44176	0.49442	1.1192	16.773	4708
460	0.44214	0.49430	1.1180	16.799	4701
480	0.44294	0.49407	1.1154	16.852	4686
494.29	0.44353	0.49390	1.1136	16.891	4675

PART 34B. ALPHA MONOCLINIC SELENIUM

Structure: Monoclinic (mP32)

Burbank 1951 correctly identified the space group as being $P2_1/n$. The following high accuracy lattice parameters were determined where the values of Cherin and Unger 1972 were corrected to 293.15 K using the thermal expansion coefficients determined by Newton and Colby 1951 (293-353 K): $\alpha_a = -1.5 \times 10^{-6}\ K^{-1}$; $\alpha_b = 84.7 \times 10^{-6}\ K^{-1}$; $\alpha_c = 63.3 \times 10^{-6}\ K^{-1}$; $\alpha_{\beta^\circ} = 5.5 \times 10^{-6}\ K^{-1}$.

Table 34d. Lattice parameters of alpha monoclinic selenium at 293.15 K

References	Original Temperature K	*a* nm	*b* nm	*c* nm	*β* °
Newton and Colby 1951	293	0.9066	0.9074	1.1599	90.87
Cherin and Unger 1972	299	0.9055	0.9079	1.1597	90.81
	Selected	0.9055 (3)	0.9079 (5)	1.1597 (6)	90.81 (5)

At 293.15 K: Density 4402 (4) kg m^{-3} Molar Volume 143.52 (12) $cm^3\ mol^{-1}$.

Cherin and Unger 1972 determined the average bond length to be 0.2336 (6) nm and the average Se-Se-Se bond angle to be 105.7 (1.6)°. Donohue 1974 gave a table of all interatomic distances less than 0.4 nm between molecules.

PART 34C. BETA MONOCLINIC SELENIUM

Structure: Monoclinic (mP32)

Burbank 1952 identified the space group as being $P2_1/a$. The following room temperature values have been determined for the lattice parameters:

Table 34e. Lattice parameters of beta monoclinic selenium at RT

References	Original Temperature K	*a* nm	*b* nm	*c* nm	*β* °
Klug 1934	RT	1.277	0.806	0.927	93.07
Burbank 1952	RT	1.285	0.807	0.931	93.13
	Selected	1.285 (1)	0.807 (1)	0.931 (1)	93.13 (8)

At RT: Density 4353 (8) kg m^{-3} Molar Volume 145.13 (26) $cm^3\ mol^{-1}$.

Burbank 1952 suggested that the ring structure was highly distorted but corrections by Marsh et al. 1953 showed the structure to be very similar to that of the alpha modification with an average bond length of 0.2337 (19) nm and the average Se-Se-Se bond angle of 105.7 (1.0)°. Donohue 1974 gave a table of all interatomic distances less than 0.4 nm between molecules.

PART 34D. RHOMBOHEDRAL SELENIUM

Structure: Rhombohedral (hR6)

Miyamoto 1980 identified the structure and gave the lattice parameters in terms of the equivalent hexagonal cell as a_h 1.1362 (1) nm c_h 0.4429 (8) nm. The values for the equivalent rhombohedral cell would be a_r 0.6724 (1) nm and α_r 115.32 (4)°. The bond length is 0.2356 (9) nm and the Se-Se-Se bond angle is 101.1 (3)°. The calculated density is 4767 (9) kg m^{-3} and the molar volume 99.40 (18) cm^3 mol^{-1}.

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35 BROMINE Br

Atomic Weight: 79.901 to 79.907 (Meija 2017)
Select 2009 value 79.904 (1) (Wieser and Coplen 2011).

Structure: Orthorhombic (oS8)

The triple point was determined by Hildenbrand et al. 1958 to be 265.90 (5) K.

35.1 Crystallographic Properties

Lattice parameters determined at 5 K, 80 K, 170 K and 250 K by Powell et al. 1984 were fitted to Equation B using the enthalpy values selected by Gurvich et al. 1989:

$$\ln (a, \text{nm}) = (H_T - H_0)\,(1.44286 \times 10^{-6} + 2.34440 \times 10^{-9}\,T + 6.30066 \times 10^{-5}/T) - 0.4205033 \quad (35a)$$

$$\ln (b, \text{nm}) = (H_T - H_0)\,(9.21006 \times 10^{-7} + 9.54540 \times 10^{-9}\,T + 9.90664 \times 10^{-5}/T) - 0.8056975 \quad (35b)$$

$$\ln (c, \text{nm}) = (H_T - H_0)\,(4.90104 \times 10^{-7} - 1.71007 \times 10^{-9}\,T + 7.61826 \times 10^{-6}/T) - 0.1399758 \quad (35c)$$

Values of the positional parameters also determined by Powell et al. 1984 were calculated as follows where for the *y* parameter the value at 80 K was not included:

$$y = -1.9415 \times 10^{-5}\,T + 1.0513 \times 10^{-8}\,T^2 + 0.1391 \quad (35d)$$

$$z = -5.1880 \times 10^{-6}\,T - 2.8883 \times 10^{-9}\,T^2 + 0.1114 \quad (35e)$$

Compared to the selected values, the lattice parameter measurements of Hawes 1959 (167 – 250 K) show drifts of 0.004 to 0.001 nm higher for the *a*-axis, 0.005 to 0.009 nm lower for the *b*-axis and 0.003 to 0.006 nm higher for the *c*-axis.

Calculation of interatomic distances in bromine

Br (1) – Br (2) = $d1 = [(2yb)^2 + (2zc)^2]^{1/2}$ (Bond length r_e)

Br (1) – Br (3) = $d2 = [b^2/4 + (0.5 - 2z)^2 c^2]^{1/2}$

Br (1) – Br (4) = $d3 = [(1 - 2y)^2 b^2 + (2zc)^2]^{1/2}$

Br (1) – Br (5) = $d4 = [a^2/4 + b^2/4]^{1/2}$

Br (1) – Br (6) = $d5 = [a^2/4 + (0.5 - 2y)^2 b^2 + (2zc)^2]^{1/2}$

Br (1) – Br (7) = $d6 = [a^2/4 + (0.5 - 2z)^2 c^2]^{1/2}$

Table 35a. Crystallographic properties of bromine

T K	α_a x 10^6 K^{-1}	α_b x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}
0	0	0	0	0
5	3.61	5.24	0.54	3.13
10	15.5	21.1	2.62	13.1
15	32.7	47.4	5.95	27.0
20	46.6	58.1	8.98	37.9
25	57.1	69.0	11.4	45.8
30	63.6	75.3	12.9	50.6
40	71.0	82.4	14.4	56.0
50	75.0	87.7	14.6	59.1
60	77.8	93.0	14.2	61.7
70	80.4	99.4	13.4	64.4
80	83.3	107	12.5	67.6
90	86.4	115	11.5	71.0
100	89.6	124	10.3	74.6
110	92.8	133	9.10	78.4
120	96.1	143	7.79	82.3
130	99.5	153	6.42	86.4
140	103	164	4.98	90.6
150	107	175	3.50	94.9
160	110	186	1.96	99.3
170	114	197	0.38	104
180	118	209	- 1.24	108
190	122	221	- 2.91	113
200	126	233	- 4.61	118
210	130	246	- 6.36	123
220	134	259	- 8.14	128
230	139	273	- 9.96	134
240	144	288	- 11.8	140
250	149	303	- 13.7	146
260	155	319	- 15.7	153
265.90	159	330	- 16.9	157

Table 35b. Crystallographic properties of bromine

T K	100 ε_0 *a*	100 ε_0 *b*	100 ε_0 c	100 ε_0 avr
0	0	0	0	0
5	< 0.001	< 0.001	< 0.001	< 0.001
10	0.005	0.008	< 0.001	0.005
15	0.017	0.023	0.003	0.014
20	0.037	0.049	0.007	0.032
25	0.063	0.080	0.012	0.053
30	0.093	0.116	0.018	0.076
40	0.161	0.196	0.032	0.129
50	0.234	0.281	0.046	0.187
60	0.311	0.371	0.061	0.248
70	0.390	0.467	0.075	0.311
80	0.472	0.570	0.087	0.377
90	0.556	0.681	0.099	0.446
100	0.644	0.801	0.110	0.519
110	0.735	0.929	0.120	0.596
120	0.830	1.067	0.129	0.677
130	0.928	1.215	0.136	0.762
140	1.029	1.374	0.141	0.852
150	1.134	1.543	0.146	0.944
160	1.242	1.723	0.148	1.042
170	1.354	1.914	0.150	1.145
180	1.470	2.117	0.149	1.252
190	1.590	2.332	0.147	1.365
200	1.713	2.559	0.143	1.482
210	1.841	2.798	0.138	1.605
220	1.973	3.051	0.130	1.732
230	2.110	3.317	0.121	1.866
240	2.251	3.597	0.111	2.006
250	2.397	3.893	0.098	2.152
260	2.549	4.204	0.083	2.304
265.90	2.642	4.395	0.073	2.395

Table 35c. Crystallographic properties of bromine

T K	*a* nm	*b* nm	*c* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.65672	0.44678	0.86938	38.403	4161
5	0.65672	0.44678	0.86938	38.404	4161
10	0.65675	0.44681	0.86939	38.409	4161
15	0.65683	0.44688	0.86940	38.420	4160
20	0.65696	0.44699	0.86948	38.439	4157
25	0.65713	0.44714	0.86953	38.463	4155
30	0.65733	0.44730	0.86953	38.491	4152
40	0.65778	0.44765	0.86966	38.553	4145
50	0.65826	0.44803	0.86978	38.619	4138
60	0.65876	0.44844	0.86991	38.689	4131
70	0.65928	0.44887	0.87003	38.763	4123
80	0.65982	0.44933	0.87014	38.839	4115
90	0.66038	0.44983	0.87024	38.920	4106
100	0.66096	0.45037	0.87034	39.005	4097
110	0.66156	0.45095	0.87042	39.095	4088
120	0.66219	0.45157	0.87050	39.189	4078
130	0.66284	0.45224	0.87056	39.288	4068
140	0.66351	0.45296	0.87061	39.393	4057
150	0.66420	0.45372	0.87065	39.503	4046
160	0.66492	0.45454	0.87067	39.618	4034
170	0.66567	0.45541	0.87068	39.738	4021
180	0.66644	0.45633	0.87068	39.864	4009
190	0.66724	0.45732	0.87066	39.998	3995
200	0.66806	0.45835	0.87063	40.137	3982
210	0.66892	0.45946	0.87058	40.282	3967
220	0.66980	0.46062	0.87051	40.435	3952
230	0.67072	0.46184	0.87044	40.594	3937
240	0.67167	0.46314	0.87034	40.761	3921
250	0.67265	0.46451	0.87023	40.936	3904
260	0.67367	0.46596	0.87010	41.120	3886
265.90	0.67430	0.46681	0.87002	41.233	3876

Table 35d. Inter-atomic distances for bromine

T K	*y*	*z*	*d*1 nm	*d*2 nm	*d*3 nm	*d*4 nm	*d*5 nm	*d*6 nm
0	0.1391	0.1114	0.2301	0.3286	0.3762	0.3971	0.3939	0.4073
5	0.1390	0.1114	0.2301	0.3286	0.3762	0.3971	0.3939	0.4073
10	0.1389	0.1113	0.2300	0.3287	0.3763	0.3972	0.3939	0.4074
15	0.1388	0.1113	0.2299	0.3287	0.3764	0.3972	0.3940	0.4074
20	0.1387	0.1113	0.2299	0.3288	0.3765	0.3973	0.3940	0.4075
25	0.1386	0.1113	0.2298	0.3289	0.3767	0.3974	0.3941	0.4076
30	0.1385	0.1112	0.2297	0.3290	0.3768	0.3975	0.3942	0.4077
40	0.1383	0.1112	0.2297	0.3292	0.3772	0.3978	0.3944	0.4080
50	0.1382	0.1111	0.2296	0.3295	0.3775	0.3981	0.3946	0.4083
60	0.1380	0.1111	0.2295	0.3297	0.3779	0.3985	0.3949	0.4085
70	0.1378	0.1110	0.2294	0.3298	0.3782	0.3988	0.3951	0.4088
80	0.1376	0.1110	0.2293	0.3302	0.3786	0.3991	0.3954	0.4091
90	0.1374	0.1109	0.2292	0.3304	0.3790	0.3995	0.3957	0.4094
100	0.1373	0.1109	0.2292	0.3307	0.3795	0.3999	0.3959	0.4097
110	0.1371	0.1108	0.2291	0.3310	0.3799	0.4003	0.3962	0.4101
120	0.1369	0.1107	0.2290	0.3313	0.3804	0.4008	0.3965	0.4104
130	0.1368	0.1107	0.2290	0.3316	0.3808	0.4012	0.3968	0.4107
140	0.1366	0.1106	0.2289	0.3320	0.3814	0.4017	0.3971	0.4111
150	0.1364	0.1106	0.2289	0.3323	0.3820	0.4022	0.3975	0.4114
160	0.1363	0.1105	0.2288	0.3327	0.3826	0.4027	0.3978	0.4118
170	0.1361	0.1104	0.2288	0.3330	0.3832	0.4033	0.3981	0.4121
180	0.1359	0.1104	0.2288	0.3334	0.3838	0.4039	0.3985	0.4125
190	0.1358	0.1103	0.2287	0.3338	0.3845	0.4045	0.3989	0.4129
200	0.1356	0.1102	0.2287	0.3343	0.3852	0.4051	0.3993	0.4133
210	0.1355	0.1102	0.2287	0.3347	0.3860	0.4058	0.3997	0.4137
220	0.1353	0.1101	0.2287	0.3352	0.3868	0.4064	0.4001	0.4141
230	0.1352	0.1101	0.2287	0.3357	0.3876	0.4072	0.4005	0.4145
240	0.1350	0.1100	0.2287	0.3362	0.3885	0.4079	0.4010	0.4149
250	0.1349	0.1099	0.2287	0.3367	0.3894	0.4087	0.4014	0.4154
260	0.1348	0.1099	0.2287	0.3373	0.3904	0.4096	0.4019	0.4159
265.90	0.1347	0.1098	0.2288	0.3376	0.3910	0.4101	0.4022	0.4161

*d*1 is the bond length (r_e).

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36 KRYPTON Kr

Atomic weight: 83.798 (2) (Meija 2017)

Structure: Face-centered cubic (cF4)

The triple point is a secondary fixed point on ITS-90 at 115.775 (1) K (Bedford et al. 1996).

36.1 Crystallographic properties of krypton

Smoothed values derived from the lattice parameter measurements of Losee and Simmons 1968b (4-115 K) were combined with dilatometric measurements of Tilford and Swenson 1972 (1-45 K). The measurements were extrapolated to the triple point. The lattice parameter was determined by Losee and Simmons 1968b to be 0.564597 (10) nm at 4.25 K and this value is selected. Urvas et al. 1967 determined 0.564591 nm at 4.25 K which is within the accuracy of the selected value. Lattice parameters obtained by Macrander 1978 along the melting line 127.34 K to 138.94 K extrapolate to agree exactly with the selected value at the triple point.

36.2 Bulk properties of krypton

Measurements of both dilatometric and length change values by Losee and Simmons 1968a were given in analytical form by Losee and Simmons 1968b leading to the vacancy parameters H_V/k = 895 K and S_V/k = 2.0. Based on the later measurements of Coufal et al. 1970 (which were shown only graphically), Korpiun and Coufal 1971 selected H_V/k = 1000 K and S_V/k =2.8 by normalizing to the selected crystallographic thermal expansion coefficient of Losee and Simmons 1968b at 80 K and therefore, this equation is selected to represent the bulk properties. Bulk volume thermal expansion coefficients of Manzhelii et al. 1967 (16-69 K) trend from 8% high initially to 2% low at 30 K and increases to an average of 2% high above 45 K. Similar measurements by Manzhelii et al. 1969 (90-114 K) drift from initially 2% high to 0.5% high at 110 K before increasing sharply to 4% high at 114 K.

Table 36a. Crystallographic properties of krypton

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_0$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	0	0.56459	0.39923	27.096	3092.7
1	0.050	< 0.0001	0.56459	0.39923	27.096	3092.7
2	0.417	< 0.0001	0.56459	0.39923	27.096	3092.7
3	1.495	0.0001	0.56460	0.39923	27.096	3092.6
4	3.833	0.0004	0.56460	0.39923	27.096	3092.6
5	8.127	0.0009	0.56460	0.39923	27.097	3092.6
6	14.61	0.0021	0.56461	0.39924	27.097	3092.5
7	23.20	0.0040	0.56462	0.39924	27.099	3092.3
8	33.50	0.0068	0.56463	0.39926	27.101	3092.0
9	44.97	0.0169	0.56466	0.39927	27.104	3091.7
10	56.97	0.0158	0.56468	0.39929	27.109	3091.2
11	69.40	0.0209	0.56471	0.39931	27.113	3090.7
12	81.47	0.0297	0.56476	0.39935	27.120	3089.9
13	93.20	0.0384	0.56481	0.39938	27.127	3089.1
14	104.5	0.0483	0.56487	0.39942	27.135	3088.2
15	115.3	0.0592	0.56493	0.39947	27.144	3087.2
16	125.6	0.0712	0.56500	0.39951	27.154	3086.1
18	144.1	0.0983	0.56515	0.39962	27.176	3083.6
20	160.6	0.1288	0.56532	0.39974	27.201	3080.7
25	193.0	0.2175	0.56582	0.40010	27.273	3072.6
30	217.7	0.3205	0.56640	0.40051	27.357	3063.1
35	237.3	0.4345	0.56705	0.40096	27.451	3052.7
40	251.5	0.5575	0.56774	0.40145	27.551	3041.5
45	264.0	0.687	0.56847	0.40197	27.658	3029.8
50	275.5	0.823	0.56924	0.40251	27.770	3017.5
55	288.3	0.965	0.57004	0.40308	27.888	3004.8
60	301.5	1.114	0.57088	0.40380	28.011	2992.6
65	315.0	1.270	0.57177	0.40430	28.141	2977.8
70	329.0	1.433	0.57269	0.40495	28.277	2963.4
75	343.3	1.604	0.57365	0.40563	28.421	2948.5
80	357.5	1.782	0.57466	0.40634	28.570	2933.0
85	372.3	1.968	0.57571	0.40709	28.727	2917.0
90	388.5	2.163	0.57681	0.40786	28.892	2900.4
95	406.0	2.366	0.57795	0.40867	29.065	2883.1
100	430.0	2.578	0.57915	0.40952	29.246	2865.3
105	459.2	2.805	0.58043	0.41043	29.440	2846.4
110	493.5	3.051	0.58183	0.41141	29.652	2826.0
115	533.0	3.317	0.58332	0.41247	29.883	2804.2
115.775	539.6	3.360	0.58357	0.41264	29.920	2800.8

$$d = a/\sqrt{2}$$

Table 36b. Bulk properties of krypton

$3\ (\varepsilon_0 L - \varepsilon_0 a) = \exp(2.8 - 1000/T)$ $\quad \alpha_L - \alpha_a = (333.3/T^2) \exp(2.8 - 1000/T)$

T K	$\alpha \times 10^6$ K	$100\ \varepsilon_0$	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
80	357.5	1.782	28.570	2933.0
85	376.3	1.968	28.727	2917.0
90	396.7	2.170	28.898	2899.8
95	423.0	2.378	29.075	2882.1
100	453.3	2.603	29.267	2863.2
105	492.7	2.844	29.474	2843.1
110	546.7	3.108	29.702	2821.3
115	606.7	3.405	29.959	2797.1
115.775	616.5	3.454	30.002	2793.1

This Table is considered to be identical to Table 36a below 80 K.

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37 RUBIDIUM Rb

Atomic weight: 85.4678 (3) (Meija 2017)

Structure: Body-centered cubic (cI2)

Alcock et al. 1994 select 312.45 (10) K for the melting point.

37.1 Crystallographic properties

There have been a significant number of determinations of the lattice parameter but because these generally show a degree of scatter then the thermal expansion over the whole temperature range is based on the volume ratios of Anderson and Swenson 1983 (4-295 K), which were reduced to length change values and combined with enthalpy values selected by Alcock et al. 1994 and fitted to Equation B:

$$\ln (L_T) = (H_T - H_0) (2.35663 \times 10^{-6} + 8.11248 \times 10^{-10} T + 6.50503 \times 10^{-6}/ T) - 1.91922 \times 10^{-2} \quad (37a)$$

This equation is specifically a representation of bulk thermal expansion but is also used for crystallographic expansion because of the lack of other data. The average thermal expansion over the range from 293.15 K to the melting point is 88 x 10^{-6} K^{-1}, whereas the direct density measurements of Basin et al. 1969 (288 – 312 K) lead to a much higher value of 96 x 10^{-6} K^{-1}. However, this is also higher than the value of 94 x 10^{-6} K^{-1} derived from the direct density measurements for cesium by Basin 1972 whereas a periodic trend suggests that it should be lower and therefore these measurements were not included in the evaluation. In comparison with lattice parameter measurements to consider the quality of the procedure used it is noted that the four values of Rosengren and Johansson 1975 (12-205 K) and the two measurements of Copley 1973 at 78 K and 197 K average 0.0002 nm low while the measurements of Kelly and Pearson 1955 at 77 K and 90 K average 0.0001 nm high. A single measurement of Hume-Rothery and Lonsdale 1945 at 90 K is 0.0009 nm high but may be subject to a wavelength calibration problem. The two measurements of Barrett 1956 at 5 K and 78 K are both 0.0006 nm low while a de Haas – van Alphen (dHvA) measurement of Gaertner and Templeton 1977 calculated as a lattice parameter value using the free electron model is 0.0003 nm low.

Table 37a. Lattice parameter of rubidium at 293.15 K

References	Original Temperature K	*a* nm	Notes
Hume-Rothery and Lonsdale 1945	292	0.5710	a
Kelley and Pearson 1955	297	0.5697	
Basin et al. 1969	293	0.5700	b
Copley 1973	303	0.5699	
	Selected	0.5699 (2)	

Notes for Table 37a

a. Not included in the average

b. From interpolated direct density measurement 1532.8 kg m^{-3}

At 293.15 K for Rb: Density 1534 (2) kg m^{-3} Molar Volume 55.73 (6) cm^3 mol^{-1}

Table 37b. Crystallographic properties of rubidium

T K	$\alpha \times 10^6$ K^{-1}	100 ε_T	*a* nm	*d* nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
0	0	- 1.901	0.5591	0.4842	52.62	1624
5	5.2	- 1.900	0.5591	0.4842	52.62	1624
10	19.3	- 1.894	0.5591	0.4842	52.63	1624
15	32.4	- 1.881	0.5592	0.4843	52.65	1623
20	41.3	- 1.863	0.5593	0.4844	52.68	1623
25	47.5	- 1.841	0.5594	0.4845	52.71	1621
30	51.1	- 1.817	0.5595	0.4846	52.75	1620
40	55.3	- 1.765	0.5598	0.4848	52.84	1618
50	58.0	- 1.709	0.5602	0.4851	52.93	1615
60	59.8	- 1.651	0.5605	0.4854	53.02	1612
70	61.1	- 1.591	0.5608	0.4857	53.11	1609
80	62.2	- 1.531	0.5612	0.4860	53.21	1606
90	63.2	- 1.469	0.5615	0.4863	53.31	1603
100	64.2	- 1.406	0.5619	0.4866	53.42	1600
110	65.0	- 1.342	0.5622	0.4869	53.52	1597
120	65.9	- 1.278	0.5626	0.4872	53.62	1594
130	66.8	- 1.212	0.5630	0.4876	53.73	1591
140	67.7	- 1.146	0.5634	0.4879	53.84	1587
150	68.6	- 1.078	0.5638	0.4882	53.95	1584
160	69.5	- 1.010	0.5641	0.4886	54.06	1581
170	70.4	- 0.941	0.5645	0.4889	54.18	1578
180	71.3	- 0.871	0.5649	0.4893	54.29	1574
190	72.1	- 0.800	0.5653	0.4896	54.41	1571
200	73.1	- 0.727	0.5658	0.4900	54.53	1567
210	74.0	- 0.654	0.5662	0.4903	54.65	1564
220	75.0	- 0.580	0.5666	0.4907	54.77	1561
230	76.0	- 0.505	0.5670	0.4911	54.89	1557
240	77.2	- 0.429	0.5675	0.4914	55.02	1553
250	78.4	- 0.352	0.5679	0.4918	55.15	1550
260	79.8	- 0.273	0.5683	0.4922	55.28	1547
270	81.2	- 0.192	0.5688	0.4926	55.41	1542
280	82.8	- 0.111	0.5693	0.4930	55.55	1539
290	84.9	- 0.027	0.5697	0.4934	55.69	1535
293.15	85.6	0	0.5699	0.4935	55.73	1534
295	86.0	0.016	0.5700	0.4936	55.76	1533
300	87.3	0.059	0.5702	0.4938	55.83	1531
305	88.8	0.103	0.5705	0.4941	55.91	1529
310	90.4	0.148	0.5707	0.4943	55.98	1527
312.45	91.2	0.170	0.5709	0.4944	56.02	1526

$$d = \sqrt{3}a/2$$

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38 STRONTIUM Sr

Atomic Weight: 87.62 (1) (Meija 2017)

Allotropy: Alpha phase: Face-centered cubic (cF4)
Beta phase: Body-centered cubic (cI2)

Both Sheldon and King 1953 and Hirst et al. 1956 reported an intermediate hexagonal close-packed (hP2) structure but Peterson and Colburn 1966 showed that this was due to hydrogen contamination. Alcock et al. 1993 selects 820 (3) K for the alpha-beta transition temperature and 1041 (2) K for the melting point.

38.1 Alpha Phase: Face-centered cubic (cF4): 0 K to 820 K

Up to 12 K thermal expansion coefficients of White 1972 (3-85 K and 283 K) were fitted to a Debye equation but at 28 K and above they were combined with the selected specific heat values of Alcock et al. 1993 and fitted to Equation A:

$$3 - 12\ \text{K}: \quad \alpha\ (\text{K}^{-1}) = -1.27560 \times 10^{-8}\, T + 1.40905 \times 10^{-10}\, T^{3} + 3.36196 \times 10^{-11}\, T^{5} - 8.00680 \times 10^{-15}\, T^{7} \qquad (38a)$$

$$28 - 283\ \text{K}: \quad \alpha\ (\text{K}^{-1}) = Cp\ (\ 8.71992 \times 10^{-7} - 5.31006 \times 10^{-11}\, T - 4.10389 \times 10^{-6}\ /T) \qquad (38b)$$

Equation 38a has an accuracy of ± 1.6 x 10^{-9} K^{-1} and equation 38b has ± 9.7 x 10^{-8} K^{-1}. Intermediate values in the range 12 K to 28 K were given by White 1972 while equation 38b was extrapolated to 293.15 K. On the basis $100\Delta\varepsilon$ length change values derived from the volume ratios of Anderson et al. 1990 (4-295 K) show a maximum deviation of 0.029 high at 100 K.

In the high temperature region length change values derived from the direct density measurements of Stankus and Tyagel'skii 1992 (293-850 K in the alpha range) were selected and fitted to the following equation:

$$\varepsilon_T = 2.14953 \times 10^{-5}\, T - 2.66113 \times 10^{-10}\, T^{2} + 4.70757 \times 10^{-12}\, T^{3} - 6.39707 \times 10^{-3} \qquad (38c)$$

Dilatometric measurements of Dzhavadov 1985 (293-780 K) were only shown graphically. However, a thermal expansion value of 22.5 (3) x 10^{-6} K^{-1} at 300 K was given and agreed with the selected value.

Table 38a. Lattice parameter of alpha strontium at 293.15 K

References	Original Temperature K	*a* nm	Notes
King 1929	RT	0.6088	a
Sheldon and King 1953	298	0.6085	
Hirst et al. 1956	298	0.6088	
Schottmiller et al. 1958	298	0.6084	
Bruzzone 1971	RT	0.6082	
Stankus and Tyagel'skii 1992	293	0.6089	b
	Selected	0.6086 (3)	

Notes for Table 38a

a. Superseded by Sheldon and King 1953 – not included in the average

b. From direct density value 2578.3 kg m^{-3}

At 293.15 K: Density 2582 (4) kg m^{-3} Molar volume 33.94 (5) cm^3 mol^{-1}

38.2 Beta Phase: Body-centered cubic: 820 K to 1041 K

Length change values derived from the direct density measurements of Stankus and Tyagel'skii 1992 (850 – 1044 K in the beta range) were fitted to the following equations:

$$a\ (\text{nm}) = 1.78861 \times 10^{-5}\, T + 0.473961 \qquad (38d)$$

$$\varepsilon_T = 3.70277 \times 10^{-5}\, T - 1.88085 \times 10^{-2} \qquad (38e)$$

The derived thermal expansion coefficient is 36.5 x 10^{-6} K^{-1}. The volume change on transition derived using the Clausius-Clapeyron equation with an initial pressure coefficient of dT/dP = – 0.10 K MPa^{-1} as measured by Jayaraman et al. 1963, and an enthalpy of transition of 850 (250) J mol^{-1} selected by Alcock et al. 1993 is a contraction of 0.10 (3) cm^3 mol^{-1} which compares with the directly determined value of 0.22 (11) cm^3 mol^{-1} from the density measurements of Stankus and Tyagel'skii 1992.

Lattice parameter values for the beta phase on samples probably saturated with hydrogen were determined as 0.485nm at 887 K by Sheldon and King 1953, 0.488 nm at 901 K by Hirst et al. 1956 and 0.487 nm at 903 K by Schottmiller at al 1958 and on the whole are notably smaller than those obtained by the direct density method as given in Table 38c on supposedly purer metal because only the alpha-beta transition was detected.

Table 38b. Crystallographic properties of alpha strontium

T K	α x 10^6 K^{-1}	100 ε_T	*a* nm	*d* nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
0	0	- 0.531	0.6054	0.4281	33.40	2623
10	0.27	- 0.531	0.6054	0.4281	33.40	2623
20	3.50	- 0.529	0.6054	0.4281	33.40	2623
30	8.20	- 0.523	0.6054	0.4281	33.41	2623
40	11.86	- 0.513	0.6055	0.4281	33.42	2622
50	14.33	- 0.500	0.6056	0.4282	33.43	2621
60	16.08	- 0.485	0.6056	0.4283	33.45	2620
70	17.32	- 0.468	0.6058	0.4283	33.46	2618
80	18.21	- 0.451	0.6059	0.4284	33.48	2617
90	18.87	- 0.432	0.6060	0.4285	33.50	2616
100	19.43	- 0.413	0.6061	0.4286	33.52	2614
110	19.84	- 0.394	0.6062	0.4286	33.54	2613
120	20.16	- 0.374	0.6063	0.4287	33.56	2611
130	20.44	- 0.353	0.6065	0.4288	33.58	2609
140	20.69	- 0.333	0.6066	0.4289	33.60	2608
150	20.91	- 0.312	0.6067	0.4290	33.62	2606
160	21.10	- 0.291	0.6068	0.4291	33.64	2604
170	21.27	- 0.270	0.6070	0.4292	33.66	2603
180	21.42	- 0.249	0.6071	04293	33.69	2601
190	21.56	- 0.227	0.6072	0.4294	33.71	2599
200	21.67	- 0.206	0.6073	0.4295	33.73	2598
210	21.78	- 0.184	0.6075	0.4296	33.75	2596
220	21.88	- 0.162	0.6076	0.4296	33.77	2594
230	21.97	- 0.140	0.6077	0.4297	33.80	2593
240	22.06	- 0.118	0.6079	0.4298	33.82	2591
250	22.14	- 0.096	0.6080	0.4299	33.84	2589
260	22.23	- 0.074	0.6081	0.4300	33.86	2588
270	22.32	- 0.052	0.6083	0.4301	33.89	2586
280	22.41	- 0.030	0.6084	0.4302	33.91	2584
290	22.52	- 0.007	0.6086	0.4303	33.93	2582
293.15	22.55	0	0.6086	0.4303	33.94	2582
300	22.60	0.015	0.6087	0.4304	33.95	2581
350	23.01	0.130	0.6094	0.4307	34.07	2572
400	23.48	0.246	0.6101	0.4314	34.19	2563
450	24.03	0.365	0.6108	0.4319	34.31	2554
500	24.64	0.487	0.6116	0.4324	34.44	2544
550	25.32	0.613	0.6123	0.4330	34.57	2535
600	26.07	0.742	0.6131	0.4335	34.70	2525
650	26.88	0.876	0.6139	0.4341	34.84	2515
700	27.76	1.013	0.6148	0.4347	34.98	2505
750	28.71	1.156	0.6156	0.4353	35.13	2494
800	29.72	1.304	0.6165	0.4357	35.28	2483
820	30.14	1.365	0.6169	0.4362	35.35	2479

$$d = a/\sqrt{2}$$

Table 38c. Crystallographic properties of beta strontium

T K	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
820	1.155	0.4886	0.4232	35.13	2494
850	1.267	0.4892	0.4236	35.24	2486
900	1.452	0.4901	0.4244	35.44	2473
950	1.637	0.4910	0.4252	35.63	2459
1000	1.822	0.4919	0.4260	35.83	2446
1041	1.974	0.4926	0.4261	35.99	2435

$$d = \sqrt{3}a/2$$

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39 YTTRIUM Y

Atomic weight: 88.90584 (1) (Meija 2017)

Allotropy: Alpha phase: Hexagonal close-packed (hP2)
Beta phase: Body-centered cubic (cI2)

Gschneidner 1990 selected 1751 K for the alpha-beta transformation temperature and 1795 K for the melting point.

39.1 Alpha Phase: Hexagonal close-packed (hP2): 0 K to 1751 K

In the high temperature region length change values derived by Touloukian et al. 1975 from the lattice parameter measurements of Spedding et al. 1961 (296-1170 K) where fitted by Touloukian et al. 1975 to accepted equations 39e and 39j as given below except for a slight correction to a 293.15 K baseline. However, an upper limit on these equations was selected as 936 K because this represents a maximum in the derived thermal expansion coefficient for the *c* axis. Above 936 K length change values derived from direct density measurements of Stankus and Basin 1980 (293-1763 K in the alpha region) were accepted and by following the procedure as given in part 39.4 it was possible to extrapolate the *a* and *c* axis thermal expansion values to 1497 K as equations 39f and 39k. At this temperature Stankus and Basin 1980 note a sharp change in the thermal expansion coefficient which is not considered as being due to pure yttrium but to an unknown major impurity. However, for consistency with values with the beta phase this change is accepted and over the range 1497 K to 1763 K the derived thermal expansion coefficient is 15.04×10^{-6} K^{-1}.

On the basis $100\Delta\varepsilon$ dilatometric measurements of Nolting et al. 1960 (298-1273 K), as given by Touloukian et al. 1975, showed very poor agreement with selected values with a first sample trending to 0.26 low and a second to 0.12 low.

In the low temperature region for the *a* axis, length change values derived by Touloukian et al. 1975, from the lattice parameter measurements of Finkel' and Vorob'ev 1967 (79-299 K) and Finkel' and Vorob'ev 1968 (81-300 K) were combined and in order to extrapolate below 80 K the derived polynomial equation was differentiated and fitted to Equation A using the specific heat values selected by Arblaster 2013. Below 25 K the thermal expansion coefficients of Pureur et al. 1986 (1.2 – 30 K) were accepted. In order to ensure a compromise between the low and high temperature data the selected thermal expansion coefficient at 200 K and its derivative and similar values from equation 39e at 293.15 K were used for interpolation but although accepted the derived thermal expansion curve is not considered to appear to behave naturally. As a result of this compromise then on the basis $100\Delta\varepsilon$ the measurements of Finkel' and Vorob'ev 1967, 1968 are initially 0.010 lower than the selected values while the *a* axis values of Meyeroff and Smith 1962 (5-273 K) are initially 0.057 high then trend towards the selected values.

In the low temperature region for the *c* axis, in agreement with Touloukian et al. 1975 the dilatometric measurements of Meyeroff and Smith 1962 (5-273 K) were accepted. Up to 40 K the values were fitted to Equation A together with the specific heat values selected by Arblaster 2013. At 125 K the selected thermal expansion and its derivative were combined with similar values obtained by extrapolating equation 39j to 200 K. Although the derived thermal expansion curve appears to behave naturally on the basis $100\Delta\varepsilon$ the actual length change values of Meyeroff and Smith 1962 now bias 0.010 low up to 150 K and then converge to the selected values. The *c* axis values of Finkel' and Vorob'ev 1967 (79-300 K) as given by Touloukian et al. 1975 are initially 0.022 high while those of Finkel' and Vorob'ev 1968 (81-300 K) reach a maximum deviation of 0.008 low at 161 K. The thermal expansion coefficients of Purier et al. 1986 (1.2-30 K) were not used for the *c* axis because the value at 20 K is 70% higher than the selected value.

39.2 Thermal expansion equations for alpha yttrium

a-axis:

0-25 K: $\alpha_a\ (K^{-1}) = -1.4 \times 10^{-9}\, T + 7.04 \times 10^{-11}\, T^3$ (39a)

25-100 K: $\alpha_a\ (K^{-1}) = C_p\ (6.61928 \times 10^{-8} + 8.73189 \times 10^{-10}\, T + 5.86249 \times 10^{-6}\, T)$ (39b)

100-200 K: $\alpha_a\ (K^{-1}) = 2.34290 \times 10^{-8}\, T + 2.10113 \times 10^{-6}$ (39c)

200-293.15 K: $\alpha_a\ (K^{-1}) = 2.82765 \times 10^{-7}\, T - 1.00638 \times 10^{-9}\, T^2 + 1.19347 \times 10^{-12}\, T^3 - 1.90586 \times 10^{-5}$ (39d)

293.15-936 K: $\varepsilon_T\, a = 7.32800 \times 10^{-6}\, T + 9.00900 \times 10^{-11}\, T^2 + 1.33000 \times 10^{-13}\, T^3 - 2.15930 \times 10^{-3}$ (39e)

936-1497 K: $\varepsilon_T\, a = 1.45733 \times 10^{-5}\, T - 8.93465 \times 10^{-9}\, T^2 + 3.80462 \times 10^{-12}\, T^3 - 4.04643 \times 10^{-3}$ (39f)

c-axis:

0-40 K: $\alpha_c\ (K^{-1}) = C_p\ (5.29537 \times 10^{-7} + 1.02482 \times 10^{-9}\, T - 2.06539 \times 10^{-6}\, T)$ (39g)

40-125 K: $\alpha_c\ (K^{-1}) = 3.47230 \times 10^{-7}\, T - 1.70901 \times 10^{-9}\, T^2 + 2.195139 \times 10^{-12}\, T^3 - 6.68961 \times 10^{-6}$ (39h)

125-200 K: $\alpha_c\ (K^{-1}) = 3.77431 \times 10^{-7}\, T - 1.89774 \times 10^{-9}\, T^2 + 3.28913 \times 10^{-12}\, T^3 - 8.22340 \times 10^{-6}$ (39i)

200-936 K: $\varepsilon_T\, c = 1.46100 \times 10^{-5}\, T + 8.47100 \times 10^{-9}\, T^2 - 3.01800 \times 10^{-12}\, T^3 - 4.93486 \times 10^{-3}$ (39j)

936-1497 K: $\varepsilon_T\, c = 1.99684 \times 10^{-5}\, T - 1.47472 \times 10^{-9}\, T^2 + 2.02839 \times 10^{-12}\, T^3 - 5.37258 \times 10^{-3}$ (39k)

General

1497-1751 K: ε_T avr = 1.53117 x 10^{-5} T – 6.56950 x 10^{-3} (39l)

Table 39a. Lattice parameters values for alpha yttrium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Notes
Spedding et al. 1956	RT	0.36476	0.57309	
Evans and Raynor 1960	298	0.36515	0.57472	
Harris and Raynor 1964	298	0.36509	0.57386	
Norman et al. 1967	295	0.36510	0.57389	
Finkel' and Vorob'ev 1967	299,300	0.36505	0.57406	a
Finkel and Vorob'ev 1968	300	0.36506	0.57408	a
Spedding and Beaudry 1971	297	0.36483	0.57317	b
Morris et al. 1981	298	0.36470	0.57279	
	Selected	0.36483 (2)	0.57317 (6)	

Notes for Table 39a

a. Values given by Touloukian et al. 1975

b. Temperature of measurement given by Gschneidner 1990

In agreement with Gschneidner 1990 the values determined by Spedding and Beaudry 1971 for electropolished wires are selected.

At 293.15 K: Density 4469 (1) kg m^{-3} Molar volume 19.894 (3) cm^3 mol^{-1}

39.3 Beta Phase: Body-centered cubic (cI2): 1751 K to 1795 K

Eash and Carlson 1960 confirmed the structure based on complete solid solubility between beta yttrium and beta thorium. Direct density measurements determined by Stankus and Basin 1980 at 1763 K and 1796 K were converted to length change values and fitted to the equations:

a (nm) = 2.07226 x 10^{-5} T + 0.375629 (39m)

ε_T = 5.12601 x 10^{-5} T – 7.08330 x 10^{-2} (39n)

The derived thermal expansion coefficient is 50.2 x 10^{-6} K^{-1}. The transition from the alpha to the beta phases leads to a molar volume contraction of 0.39%. The actual direct density measurements of Stankus and Basin 1980 are 0.38% greater than the calculated values, in exact agreement with the difference obtained at 293 K.

39.4 Extension of *a* and *c* axes thermal expansion values for alpha yttrium above 936 K

The average selected length change value and derived thermal expansion coefficient at 936 K were combined with length change values obtained from the direct density measurements of Stankus and Basin 1980 at 1400 K and 1497 K and fitted to the equation:

$$\varepsilon_T \text{ avr} = 1.63703 \times 10^{-5} T - 6.44684 \times 10^{-9} T^2 + 3.21221 \times 10^{-12} T^3 - 4.48795 \times 10^{-3} \quad (39o)$$

The c/a ratio trend with temperature as given in Table 39d was fitted in the range 600 K to 936 K to the equation:

$$c/a = 2.02121 \times 10^{-5} T + 1.58140 \times 10^{-9} T^2 + 1.564519 \quad (39p)$$

This equation was extrapolated to 1497 K and was combined with equation 39o to give individual length change values for the *a* and *c* axes above 936 K which were then fitted to give equations 39f and 39k.

Table 39b. Crystallographic Properties of alpha yttrium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
0	0	0	0	- 0.148	- 0.399	- 0.232
10	0.056	0.083	0.065	- 0.148	- 0.399	- 0.232
20	0.54	0.84	0.64	- 0.148	- 0.398	- 0.232
30	1.53	2.61	1.90	- 0.148	- 0.397	- 0.230
40	2.25	4.72	3.08	- 0.145	- 0.393	- 0.228
50	2.83	6.76	4.14	- 0.143	- 0.387	- 0.224
60	3.27	8.62	5.06	- 0.140	- 0.380	- 0.220
70	3.64	10.25	5.84	- 0.136	- 0.370	- 0.214
80	3.94	11.65	6.51	- 0.132	- 0.359	- 0.208
90	4.21	12.85	7.09	- 0.128	- 0.347	- 0.201
100	4.44	13.87	7.59	- 0.124	- 0.334	- 0.194
110	4.68	14.72	8.03	- 0.119	- 0.320	- 0.186
120	4.91	15.43	8.42	- 0.115	- 0.305	- 0.178
130	5.15	16.00	8.76	- 0.110	- 0.289	- 0.169
140	5.38	16.45	9.07	- 0.104	- 0.273	- 0.160
150	5.62	16.79	9.34	- 0.099	- 0.256	- 0.151
160	5.85	17.06	9.59	- 0.093	- 0.239	- 0.142
170	6.08	17.25	9.81	- 0.087	- 0.222	- 0.132
180	6.32	17.41	10.02	- 0.081	- 0.205	- 0.122
190	6.55	17.54	10.22	- 0.074	- 0.187	- 0.112
200	6.78	17.67	10.41	- 0.068	- 0.170	- 0.102
210	6.99	17.80	10.59	- 0.061	- 0.152	- 0.091
220	7.15	17.92	10.74	- 0.054	- 0.134	- 0.081
230	7.26	18.05	10.86	- 0.047	- 0.116	- 0.070
240	7.34	18.17	10.95	- 0.039	- 0.098	- 0.059
250	7.38	18.29	11.02	- 0.032	- 0.080	- 0.049
260	7.40	18.41	11.07	- 0.025	- 0.062	- 0.037
270	7.41	18.53	11.12	- 0.017	- 0.043	- 0.026
280	7.41	18.65	11.16	- 0.010	- 0.025	- 0.015
290	7.41	18.76	11.20	- 0.002	- 0.006	- 0.004
293.15	7.42	18.80	11.21	0	0	0
300	7.42	18.88	11.24	0.005	0.013	0.008
400	7.46	19.90	11.60	0.079	0.207	0.122
500	7.51	20.73	11.91	0.154	0.411	0.240
600	7.56	21.38	12.17	0.230	0.623	0.361
700	7.63	21.85	12.37	0.306	0.841	0.484
800	7.70	22.13	12.51	0.383	1.063	0.610
900	7.79	22.25	12.61	0.461	1.288	0.736
1000	8.07	22.60	12.97	0.540	1.515	0.865
1100	8.67	23.67	13.67	0.624	1.751	0.999
1200	9.50	24.70	14.56	0.715	1.997	1.142
1300	10.55	25.84	15.64	0.816	2.255	1.296
1400	11.82	27.08	16.91	0.928	2.526	1.461
1497	13.26	28.39	18.31	1.051	2.802	1.635

Table 39c. Crystallographic Properties of alpha yttrium

T K	*a* nm	*c* nm	*c*/*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.36429	0.57088	1.5671	0.35456	19.756	4500
10	0.36429	0.57088	1.5671	0.35456	19.756	4500
20	0.36429	0.57089	1.5671	0.35456	19.756	4500
30	0.36429	0.57090	1.5671	0.35457	19.757	4500
40	0.36430	0.57092	1.5672	0.35458	19.758	4500
50	0.36431	0.57095	1.5672	0.35459	19.760	4499
60	0.36432	0.57099	1.5673	0.35461	19.763	4499
70	0.36433	0.57105	1.5674	0.35464	19.766	4498
80	0.36435	0.57111	1.5675	0.35467	19.770	4497
90	0.36436	0.57118	1.5676	0.35470	19.774	4496
100	0.36438	0.57126	1.5678	0.35474	19.778	4495
110	0.36439	0.57134	1.5679	0.35478	19.783	4494
120	0.36441	0.57142	1.5681	0.35482	19.788	4493
130	0.36443	0.57151	1.5682	0.35486	19.793	4492
140	0.36445	0.57161	1.5684	0.35491	19.798	4491
150	0.36447	0.57170	1.5686	0.35495	19.804	4489
160	0.36449	0.57180	1.5688	0.35500	19.809	4488
170	0.36451	0.57190	1.5689	0.35504	19.815	4487
180	0.36453	0.57200	1.5691	0.35509	19.821	4485
190	0.36456	0.57210	1.5693	0.35514	19.827	4484
200	0.36458	0.57220	1.5695	0.35519	19.832	4483
210	0.36461	0.57230	1.5696	0.35524	19.839	4481
220	0.36463	0.57340	1.5698	0.35529	19.846	4480
230	0.36466	0.57250	1.5700	0.35534	19.852	4478
240	0.36469	0.57261	1.5701	0.35539	19.858	4477
250	0.36471	0.57271	1.5703	0.35544	19.865	4475
260	0.36474	0.27282	1.5705	0.35549	19.872	4474
270	0.36477	0.57292	1.5707	0.35554	19.878	4473
280	0.36479	0.57303	1.5708	0.35560	19.885	4471
290	0.36482	0.57314	1.5710	0.35565	19.892	4470
293.15	0.36483	0.57317	1.5711	0.35567	19.894	4469
300	0.36485	0.57324	1.5712	0.35570	19.898	4468
400	0.36512	0.57436	1.5731	0.35624	19.967	4453
500	0.36539	0.57553	1.5751	0.35681	20.037	4437
600	0.36567	0.57640	1.5772	0.35739	20.110	4421
700	0.36595	0.57799	1.5794	0.35799	20.184	4405
800	0.36623	0.57926	1.5817	0.35860	20.259	4388
900	0.36651	0.58055	1.5840	0.35922	20.336	4372
1000	0.36680	0.58185	1.5863	0.35984	20.414	4355
1100	0.36711	0.58321	1.5887	0.36049	20.496	4338
1200	0.36744	0.58462	1.5911	0.36118	20.583	4319
1300	0.36781	0.58610	1.5935	0.36190	20.678	4300
1400	0.36822	0.58765	1.5959	0.36267	20.778	4279
1497	0.36866	0.58923	1.5983	0.36346	20.886	4257

$$d1 = (a^2/3 + c^2/4)^{½} \qquad d2 = a$$

Table 39d. Bulk properties of alpha yttrium

T K	100 ε_T	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1497	1.635	20.886	4257
1500	1.640	20.889	4256
1550	1.716	20.936	4247
1600	1.793	20.983	4237
1650	1.869	21.030	4227
1700	1.946	21.078	4218
1750	2.023	21.125	4208
1751	2.024	21.126	4208

This Table is considered to be identical to Tables 39b and 39c below 1497 K

Table 39e. Crystallographic properties of beta yttrium

T K	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1751	1.892	0.4119	0.3567	21.04_5	4225
1795	2.118	0.4128	0.3575	21.18_5	4197

$$d = \sqrt{3}a/2$$

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40 ZIRCONIUM Zr

Atomic Weight: 91.224 (2) (Meija 2017)

Allotropy: Alpha phase: Hexagonal close-packed (hP2)
Beta phase: Body-centered cubic (cI2)

Fernández-Guillermet 1987 selects 1139 K for the alpha-beta transformation temperature while the melting point is a secondary fixed point on ITS-90 at 2127 (8) K (Bedford et al. 1996).

40.1 Alpha Phase: Hexagonal close-packed (hP2): 0 K to 1139 K

Anisotropic dilatometric measurements on single crystals by Lloyd 1963 (290-1133 K) and Couterne and Cizeron 1969 (293-1023 K) show marked disagreement. Assuming selected values for the beta phase are correct (see below) then extrapolation to the transition temperature leads to a volume contraction of 0.51% for the measurements of Lloyd and 0.69% for the measurements of Couterne and Cizeron. Based on the Clausius-Clapeyron equation using a slope of the temperature-pressure transition as determined by Jayaraman et al. 1963 to be – 2.4 K/kbar and an enthalpy of transition selected by Fernández-Guillermet 1987 as 4106 J mol^{-1} then the transition is a contraction of – 0.087 cm^3 mol^{-1} (– 0.61%) which is exactly halfway between the two experimental values. Because there does not appear any valid reason to choose between the two sets of thermal expansion measurements they have been averaged to represent the thermal expansion between 293.15 K and 1139 K:

$$\varepsilon_T a = 3.92916 \times 10^{-6} T + 1.99810 \times 10^{-9} T^2 - 7.27493 \times 10^{-13} T^3 - 1.30522 \times 10^{-3} \quad (40a)$$

$$\varepsilon_T c = 4.65355 \times 10^{-6} T + 4.24666 \times 10^{-9} T^2 + 4.46282 \times 10^{-13} T^3 - 1.74038 \times 10^{-3} \quad (40b)$$

On the basis $100\Delta\varepsilon$ the measurements of Lloyd trend to 0.030 lower and those of Couterne and Cizeron up to 0.028 higher. Reduced to average values, length change values derived from the lattice parameter measurements of Skinner and Johnston 1953 (298-1164 K in the alpha range) scatter 0.056 low to 0.037 high while those of Russell 1954 (283-852 K) scatter 0.078 low to 0.089 high. The earlier measurements of Couterne and Cizeron 1966 (373-973 K) trend to 0.080 lower. Bulk dilatometric measurements are not usually considered for anisotropic materials because of possible orientation effects. However, those of Petukhov 2003-2006 (343-1139 K in the alpha range) are considered because of the selection of these values for the beta phase. They trend 0.006 high up to 1100 K and then scatter 0.002 to 0.025 low above this temperature possibly due to pre-transition effects. The measurements of Amonenko et al. 1964 (444-1147 K in the alpha phase) are also considered but were shown only graphically with actual data points being given by Touloukian et al. 1975 and on average these bias 0.035 low above 1000 K. Selected values in the high temperature region by Goldak et al. 1966 closely follow those of Lloyd 1963.

In the low temperature region length changes derived from the lattice parameter values of Goldak et al. 1966 (4.2–300 K) generally are incompatible with the high temperature selected values. However, it was found that when equation 40a was extrapolated to 185 K and the derived length change values fitted to equation B utilizing the enthalpy values of Fernández-Guillermet 1987, the agreement is obtained at 4.2 K with the measurements of Goldak et al. 1966 and therefore, these values were considered to be self-consistent. Applying the same principal to the c-axis equation 40b did not reproduce the Goldak et al. 1966 values. However, constraining equation B at low temperatures then a self-consistent set of values can be obtained if equation 40b was extrapolated only to 250 K. Therefore, equation 40c represents the *a* axis thermal expansion from 0 K to 185 K and equation 40d represents the *c* axis thermal expansion from 0 K to 250 K:

$$\ln(L_a) = (H_T - H_0)\,(\,1.68265 \times 10^{-7} + 2.60259 \times 10^{-11}\,T + 8.53854 \times 10^{-6}/T) - 1.11461 \times 10^{-3} \quad (40c)$$

$$\ln(L_c) = (H_T - H_0)\,(\,2.28814 \times 10^{-7} + 1.01449 \times 10^{-10}\,T + 1.82838 \times 10^{-7}/T) - 1.40903 \times 10^{-3} \quad (40d)$$

Although the selected values required a large degree of interpolation it was found that for average length change values that on the basis $100\Delta\varepsilon$ that the dilatometric measurements of Altman et al. 1954 (20-300K) were reproduced to within 0.001 from 80 to 120 K and with agreement to better than 0.001 above this temperature while measurements on a 7.7 mm long sample by Erfling 1939, 1942 (59-293 K) showed a bias only 0.002 low. Apart from the values at 4.2 K, the measurements of Goldak et al. 1966 for both axes bias 0.004 low.

Table 40a. Lattice parameter of alpha zirconium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Note
Treco 1953	298	0.32324	0.51478	
Skinner and Johnston 1953	298	0.32331	0.51476	
Russell 1954	293	0.32313	0.51477	
Lichter 1960	302	0.32317	0.51476	
Richter et al. 1962	295	0.32328	0.51485	
Goldak, et al. 1966	298	0.32332	0.51481	
Norman et al. 1967	295	0.32338	0.51473	a
	Selected	0.32324 (8)	0.51478 (4)	

Note for Table 40a

a. The *a*-axis value was not included in the fit

At 293.15 K: Density 6504 (3) kg m^{-3} Molar volume 14.026 (7) cm^3 mol^{-1}.

40.2 Beta Phase: Body-centered cubic (cI2): 1139 K to 2127 K

Dilatometric measurements of Petukhov 2003-2006 (1142-1832 K) and Amonenko et al. 1964 (1155-1740 K) were averaged. Again the latter measurements were shown only graphically with actual data points being given by Touloukian et al. 1975. Because of post-transition effects the measurements were only evaluated in the ranges 1207-1832 K and 1217-1740 K respectively but are considered as representing the thermal expansion from 1139 K to the melting point:

$$a\ (\text{nm}) = 2.28553 \times 10^{-6}\,T + 5.31605 \times 10^{-10}\,T^{2} + 0.358070 \qquad (40e)$$

$$\varepsilon_T = 6.35212 \times 10^{-6}\,T + 1.47748 \times 10^{-9}\,T^{2} - 4.82300 \times 10^{-3} \qquad (40f)$$

Equation 40e extrapolates to 0.3588 nm in the room temperature region in exact agreement with a value of 0.3588 (1) nm determined by Benites et al. 2000 by extrapolating Zr-Nb alloys to pure Zr. On these grounds equations 40e and 40f were considered to be self-consistent and justified the extrapolation to the melting point. The molar volume change at the alpha-beta transition temperature at 1139 K is selected as a decrease of 0.61%.

The lattice parameter determined by Skinner and Johnston 1953 at 1252 K is only 0.00012 (20) nm lower than the selected value but on the basis $100\Delta\varepsilon$ the dilatometric measurements of Skinner and Johnston 1953 (1166-1584 K), show an average bias of 0.058 low. Lattice parameters determined by Heiming et al. 1991, 1992 (1173-1823 K) trend from 0.0001 to 0.0004 nm lower but this is within the accuracy of ± 0.0005 nm assigned to these values. Direct density measurements of Paradis and Rhim 1999 (1250-2100 K) trend from 1.1% to 2.0% higher than the selected values.

Table 40b. Crystallographic properties of alpha zirconium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
0	0	0	0	- 0.111	- 0.141	- 0.121
10	0.09	0.03	0.07	- 0.111	- 0.141	- 0.121
20	0.50	0.24	0.42	- 0.111	- 0.141	- 0.121
30	1.29	0.80	1.13	- 0.110	- 0.140	- 0.120
40	2.00	1.48	1.83	- 0.109	- 0.139	- 0.119
50	2.60	2.17	2.46	- 0.106	- 0.137	- 0.117
60	3.11	2.84	3.02	- 0.103	- 0.135	- 0.114
70	3.48	3.41	3.46	- 0.100	- 0.132	- 0.111
80	3.75	3.88	3.79	- 0.096	- 0.128	- 0.107
90	3.93	4.26	4.04	- 0.093	- 0.124	- 0.103
100	4.07	4.59	4.24	- 0.089	- 0.119	- 0.099
110	4.17	4.86	4.40	- 0.085	- 0.115	- 0.095
120	4.25	5.09	4.53	- 0.080	- 0.110	- 0.090
130	4.31	5.29	4.64	- 0.076	- 0.105	- 0.086
140	4.38	5.49	4.75	- 0.072	- 0.099	- 0.081
150	4.44	5.67	4.83	- 0.067	- 0.094	- 0.076
160	4.49	5.82	4.94	- 0.063	- 0.088	- 0.071
170	4.54	5.97	5.01	- 0.058	- 0.082	- 0.066
180	4.57	6.10	5.08	- 0.054	- 0.076	- 0.061
190	4.61	6.23	5.15	- 0.049	- 0.070	- 0.056
200	4.64	6.34	5.21	- 0.045	- 0.063	- 0.051
210	4.67	6.45	5.27	- 0.040	- 0.057	- 0.046
220	4.70	6.56	5.32	- 0.035	- 0.051	- 0.040
230	4.73	6.66	5.38	- 0.030	- 0.044	- 0.035
240	4.76	6.76	5.43	- 0.026	- 0.037	- 0.030
250	4.79	6.86	5.48	- 0.021	- 0.031	- 0.024
260	4.82	6.95	5.53	- 0.016	- 0.024	- 0.019
270	4.85	7.05	5.58	- 0.011	- 0.017	- 0.013
280	4.88	7.14	5.63	- 0.006	- 0.010	- 0.007
290	4.91	7.23	5.68	- 0.002	- 0.002	- 0.002
293.15	4.91	7.26	5.69	0	0	0
300	4.93	7.32	5.73	0.003	0.005	0.004
400	5.18	8.26	6.20	0.054	0.083	0.064
500	5.38	9.22	6.66	0.107	0.170	0.128
600	5.53	10.20	7.09	0.161	0.268	0.197
700	5.64	11.21	7.50	0.217	0.370	0.270
800	5.71	12.24	7.89	0.274	0.493	0.347
900	5.74	13.30	8.26	0.332	0.621	0.428
1000	5.72	14.38	8.61	0.389	0.761	0.513
1100	5.66	15.48	8.93	0.447	0.911	0.601
1139	5.62	15.91	9.05	0.469	0.973	0.637

Table 40c. Crystallographic properties of alpha zirconium

T K	*a* nm	*c* nm	*c*/*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.32288	0.51406	1.5921	0.31751	13.975	6528
10	0.32288	0.51406	1.5921	0.31751	13.975	6528
20	0.32288	0.51406	1.5921	0.31751	13.975	6528
30	0.32288	0.51406	1.5921	0.31751	13.975	6528
40	0.32289	0.51406	1.5921	0.31752	13.976	6527
50	0.32290	0.51407	1.5921	0.31752	13.977	6527
60	0.32291	0.51409	1.5921	0.31753	13.978	6526
70	0.32292	0.51410	1.5921	0.31754	13.979	6526
80	0.32293	0.51412	1.5921	0.31755	13.981	6525
90	0.32294	0.51414	1.5921	0.31757	13.982	6524
100	0.32295	0.51417	1.5921	0.31758	13.984	6523
110	0.32297	0.51419	1.5921	0.31760	13.986	6523
120	0.32298	0.51422	1.5921	0.31761	13.988	6522
130	0.32299	0.51424	1.5921	0.31763	13.990	6521
140	0.32301	0.51427	1.5921	0.31764	13.992	6520
150	0.32302	0.51430	1.5921	0.31766	13.994	6519
160	0.32304	0.51433	1.5922	0.31768	13.996	6518
170	0.32305	0.51436	1.5922	0.31769	13.998	6517
180	0.32307	0.51439	1.5922	0.31771	14.000	6516
190	0.32308	0.51442	1.5922	0.31773	14.002	6515
200	0.32310	0.51445	1.5923	0.31775	14.004	6514
210	0.32311	0.51449	1.5923	0.31776	14.006	6513
220	0.32313	0.51452	1.5923	0.31778	14.009	6512
230	0.32314	0.51455	1.5924	0.31780	14.011	6511
240	0.32316	0.51459	1.5924	0.31782	14.013	6510
250	0.32317	0.51462	1.5924	0.31784	14.016	6509
260	0.32319	0.51466	1.5924	0.31786	14.018	6508
270	0.32320	0.51469	1.5925	0.31788	14.020	6507
280	0.32322	0.51473	1.5925	0.31790	14.023	6506
290	0.32324	0.51477	1.5926	0.31792	14.025	6504
293.15	0.32324	0.51478	1.5926	0.31793	14.026	6504
300	0.32325	0.51481	1.5926	0.31794	14.027	6503
400	0.32341	0.51521	1.5930	0.31816	14.052	6492
500	0.32359	0.51566	1.5936	0.31840	14.080	6479
600	0.32376	0.51616	1.5943	0.31866	14.109	6466
700	0.32394	0.51671	1.5951	0.31895	14.140	6452
800	0.32413	0.51732	1.5960	0.31925	14.172	6437
900	0.32431	0.51798	1.5972	0.31959	14.207	6421
1000	0.32450	0.51870	1.5985	0.31994	14.243	6405
1100	0.32468	0.51947	1.5999	0.32032	14.280	6388
1139	0.32476	0.51979	1.6006	0.32047	14.295	6381

$$d1 = (a^2/3 + c^2/4)^{1/2} \qquad d2 = a$$

Table 40d. Crystallographic properties of beta zirconium

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1139	9.68	0.433	0.36136	0.31295	14.209	6420
1200	9.85	0.493	0.36158	0.31314	14.234	6409
1300	10.13	0.593	0.36194	0.31345	14.277	6390
1400	10.42	0.697	0.36231	0.31377	14.321	6370
1500	10.70	0.803	0.36269	0.31410	14.366	6350
1600	10.98	0.912	0.36309	0.31444	14.413	6329
1700	11.26	1.025	0.36349	0.31479	14.461	6308
1800	11.54	1.140	0.36391	0.31515	14.511	6287
1900	11.82	1.258	0.36433	0.31552	14.562	6265
2000	12.10	1.379	0.36477	0.31590	14.614	6242
2100	12.37	1.503	0.36521	0.31628	14.668	6219
2127	12.45	1.537	0.36534	0.31639	14.682	6213

$$d = \sqrt{3}a/2$$

References for Zirconium

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41 NIOBIUM Nb

Atomic weight: 92.90637 (1) (Meija 2017)

Structure: Body-centered cubic (cI2)

The superconducting transition temperature at 9.2880 (25) K and the melting point at 2745 (7) K are secondary fixed point on ITS-90 (Bedford et al. 1996).

41.1 Allotropy

As with vanadium and tantalum, dilatometric measurements of Bollinger et al. 2011 suggested a structural distortion below 300 K leading to structure which is not cubic. However, lattice parameter measurements of both Smirnov and Finkel' 1965 and Roberge 1975 suggest that the structure remains body-centered cubic down to at least 120 K and even Bollinger et al. 2011 found the structure to be cubic down to 60 K in contradiction to their dilatometric measurements. Anelastic measurements on high purity metal by Cordero 2012 (0-300 K) showed no evidence of a martensitic transformation. Therefore, until the measurements of Bollinger et al. 2011 have been independently verified and the supposed new low temperature structure has been fully characterized then it is assumed that the structure remains body-centered cubic over the whole temperature range.

41.2 Low temperature

In the superconducting region specific heat measurements of White 1962 (6-9 K) were extrapolated below 6 K and leads to negative thermal expansion coefficients in agreement with the observations of Popov and Pervakov 1982 (4.5-10 K). Above the superconducting temperature the measurements of White 1962 (10-85 K) were combined with those of Lebedev et al. 1969 (8-282 K) and Radcliffe et al. 1983 (10-290 K) where the latter measurements were only considered below 100 K. Above 30 K the thermal expansion can be represented by the equations:

$$30 - 100\ \text{K}: \quad \alpha\ (\text{K}^{-1}) = -9.76552 \times 10^{-8}\,T + 4.79390 \times 10^{-9}\,T^{2} - 5.32669 \times 10^{-11}\,T^{3} + 1.96357 \times 10^{-13}\,T^{4} - 5.34302 \times 10^{-7} \qquad (41a)$$

$$100 - 293.15\ \text{K}: \quad \alpha\ (\text{K}^{-1}) = 7.34499 \times 10^{-8}\,T - 2.75203 \times 10^{-10}\,T^{2} + 3.59929 \times 10^{-13}\,T^{3} + 1.23693 \times 10^{-7} \qquad (41b)$$

Where the selected value of thermal expansion at 293.15 K is derived from the measurements given in Table 41a:

Table 41a. Room temperature thermal expansion values for niobium

References	$\alpha \times 10^6$ K^{-1}	Method
Lebedev et al. 1969	7.10	Extrapolated from 211 to 282 K
Lisovskii 1972	7.08	Value given at 300 K
Radcliffe et al. 1983	7.06	Value given at 290 K
De Camargo et al. 1987	7.05	From equation
Selected	7.07	

Linkoaho and Rantavuori 1970 obtain 7.2 (2) x 10^{-6} K^{-1} at 300 K in satisfactory agreement while the lattice parameter measurements of Straumanis and Zyszczynski 1970 (288-338 K) lead to a mean value of 7.6 x 10^{-6} K^{-1}.

On the basis $100\Delta\varepsilon$ selected length change values were confirmed by dilatometric measurements of Erfling 1942 (61-313 K) which are initially only 0.005 high then agreed exactly with the selected values above 200 K while the measurements of De Camargo et al. 1987 (75-300 K) agree with the selected values to within 0.002. Lattice parameter measurements of Smirnov and Finkel' 1965 (128-396 K) were only shown graphically with actual data points as length change values given by Touloukian et al. 1975. Measurements of Hidnert and Krider 1933 (138-575 K) were not considered in the evaluation because the metal used contained 0.93% tin and 0.26% iron.

41.3 High temperature

Dilatometric measurements of Heal 1958 (291-1173 K), Johnson et al. 1968 (298-1773 K), Petukov et al. 1977 (1261-2289 K), Petukov et al. 1978 (1198-1996 K) and Miiller and Cezairliyan 1988, 1991 (1500-2700 K) were combined to give the following equation with an overall accuracy on the basis $\pm 100\varepsilon_T$ of ± 0.008:

$$\varepsilon_T = 6.01076 \times 10^{-6} T + 2.19939 \times 10^{-9} T^2 - 9.83941 \times 10^{-13} T^3 + 2.32275 \times 10^{-16} T^4 - 1.92799 \times 10^{-3} \quad (41c)$$

Because the selected high temperature values are dilatometric measurements they cannot truly be considered as representing the crystallographic properties because of the onset of thermal vacancy effects. The enthalpy of vacancy formation (H_V) has been determined using positron annihilation Doppler broadening by Maier et al. 1979 to be 2.6 (3) eV. Estimating the vacancy concentration parameter (C_V) at 1.0 x 10^{-3} for refractory metals would lead to an entropy of vacancy formation of S_V/k = 4.1. However, because of the speculation over the value of C_V no thermal vacancy corrections were applied.

Direct density measurements of Paradis et al. 2001 (1500-2740 K) trend from 1.2% to 3.3% higher. On the basis $100\Delta\varepsilon$ deviations of dilatometric and lattice parameter values converted to length change values are given in Table 41c and Table 41d.

Table 41b. Lattice parameter values of niobium at 293.15 K

References	Original Temperature K	*a* nm	Notes
Neuburger 1936	293	0.33009	
Edwards et al. 1951	291	0.33006	
Seybolt 1954	RT	0.33003	a
Bolef 1961	300	0.33008	b
Gebhardt and Rothenbacher 1963a, 1963b	293	0.33001	a
Smirnov and Finkel' 1965	293	0.33009	c
Gebhardt et al. 1966	293	0.33002	a
Vasyutinskiy et al. 1966	293	0.33002	c
Barns 1968	298	0.33002	
Straumanis and Zyszczynski 1970	288, 298	0.33005	d
Fisher et al. 1975	298	0.33008	e
Morris et al. 1982	298	0.33032	f
	Selected	0.33005 (4)	

Notes for Table 41a

a. Extrapolated to zero oxygen content

b. From direct density measurement 8578 kg m^{-3} at 300 K

c. Value given by Touloukian et al. 1975

d. As an addition a direct density measurement 8581.6 (3) kg m^{-3} at 298 K leads to the same value of lattice parameter at 293.15 K as obtained from the lattice parameter measurement

e. From direct density measurement 8579 kg m^{-3} at 298 K

f. Not included in the average

In addition, Taylor and Doyle 1967 obtained 0.32988 (1) nm for ultrapure niobium but this value was rejected by Donohue 1974 as being too divergent. Because this value has not been verified by other sources then the consensus value obtained above was selected.

At 293.15 K: Density 8582 (3) kg m^{-3} Molar volume 10.826 (4) cm^3 mol^{-1}.

41.4 Deviations of experimental values from the selected values

Table 41c. Lattice parameter values

References	Temperature Range K	Deviations 100Δε
Edwards et al. 1951	291-2073	Scatter 0.021 low to 0.14 high
Smirvov and Finkel' 1965	128-396	Trend from 0.067 high to 0.041 low
Vasyutinskiy et al. 1966	293-2616	Shows scatter but can be considered as trending 0.12 high at 1270 K to 0.035 low at 2616 K
Frantsevich et al. 1967	293, 1473	0.009 low at 1473 K
Roberge 1975	120-295	Trends from 0.016 high

Table 41d. Dilatometric values

References	Temperature Range K	Deviations 100Δε
Tottle 1957	291-1273	Trends to 0.015 low
Fieldhouse et al. 1958	300-1824	Trends to average 0.15 high above 1500 K
Amonenko et al. 1964	293-2273	Trends from 0.05 low at 1071 K to 0.10 high at 2273 K
Ul'yanov et al. 1964	299-1307	Trends to 0.037 high at 1307 K
Conway et al. 1965	298-2281	Run I: 556-2281 K: Scatters 0.079 low to 0.084 high; Run II: 1274-2074 K: trends to maximum low of 0.064 at 1802 K; Run III: 484-2281 K: Trends from 0.059 low at 1274 K to 0.009 high at 2281 K; Run IV: 298-2064 K: Scatters 0.017 low to 0.052 high
Prindatseva and Solov'yeva 1965	293-1173	Run I: 293, 1073 K: 0.004 low at 1073 K; Run II: 293-1173 K: Trends to 0.017 low
Conway and Losekamp 1966	421-2355	Run I: 578-2272 K: Trends from 0.11 low at 1380 K to 0.047 high at 2272 K; Run II: 421-2355 K: Trends from 0.13 low at 1633 K to 0.032 low at 2355 K; Run III: 497-2305 K: Trends from 0.11 low at 1604 K to 0.032 low at 2305 K
Harris and Peacock 1966	77-387	Average bias 0.007 high below room temperature and average bias 0.008 low above
Mochalov and Ivanov 1969	293-2417	Trends from 0.054 high at 2010 K to 0.027 high at 2417 K
Hubbell and Brotzen 1972	83, 373	0.048 low and 0.012 high
Lisovskii 1972	55-300	Trends from 0.012 high
Righini et al. 1986	1000-2600	Trends to 0.038 high

Table 41e. Low temperature crystallographic properties of niobium

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	- 0.147	0.32956	0.28541	10.778	8620
5	- 0.001	- 0.147	0.32956	0.28541	10.778	8620
9.288	0.018	- 0.147	0.32956	0.28541	10.778	8620
10	0.044	- 0.147	0.32956	0.28541	10.778	8620
20	0.28	- 0.147	0.32956	0.28541	10.778	8620
30	0.64	- 0.147	0.32957	0.28541	10.778	8620
40	1.39	- 0.146	0.32957	0.28542	10.779	8620
50	2.21	- 0.144	0.32958	0.28542	10.779	8619
60	2.97	- 0.141	0.32958	0.28543	10.780	8618
70	3.63	- 0.138	0.32959	0.28544	10.781	8618
80	4.17	- 0.134	0.32961	0.28545	10.782	8617
90	4.63	- 0.130	0.32962	0.28546	10.784	8615
100	5.08	- 0.125	0.32964	0.28547	10.785	8614
110	5.35	- 0.120	0.32966	0.28549	10.787	8613
120	5.60	- 0.114	0.32967	0.28551	10.789	8611
130	5.81	- 0.108	0.32969	0.28552	10.791	8610
140	6.00	- 0.103	0.32971	0.28554	10.793	8608
150	6.16	- 0.096	0.32973	0.28556	10.794	8607
160	6.30	- 0.090	0.32975	0.28557	10.797	8605
170	6.43	- 0.084	0.32977	0.28559	10.799	8604
180	6.53	- 0.077	0.32979	0.28561	10.801	8602
190	6.61	- 0.071	0.32982	0.28563	10.803	8600
200	6.68	- 0.064	0.32984	0.28565	10.805	8598
210	6.75	- 0.057	0.32986	0.28567	10.807	8597
220	6.80	- 0.051	0.32988	0.28569	10.809	8595
230	6.84	- 0.044	0.32991	0.28571	10.812	8593
240	6.88	- 0.037	0.32993	0.25873	10.814	8591
250	6.91	- 0.030	0.32995	0.28575	10.816	8590
260	6.94	- 0.023	0.32997	0.28577	10.818	8588
270	6.98	- 0.016	0.33000	0.28579	10.821	8586
280	7.01	- 0.009	0.33002	0.28581	10.823	8584
290	7.06	- 0.002	0.33004	0.28583	10.825	8583
293.15	7.07	0	0.33005	0.28583	10.826	8582

$$d = \sqrt{3}a/2$$

Table 41f. High temperature crystallographic properties of niobium

T K	$\alpha \times 10^{-6}$ K^{-1}	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
293.15	7.07	0	0.33005	0.28583	10.826	8582
300	7.09	0.005	0.33007	0.28585	10.827	8581
400	7.35	0.077	0.33030	0.28605	10.851	8562
500	7.58	0.152	0.33055	0.28627	10.875	8543
600	7.77	0.229	0.33081	0.28649	10.900	8523
700	7.94	0.308	0.33107	0.28671	10.926	8503
800	8.08	0.388	0.33133	0.28694	10.952	8483
900	8.22	0.470	0.33160	0.28717	10.979	8462
1000	8.34	0.553	0.33188	0.28741	11.006	8441
1100	8.46	0.638	0.33215	0.28765	11.034	8420
1200	8.58	0.723	0.33244	0.28790	11.062	8398
1300	8.71	0.810	0.33272	0.28815	11.091	8377
1400	8.85	0.899	0.33302	0.28840	11.120	8355
1500	9.01	0.989	0.33331	0.28866	11.150	8332
1600	9.20	1.081	0.33362	0.28892	11.181	8309
1700	9.41	1.175	0.33393	0.28919	11.212	8286
1800	9.66	1.272	0.33425	0.28947	11.264	8263
1900	9.95	1.371	0.33458	0.28975	11.277	8238
2000	10.28	1.474	0.33491	0.29004	11.311	8213
2100	10.67	1.580	0.33526	0.29035	11.347	8188
2200	11.11	1.690	0.33563	0.29066	11.384	8161
2300	11.61	1.806	0.33601	0.29099	11.423	8133
2400	12.17	1.927	0.33641	0.29134	11.464	8104
2500	12.81	2.054	0.33683	0.29170	11.507	8074
2600	13.53	2.189	0.33727	0.29209	11.552	8042
2700	14.32	2.331	0.33774	0.29249	11.601	8009
2745	14.71	2.398	0.33796	0.29269	11.623	7993

$$d = \sqrt{3}a/2$$

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42 MOLYBDENUM Mo

Atomic weight: 95.95 (1) (Meija 2017)

Structure: Body-centered cubic (cI2)

The melting point is a secondary fixed point on ITS-90 at 2895 (4) K (Bedford et al. 1996).

42.1 Low temperature

The thermal expansion coefficients of Lebedev et al. 1969 (10-285 K) and White et al. 1978 (4-100, 283 K) were combined but also take into account the thermal expansion coefficients determined by White et al. 1978 as 5.10 x 10^{-6} K^{-1} at 283 K and Lisovskii 1972 as 5.09 x 10^{-6} K^{-1} at 300 K. Above 80 K the values can be represented by the following equations where the accuracy for the 80 to 140 K range is 3 x 10^{-8} K^{-1} and for the 140 to 293.15 K range is 6 x 10^{-8} K^{-1}:

$$80\text{ -}140\text{ K:}\quad \alpha\,(K^{-1}) = 1.78037 \times 10^{-7}\,T - 1.05853 \times 10^{-9}\,T^{2} + 2.30993 \times 10^{-12}\,T^{3} - 6.59778 \times 10^{-6} \qquad (42a)$$

$$140\text{ - }293.15\text{ K:}\quad \alpha\,(K^{-1}) = 6.93461 \times 10^{-8}\,T - 2.48633 \times 10^{-10}\,T^{2} + 3.13946 \times 10^{-13}\,T^{3} - 1.76834 \times 10^{-6} \qquad (42b)$$

On the basis 100Δε smoothed dilatometric measurements of Nix and MacNair 1942 (86-298 K) show a bias of only 0.001 low while the values of Erfling 1939 (78-273 K) show a bias of only 0.001 high. Dilatometric measurements of Davidson and Brotzen 1968 (73-373 K) and Lisovskii 1972 (55-300 K) were shown only graphically with actual data points given by Touloukian et al. 1975. The deviations of the lattice parameter and dilatometric measurements from the selected values are considered in Part 42.3 Lattice parameter measurements of Straumanis and Woodard 1971 (40-180 K) were also only shown graphically and were not related to a room temperature value. Values of Amitin et al. 1981 (80-300 K) were also only shown graphically. The lattice parameter measurements of Straumanis and Shodhan 1968 (288-338 K) lead to a mean thermal thermal expansion coefficient of 4.89 x 10^{-6} K^{-1} which is 4% lower than the selected value.

42.2 High Temperature

Dilatometric measurements of Petukhov et al. 1976 (400-2819 K), Amatuni et al. 1976 (1073-2273 K), Petukhov et al. 1977 (1274-2427 K) and Miiller and Cezairliyan 1985, 1991 (1500-2800 K) were combined to give the selected equation:

$$\varepsilon_T = 4.17633 \times 10^{-6}\,T + 1.90575 \times 10^{-9}\,T^{2} - 8.41763 \times 10^{-13}\,T^{3} + 2.31673 \times 10^{-16}\,T^{4} - 1.36857 \times 10^{-3} \qquad (42c)$$

Because the selected high temperature values are dilatometric measurements they cannot truly be considered as representing the crystallographic properties because of the onset of thermal vacancy effects. The enthalpy of vacancy formation (H_V) has been determined by three different techniques:

Table 42a. Thermal vacancy parameters for molybdenum

References	Method	H_V eV
Ziegler and Schaefer 1987	Positron lifetime spectroscopy	3.6 (2)
Maier et al. 1979	Doppler broadening	3.0 (2)
Schaffer 1987	Mean lifetimes	3.0 (2)
	Average	3.2 (4)

Estimating the vacancy concentration parameter (C_V), at 1.0 x 10^{-3} for refractory metals would lead to an entropy of vacancy formation of S_V/k = 5.9. However, because of the speculation over the value of C_V no thermal vacancy corrections were applied.

Table 42b. Lattice parameter values of molybdenum at 293.15 K

References	Original Temperature K	*a* nm
Owen and Iball 1932	289.7	0.31469
Jette and Foote 1935	298	0.31475
Lu and Chang 1941	293	0.31468
Edwards et al. 1951	291	0.31476
Geach and Summers Smith 1951-1952	293	0.31470
Swanson and Tatge 1953	298	0.31473
Geach and Summers Smith 1953-1954	293	0.31469
Anderson and Hume Rothery 1960	293	0.31469
Taylor et al. 1961, 1962	296	0.31471
Ross and Hume Rothery 1963	294.7	0.31472
Niemec 1963	RT	0.31471
Casselton and Hume Rothery 1964	RT	0.31468
Catterall and Barker 1965	295	0.31470
Clark and Knight 1965	294	0.31473
Straumanis and Shodhan 1968	298.2	0.31471
Woodward and Straumanis 1971	295.6	0.31471
	Selected	0.31471 (2)

At 293.15 K: Density 10223 (3) kg m^{-3} Molar volume 9.385 (2) cm^3 mol^{-1}.

The measurements of Petukhov et al. 1976 are considered as replacing earlier measurements of Chekhovskoi and Petukhov 1970 (1185-2470 K) and Petukhov and Chekhovskoi 1972 (2023-2819 K). Volume ratios obtained from rapid pulse heating measurements of Hixson and Winkler 1992 (1917-2896 K) when converted to length change values scatter from 0.20 low to 0.069 high. Direct density measurements of Paradis et al. 2002a (2170-2890 K) trend from 0.2% high to 0.8% low. Thermal expansion coefficients of Zhao et al. 2000 (298-1475 K) trend to 36% higher than the selected values. The dilatometric measurements of Nasekovskii 1969 (77-1700 K), Chekhovskoi et al. 1987 (1100-2600 K), and Chanchani and Hall 1990 (1500-2200 K) were only shown graphically.

42.3 Deviations of experimental values from the selected values

Table 42c. Dilatometric values

References	Temperature Range K	Deviations 100Δε
Schad and Hidnert 1919	131-578	Trends from initially 0.004 high then scatters 0.006 low to 0.005 high above room temperature
Hidnert and Gero 1924	289-783	22 runs average trend to 0.013 low
Worthing 1926	300-2400	Trends to 0.055 low
Burger 1934	298-823	Trends to average 0.012 high above 500 K
Demarquay 1945	293-2273	Scatters 0.052 to 0.001 low
Apblett and Pellini 1952	294-1922	Trends to 0.077 low at 1255 K then to 0.033 low at 1922 K
Fieldhouse et al. 1956	319-1850	Trends to 0.043 low at 1305 K then to 0.046 high at 1850 K
Lucks and Deem 1956	297-1866	Trends to 0.026 low at 1089 K then to 0.010 high
Lucks and Deem 1958	297-1866	Trends to 0.025 low at 1033 K then to 0.007 high
Rasor and McClelland 1957, 1960	301-2864	Run 1: 308-2852 K: Scatter 0.087 low to 0.048 high; Run 2: 311-2759 K: Average 0.027 high above 2400 K Run 3: 301-2864 K: Trends to 0.085 high at 2221 K to 0.061 low at 2864; Run 4: 1143-2804 K: Average 0.026 low above 2600 K
Levingstein 1961	297-1422	Trends to average 0.070 high above 1300 K
Baskin et al. 1961	291, 673	0.005 low at 673 K
Denman 1962	355-1366	Trends to average 0.005 low above 500 K
Amonenko et al. 1964	552-2273	Scatter 0.024 low to 0.010 high
Totskii 1964	273-1373	Trends to 0.008 low
Abuzov and Zelenkov 1964	293-873	Trends to 0.068 low
Valentich 1965	293-799	Trends to 0.045 low
Yagee and Styles 1965	288-1240	Trends to 0.029 high
Pridantseva and Solov'yeva 1965	293-1073	Run 1: 1073 K: 0.023 low; Run 2: 293-973 K: Trends 0.016 to 0.006 low
Conway and Losekamp 1966	298-2773	Rod: 298-2773: Trends to average 0.092 above 2000 K Sheet PM: 298-2523 K: Trends to average 0.059 high above 1800 K; Sheet AC: 298-2523 K: Trends to 0.10 high
Conway and Flagella 1967	298-2778	Run 1: 298-2765 K: Trends to 0.15 high; Run 2: 298-2778 K: Trends to average 0.12 high above 2400 K; Run 3: 298-2748 K: Trends to minimum 0.043 low at 1253 K to 0.15 high at 2748 K
Mulyakaev et al. 1967	293-1374	Trends to 0.078 low
Davidson and Brotzen 1968	73-373	Trends 0.015 low to 0.008 high
Mochalov and Ivanov 1969	293-2394	Trends to 0.047 high at 1312 K then to average 0.097 low above 2300 K
Velentich 1969	396-2476	Trends to 0.075 high at 1601 K then to 0.030 low at 2476 K
Hubbell and Brotzen 1972	83, 373	0.015 low and 0.002 low
Lisovskii 1972	55-300	Trends from maximum 0.006 high at 120 K to agree with selected values.
Shevchenko et al. 1986	373-673	Trends to 0.007 low
Onufriev et al. 1986	1900-2500	Trends 0.003 low to 0.009 low
Suh et al. 1988	293-1200	Trends to 0.039 high
Reiter and Kaschnitz 2002	1200-2300	Average bias 0.006 high

Table 42d. Lattice parameter values

References	Temperature Range K	Deviations 100Δε
Edwards et al. 1951	291-2073	Trends from 0.044 low at 1162 K to 0.028 high at 2073 K
Ross and Hume Rothery 1963	295-1733	Trends from 0.039 high at 1432 K to 0.042 low at 1921 K
Clark and Knight 1965	294-1477	Trends to 0.033 low
Pawar 1967	309-799	Average bias 0.017 high
Frantsevich et al. 1967	293, 1473	0.095 low at 1473 K
Woodward and Straumanis 1972	140-296	Trends from 0.008 low to 0.004 high
Waseda et al. 1975	298-2614	Trends to average of 0.057 high above 2200 K

42.4 Comparison with previous evaluations in the high temperature region

Choudhury and Brooks 1984 gave their review in the form of equations and tabulated thermal expansion coefficients which leads to a value at 2890 K which is 12% lower than the selected value. Touloukian et al. 1975 did not have access to any of the values used in the present evaluation but on the basis 100Δε their values differ by 0.027 low at 1200 K increasing to 0.009 high at 2600 K before increasing rapidly to 0.047 high at 2800 K. More recent reviews are generally based on the same measurements as selected in the present review and as a result the values of Fokin and Chekovskoi 1991 average only 0.002 low above 700 K while those of Wang and Reeber 1998 trended from only 0.004 low at 1100 K to an average of 0.002 high above 1800 K. Selected values of White 1998 bias 0.007 low above 1000 K. Bodryakov 2014 reported the results as volume thermal expansion. When corrected to linear thermal expansion the deviation in the high temperature region is from 1.0% low at 300 K to 3.1% low at 800 K to 3.5% high at 1700 K to 5.6% low at the melting point. However, Bodryakov 2014 did not directly mention in the evaluation the inclusion of the important high precision dilatometric measurements used in the present evaluation.

Table 42e. Low temperature crystallographic properties of molybdenum

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	- 0.0956	0.31441	0.27229	9.359	10253
10	0.006	- 0.0956	0.31441	0.27229	9.359	10253
20	0.035	- 0.0956	0.31441	0.27229	9.359	10253
30	0.125	- 0.0956	0.31441	0.27229	9.359	10253
40	0.33	- 0.0953	0.31441	0.27229	9.359	10253
50	0.67	- 0.0948	0.31441	0.27229	9.359	10253
60	1.12	- 0.0940	0.31441	0.27229	9.359	10253
70	1.59	- 0.0926	0.31442	0.27229	9.359	10252
80	2.05	- 0.0908	0.31442	0.27230	9.360	10252
90	2.54	- 0.0885	0.31443	0.27231	9.360	10251
100	2.93	- 0.0858	0.31444	0.27231	9.361	10250
110	3.25	- 0.0827	0.31445	0.27232	9.362	10249
120	3.52	- 0.0793	0.31446	0.27233	9.363	10248
130	3.73	- 0.0757	0.31447	0.27234	9.364	10247
140	3.93	- 0.0718	0.31448	0.27235	9.365	10245
150	4.10	- 0.0678	0.31450	0.27236	9.366	10244
160	4.25	- 0.0636	0.31451	0.27237	9.368	10243
170	4.38	- 0.0593	0.31452	0.27239	9.369	10242
180	4.49	- 0.0549	0.31454	0.27240	9.370	10240
190	4.59	- 0.0503	0.31455	0.27241	9.371	10239
200	4.67	- 0.0457	0.31457	0.27242	9.373	10237
210	4.74	- 0.0410	0.31458	0.27244	9.374	10236
220	4.80	- 0.0362	0.31460	0.27245	9.375	10234
230	4.85	- 0.0314	0.31461	0.27246	9.377	10233
240	4.89	- 0.0266	0.31463	0.27247	9.378	10231
250	4.93	- 0.0216	0.31464	0.27249	9.379	10230
260	4.97	- 0.0167	0.31466	0.27250	9.381	10228
270	5.01	- 0.0117	0.31467	0.27251	9.382	10227
280	5.05	- 0.0067	0.31469	0.27253	9.384	10225
290	5.09	- 0.0016	0.31470	0.27254	9.385	10224
293.15	5.10	0	0.31471	0.27255	9.385	10223

$$d = \sqrt{3}a/2$$

Table 42f. High temperature crystallographic properties of molybdenum

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
293.15	5.10	0	0.31471	0.27255	9.385	10223
300	5.12	0.003	0.31472	0.27256	9.386	10222
400	5.35	0.056	0.31489	0.27270	9.401	10206
500	5.56	0.111	0.31506	0.27285	9.417	10189
600	5.76	0.167	0.31524	0.27300	9.433	10172
700	5.92	0.226	0.31542	0.27316	9.449	10154
800	6.07	0.286	0.31561	0.27333	9.466	10136
900	6.22	0.347	0.31580	0.27349	9.482	10118
1000	6.36	0.410	0.31600	0.27367	9.501	10099
1100	6.52	0.475	0.31620	0.27384	9.520	10079
1200	6.68	0.541	0.31641	0.27402	9.539	10059
1300	6.86	0.609	0.31663	0.27421	9.558	10039
1400	7.06	0.679	0.31685	0.27440	9.578	10018
1500	7.28	0.752	0.31708	0.27460	9.599	9996
1600	7.54	0.826	0.31731	0.27480	9.620	9974
1700	7.84	0.904	0.31755	0.27501	9.642	9951
1800	8.18	0.985	0.31781	0.27523	9.665	9927
1900	8.57	1.069	0.31807	0.27546	9.690	9902
2000	9.01	1.158	0.31835	0.27570	9.715	9876
2100	9.51	1.252	0.31865	0.27596	9.742	9849
2200	10.07	1.351	0.31896	0.27623	9.771	9820
2300	10.70	1.456	0.31929	0.27652	9.801	9789
2400	11.41	1.568	0.31965	0.27682	9.834	9757
2500	12.20	1.688	0.32002	0.27715	9.869	9923
2600	13.07	1.816	0.32043	0.27750	9.906	9686
2700	14.02	1.954	0.32086	0.27787	9.947	9647
2800	15.08	2.103	0.32133	0.27828	9.990	9605
2895	16.17	2.254	0.32180	0.27869	10.035	9562

$$d = \sqrt{3}a/2$$

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43 TECHNETIUM Tc

Atomic mass ^{98}Tc: 97.907211 (4) (Wang et al. 2017)
Atomic mass ^{99}Tc: 98.9062497 (10) (Wang et al. 2017)

^{98}Tc has the longest half life at 4.2 x 10^6 y while ^{99}Tc is the "most useful" isotope with a half life of 2.11 x 10^5 y (Audi et al. 2017).

Structure: Hexagonal close-packed (hP2)

Fernández Guillermet and Grimvall 1989 select 2430 (30) K for the melting point while Trainor and Brodsky 1975 determined the superconducting temperature to be 7.86 K.

In the high temperature region dilatometric measurements of Shirasu and Minato 2002 (323-1300 K) were corrected from a 323 K base to a 293.15 K base and were used to represent the thermal expansion from 293.15 to 1300 K:

$$\varepsilon_T \text{ avr} = 8.55208 \times 10^{-6} T - 1.04826 \times 10^{-9} T^2 + 9.20624 \times 10^{-13} T^3 - 2.44015 \times 10^{-3} \quad (43a)$$

Marples and Koch 1972 determined the lattice parameters at 4.2 K and 298 K and also mean thermal expansion coefficients from 150 K to 298 K. Average length change values from these measurements together with the assumptions that $\alpha = 0$ at 4.2 K and $\alpha = 8.17483 \times 10^{-6}$ K^{-1} at 293.15 K as derived from Equation 43a leads to the following equation which is considered to represent the thermal expansion below 293.15 K:

$$\varepsilon_T \text{ avr} = -3.25057 \times 10^{-7} T + 3.93550 \times 10^{-8} T^2 - 1.05198 \times 10^{-10} T^3 + 1.24514 \times 10^{-13} T^4 - 1.55612 \times 10^{-3} \quad (43b)$$

Based on the *c*/*a* ratios determined from the lattice parameter measurements of Marples and Koch 1972 corrected to the presently accepted lattice parameter values then the ratio can be considered to be 1.6046_6 at 4.2 K increasing to 1.6047_7 at 150 K with this value being constant up to 293.15 K. Above this temperature the behavior is unknown but because over the range 150 K to 293.15 K $\alpha_a = \alpha_c$ then it is speculated that the ratio remains constant at 1.6047_7 from 150 K to 1300 K. Therefore, above room temperature it is assumed that $\varepsilon_T \text{ avr} = \varepsilon_T a = \varepsilon_T c$. Because of the possibility of anisotropic effects in the measurements of Shirasu and Minato 2002 and the fact that Equation 43a shows a minimum in the derived thermal expansion coefficient at 380 K, it is considered that although Equations 43a and 43b lead to satisfactory length change values they are too insensitive to derive meaningful thermal expansion coefficient values.

Table 43a. Lattice parameter values of technetium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Note
Baker 1965	RT	0.27416	0.44000	
Marples and Koch 1972	298	0.27407	0.43981	
Haines et al. 1980	RT	0.27376	0.43952	a
	Selected	0.27412 (4)	0.43990 (10)	

Note for Table 43a

a. Not included in the average

At 293.15 K for Tc: Density ^{98}Tc 11359 (4) kg m^{-3} Density ^{99}Tc 11475 (4) kg m^{-3}
Molar volume 8.620 (3) cm^3 mol^{-1}.

Table 43b. Crystallographic properties of technetium

T K	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
0	- 0.153	- 0.160	- 0.156
10	- 0.153	- 0.160	- 0.156
20	- 0.153	- 0.159	- 0.155
30	- 0.151	- 0.157	- 0.153
40	- 0.150	- 0.155	- 0.151
50	- 0.147	- 0.152	- 0.149
60	- 0.144	- 0.148	- 0.146
70	- 0.141	- 0.144	- 0.142
80	- 0.137	- 0.140	- 0.138
90	- 0.133	- 0.135	- 0.134
100	- 0.128	- 0.131	- 0.129
110	- 0.123	- 0.125	- 0.124
120	- 0.118	- 0.119	- 0.118
130	- 0.113	- 0.113	- 0.113
140	- 0.107	- 0.107	- 0.107
150	- 0.101	- 0.101	- 0.101
160	- 0.095	- 0.095	- 0.095
170	- 0.089	- 0.089	- 0.089
180	- 0.082	- 0.082	- 0.082
190	- 0.076	- 0.076	- 0.076
200	- 0.069	- 0.069	- 0.069
210	- 0.062	- 0.062	- 0.062
220	- 0.055	- 0.055	- 0.055
230	- 0.048	- 0.048	- 0.048
240	- 0.041	- 0.041	- 0.041
250	- 0.033	- 0.033	- 0.033
260	- 0.026	- 0.026	- 0.026
270	- 0.018	- 0.018	- 0.018
280	- 0.011	- 0.011	- 0.011
290	- 0.003	- 0.003	- 0.003
293.15	0	0	0
300	0.006	0.006	0.006
400	0.087	0.087	0.087
500	0.169	0.169	0.169
600	0.251	0.251	0.251
700	0.335	0.335	0.335
800	0.420	0.420	0.420
900	0.508	0.508	0.508
1000	0.598	0.598	0.598
1100	0.692	0.692	0.692
1200	0.790	0.790	0.790
1300	0.893	0.893	0.893

Table 43c. Crystallographic properties of technetium

T K	*a* nm	*c* nm	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$ ^{98}Tc	Density $kg\ m^{-3}$ ^{99}Tc
0	0.27370	0.43919	0.27054	8.579	11412	11528
10	0.27370	0.43920	0.27054	8.579	11412	11528
20	0.27370	0.43920	0.27055	8.580	11412	11528
30	0.27370	0.43921	0.27055	8.580	11411	11528
40	0.27371	0.43922	0.27056	8.581	11410	11527
50	0.27372	0.43923	0.27057	8.581	11409	11526
60	0.27373	0.43925	0.27058	8.582	11408	11525
70	0.27373	0.43926	0.27059	8.583	11407	11524
80	0.27374	0.43928	0.27061	8.584	11406	11522
90	0.27376	0.43931	0.27062	8.585	11404	11521
100	0.27377	0.43933	0.27063	8.586	11403	11519
110	0.27378	0.43935	0.27065	8.588	11401	11517
120	0.27380	0.43938	0.27066	8.589	11399	11515
130	0.27381	0.43940	0.27068	5.590	11397	11514
140	0.27383	0.43943	0.27068	8.592	11395	11512
150	0.27384	0.43945	0.27070	8.593	11393	11509
160	0.27386	0.43948	0.27071	8.595	11391	11507
170	0.27388	0.43951	0.27073	8.597	11389	11505
180	0.27389	0.43954	0.27075	8.598	11387	11503
190	0.27391	0.43957	0.27077	8.600	11384	11501
200	0.27393	0.43960	0.27078	8.602	11382	11498
210	0.27395	0.43963	0.27080	8.604	11380	11496
220	0.27397	0.43966	0.27082	8.605	11377	11494
230	0.27399	0.43969	0.27084	8.607	11375	11491
240	0.27401	0.43972	0.27086	8.609	11373	11489
250	0.27403	0.43975	0.27088	8.611	11370	11486
260	0.27405	0.43979	0.27090	8.613	11368	11484
270	0.27407	0.43982	0.27092	8.615	11365	11481
280	0.27409	0.43985	0.27094	8.617	11362	11478
290	0.27411	0.43989	0.27096	8.619	11360	11475
293.15	0.27412	0.43990	0.27097	8.620	11359	11475
300	0.27414	0.43992	0.27099	8.621	11357	11473
400	0.27436	0.44028	0.27121	8.642	11329	11445
500	0.27458	0.44064	0.27143	8.663	11301	11417
600	0.27481	0.44101	0.27165	8.685	11273	11389
700	0.27504	0.44137	0.27188	5.706	11245	11360
800	0.27527	0.44175	0.27211	8.729	11217	11331
900	0.27551	0.44213	0.27235	8.752	11187	11302
1000	0.27576	0.44253	0.27259	8.775	11157	11271
1100	0.27602	0.44295	0.27288	8.800	11126	11239
1200	0.27629	0.44338	0.27311	8.826	11094	11207
1300	0.27657	0.44383	0.27339	8.853	11060	11173

$$d1 = (a^2/3 + c^2/4)^{½} \qquad d2 = a$$

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44 RUTHENIUM Ru

This review is based on the assessment of Arblaster 2013

Atomic Weight: 101.07 (2) (Meija 2017)

Structure: Hexagonal close packed (hP2)

The melting point is a secondary fixed point on ITS-90 at 2606 (10) K (Bedford et al. 1996).

Lattice parameter measurements were carried out by Owen and Roberts 1936, 1937 (323-873 K), Hall and Crangle 1957 (799-1557 K), Ross and Hume-Rothery 1963 (1793-2453 K), Finkel' et al. 1971 (80-300 K) and Schröder et al. 1972 (84-1982 K) and dilatometic measurements by Shirasu and Minato 2002 (323-1300 K). The measurements of Hall and Crangle 1957, Ross and Hume-Rothery 1963 and Finkel' et al. 1971 were given in the form of graphs with actual data points given by Touloukian et al. 1975.

44.1 High temperature region

Length change values derived from the measurements of Owen and Roberts 1936, 1937 and Ross and Hume-Rothery 1963 agree satisfactorily and were combined to give the following equations to represent the thermal expansion from 293.15 K to the melting point. On the basis ± 100ε_T equation 44a is accurate to ± 0.009 and equation 44b accurate to ± 0.025:

$$\varepsilon_T\, a = 4.93471 \times 10^{-6}\, T + 1.34455 \times 10^{-9}\, T^{2} + 1.61958 \times 10^{-13}\, T^{3} - 1.56642 \times 10^{-3} \quad (44a)$$

$$\varepsilon_T\, c = 7.52727 \times 10^{-6}\, T + 2.06251 \times 10^{-9}\, T^{2} + 2.61425 \times 10^{-13}\, T^{3} - 2.39045 \times 10^{-3} \quad (44b)$$

On the basis 100$\Delta\varepsilon$ the measurements of Hall and Crangle 1957 deviate continuously from selected values to be 0.14 low at the experimental limit at 1557 K. Above room temperature the *a*-axis values of Schröder et al. 1972 initially trend to 0.080 low at 1300 K before increasing to 0.089 high at 1982 K while the *c*-axis values show a similar trend deviating to 0.072 low at 1100 K before increasing sharply to 0.35 high at 1982 K. The dilatometric measurements of Shirasu and Minato trend to 0.10 low.

44.2 Low temperature region

In the low temperature region the measurements of Finkel' et al. 1971 were smoothed by fitting to equations 44e and 44f as given in Part 44.3. Derived thermal expansion coefficients at 293.15 K of 6.5 x 10^{-6} K^{-1} for the *a* axis and 11.5 x 10^{-6} K^{-1} for the *c* axis are notably higher than those derived from equations 44a and 44b and indicate the degree of incompatibility between the high and low temperature data. Various manipulations of subsets of the low temperature measurements to try and reconcile the differences proved

to be unsatisfactory and therefore the measurements of Finkel' et al. 1971 were rejected. Because the high and low temperature measurements could not be reconciled then in order to extrapolate below room temperature equations 44a and 44b were differentiated in order to obtain thermal expansion values, α*, which when converted to thermodynamic thermal expansion. α, and these values at 293.15 K, and over the range 300 to 800 K at 50 K intervals, were then fitted to Equation A using the high temperature specific heat equation 44g as given in Part 44.4. These equations were then extrapolated below room temperature in order to represent the thermal expansion to absolute zero:

$$\alpha_a\,(K^{-1}) = Cp\,(1.92207 \times 10^{-7} + 8.09046 \times 10^{-11}\,T + 7.16082 \times 10^{-6}/\,T) \qquad (44c)$$

$$\alpha_c\,(K^{-1}) = Cp\,(2.93088 \times 10^{-7} + 1.24609 \times 10^{-10}\,T + 1.09421 \times 10^{-5}/\,T) \qquad (44d)$$

As a judgment of the uncertainty in this procedure it is noted that on the basis 100Δε that the *a*-axis values of Finkel' et al. 1971 show a maximum deviation of only 0.006 low at 80 K while for the *c*-axis there is initial agreement and a maximum deviation of only 0.010 low at 220 K. The low temperature measurements of Schröder et al. 1972 for the *a*-axis are a maximum of 0.027 low at 84 K and then converge towards the selected value while for the **c**-axis the difference is initially 0.026 low at 84 K but there is agreement to better than 0.001 above 210 K.

Table 44a. Lattice parameter of ruthenium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Notes
Owen et al. 1935	291	0.27044	0.42818	a
Owen and Roberts 1936	291	0.27042	0.42819	a
Owen and Roberts 1937	293	0.27040	0.42819	a
Ross and Hume-Rothery 1963	303	0.27042	0.42799	a, b
Finkel' et al. 1971	293	0.27062	0.42815	a, b
Hallawell and Hume-Rothery 1954	298	0.27058	0.42817	
Swanson et al. 1955	300	0.27059	0.42819	
Hall and Crangle 1957	RT	0.27058	0.42805	
Anderson and Hume-Rothery 1960	293	0.27058	0.42814	
Černohorský 1960	295	0.27059	0.42812	
Savitskii et al. 1962	RT	0.27059	0.42819	
Schmitz-Pranghe and Dünner 1972	284	0.27056	0.42826	
	Selected	0.27058 (2)	0.42816 (7)	

Notes for Table 44a

a. Not included in the average

b. Lattice parameter values were given by Touloukian et al. 1975

At 293.15 K: Density 12364 (3) kg m^{-3} Molar volume 8.174 (2) cm^3 mol^{-1}.

Part 44.3: Thermal expansion equations derived from the measurements of Finkel' et al. 1971

a-axis: 80 – 289 K *c*-axis: 80 – 285 K

$$\varepsilon_T a = 3.25082 \times 10^{-6} T + 4.63332 \times 10^{-9} T^2 + 2.07266 \times 10^{-12} T^3 - 1.40337 \times 10^{-3} \quad (44e)$$

$$\varepsilon_T c = 3.44170 \times 10^{-6} T + 2.91501 \times 10^{-9} T^2 + 2.44946 \times 10^{-11} T^3 - 1.87652 \times 10^{-3} \quad (44f)$$

Part 44.4 Specific heat values for ruthenium

This is an extension of the Tables given by Arblaster 1995. The high temperature specific heat equation 44g covering the range 298.15 to 2606 K is derived by differentiating the selected enthalpy equation. C_p values are given in J mol^{-1} K^{-1}

Table 44b. Low temperature specific heat values for ruthenium

T K	10	15	20	25	30	35	40	45	50
C_p	0.0438	0.0955	0.186	0.359	0.731	1.233	1.877	2.707	3.982
T K	60	70	80	90	100	110	120	130	140
C_p	5.838	7.991	10.000	11.839	13.455	14.854	16.071	17.130	18.050
T K	150	160	170	180	190	200	210	220	230
C_p	18.837	19.509	20.093	20.607	21.066	21.480	21.857	22.200	23.514
T K	240	250	260	270	280	290	293.15	298.15	300
C_p	22.796	23.047	23.277	23.490	23.693	23.889	23.950	24.046	24.071

High temperature specific heat equation for ruthenium:

$$C_p (J\ mol^{-1} K^{-1}) = 7.28378 \times 10^{-3} T - 2.703021 \times 10^{-6} T^2 + 1.50844 \times 10^{-9} T^3 - 97572.6 / T^2 + 23.1728 \quad (44g)$$

Table 44c. Low temperature crystallographic properties of ruthenium

All values are estimated.

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
0	0	0	0	- 0.113	- 0.172	- 0.132
10	0.04	0.06	0.05	- 0.113	- 0.172	- 0.132
20	0.10	0.16	0.12	- 0.113	- 0.172	- 0.132
30	0.32	0.48	0.37	- 0.112	- 0.171	- 0.132
40	0.70	1.07	0.83	- 0.112	- 0.171	- 0.131
50	1.25	1.91	1.47	- 0.111	- 0.169	- 0.130
60	1.85	2.82	2.17	- 0.109	- 0.167	- 0.129
70	2.39	3.66	2.82	- 0.107	- 0.163	- 0.126
80	2.88	4.40	3.39	- 0.105	- 0.159	- 0.123
90	3.30	5.04	3.88	- 0.102	- 0.155	- 0.119
100	3.66	5.58	4.30	- 0.098	- 0.149	- 0.115
110	3.95	6.03	4.65	- 0.094	- 0.144	- 0.111
120	4.20	6.42	4.94	- 0.090	- 0.137	- 0.106
130	4.42	6.74	5.19	- 0.086	- 0.131	- 0.101
140	4.60	7.02	5.40	- 0.081	- 0.124	- 0.096
150	4.75	7.25	5.58	- 0.077	- 0.117	- 0.090
160	4.88	7.44	5.73	- 0.072	- 0.109	- 0.084
170	4.98	7.61	5.86	- 0.067	- 0.102	- 0.079
180	5.08	7.75	5.97	- 0.062	- 0.094	- 0.073
190	5.17	7.89	6.07	- 0.057	- 0.086	- 0.067
200	5.25	8.01	6.17	- 0.052	- 0.079	- 0.061
210	5.32	8.12	6.25	- 0.046	- 0.070	- 0.054
220	5.38	8.22	6.33	- 0.041	- 0.062	- 0.048
230	5.45	8.31	6.40	- 0.036	- 0.054	- 0.042
240	5.50	8.40	6.47	- 0.030	- 0.046	- 0.035
250	5.58	8.48	6.55	- 0.024	- 0.037	- 0.029
260	5.63	8.56	6.61	- 0.019	- 0.029	- 0.022
270	5.68	8.63	6.66	- 0.013	- 0.020	- 0.016
280	5.71	8.70	6.71	- 0.008	- 0.011	- 0.009
290	5.75	8.77	6.76	- 0.002	- 0.003	- 0.002
293.15	5.77	8.80	6.78	0	0	0

Table 44d. Low temperature crystallographic properties of ruthenium

All values are estimated.

T K	*a* nm	*c* nm	*c*/*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.27028	0.42742	1.5814	0.26462	8.142	12414
10	0.27028	0.42742	1.5814	0.26462	8.142	12414
20	0.27028	0.42743	1.5814	0.26462	8.142	12414
30	0.27028	0.42743	1.5814	0.26462	8.142	12414
40	0.27028	0.42743	1.5814	0.26462	8.142	12413
50	0.27028	0.42744	1.5815	0.26462	8.142	12413
60	0.27028	0.42745	1.5815	0.26463	8.143	12412
70	0.27029	0.42746	1.5815	0.26464	8.144	12411
80	0.27030	0.42748	1.5815	0.26465	8.144	12410
90	0.27031	0.42750	1.5815	0.26466	8.145	12409
100	0.27031	0.42752	1.5816	0.26467	8.146	12407
110	0.27033	0.42755	1.5816	0.26468	8.147	12406
120	0.27034	0.42757	1.5816	0.26470	8.148	12404
130	0.27035	0.42760	1.5817	0.26471	8.150	12402
140	0.27036	0.42763	1.5817	0.26473	8.151	12400
150	0.27037	0.42766	1.5817	0.26475	8.152	12398
160	0.27039	0.42769	1.5818	0.26476	8.154	12396
170	0.27040	0.42772	1.5818	0.26478	8.155	12394
180	0.27041	0.42776	1.5819	0.26480	8.156	12391
190	0.27043	0.42779	1.5819	0.26482	8.158	12389
200	0.27044	0.42782	1.5820	0.26484	8.159	12387
210	0.27045	0.42786	1.5820	0.26485	8.161	12385
220	0.27046	0.42789	1.5820	0.26487	8.162	12382
230	0.27048	0.42793	1.5821	0.26489	8.164	12380
240	0.27050	0.42796	1.5821	0.26491	8.166	12377
250	0.27051	0.42800	1.5822	0.26493	8.167	12375
260	0.27053	0.42804	1.5822	0.26495	8.169	12373
270	0.28054	0.42807	1.5823	0.26497	8.170	12370
280	0.27056	0.42811	1.5823	0.26499	8.172	12368
290	0.27058	0.42815	1.5824	0.26501	8.174	12365
293.15	0.27058	0.42816	1.5824	0.26502	8.174	12364

$$d1 = (a^2/3 + c^2/4)^{½} \qquad d2 = a$$

Table 44e. High temperature crystallographic properties of ruthenium

T K	α_a x 10^{-6} K^{-1}	α_c x 10^{-6} K^{-1}	α_{avr} x 10^{-6} K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
293.15	5.77	8.80	6.78	0	0	0
300	5.79	8.83	6.80	0.004	0.006	0.005
400	6.09	9.29	7.16	0.063	0.097	0.074
500	6.40	9.73	7.52	0.126	0.192	0.148
600	6.72	10.25	7.90	0.191	0.292	0.225
700	7.05	10.76	8.28	0.260	0.398	0.306
800	7.39	11.27	8.68	0.333	0.509	0.391
900	7.73	11.80	9.09	0.409	0.625	0.481
1000	8.09	12.34	9.51	0.488	0.746	0.574
1100	8.46	12.90	9.94	0.571	0.873	0.672
1200	8.83	13.47	10.38	0.658	1.006	0.774
1300	9.22	14.05	10.83	0.749	1.145	0.881
1400	9.61	14.65	11.29	0.844	1.291	0.993
1500	10.02	15.26	11.76	0.943	1.442	1.109
1600	10.43	15.88	12.24	1.046	1.600	1.231
1700	10.85	16.51	12.74	1.154	1.765	1.357
1800	11.28	17.16	13.24	1.266	1.936	1.489
1900	11.71	17.82	13.75	1.382	2.115	1.626
2000	12.16	18.49	14.27	1.505	2.300	1.768
2100	12.61	19.17	14.80	1.629	2.493	1.916
2200	13.08	19.86	15.34	1.760	2.693	2.070
2300	13.55	20.56	15.89	1.895	2.901	2.230
2400	14.03	21.28	16.44	2.036	3.117	2.395
2500	14.51	22.00	17.01	2.182	3.340	2.566
2600	15.01	22.74	17.58	2.333	3.571	2.744
2606	15.04	22.78	17.62	2.342	3.586	2.755

Table 44f. High temperature crystallographic properties of ruthenium

T K	*a* nm	*c* nm	*c*/*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
293.15	0.27058	0.42816	1.5824	0.26502	8.174	12364
300	0.27059	0.42819	1.5824	0.26503	8.175	12363
400	0.27075	0.42857	1.5829	0.26524	8.193	12337
500	0.27092	0.42898	1.5834	0.26547	8.211	12310
600	0.27110	0.42941	1.5840	0.26570	8.230	12281
700	0.27128	0.42986	1.5845	0.26595	8.250	12251
800	0.27148	0.43034	1.5851	0.26620	8.271	12220
900	0.27169	0.43083	1.5858	0.26647	8.293	12188
1000	0.27190	0.43135	1.5864	0.26676	8.316	12154
1100	0.27213	0.43190	1.5871	0.26706	8.340	12118
1200	0.27236	0.43247	1.5878	0.26737	8.366	12082
1300	0.27261	0.43306	1.5886	0.26769	8.392	12043
1400	0.27286	0.43369	1.5894	0.26803	8.420	12003
1500	0.27313	0.43434	1.5902	0.26838	8.449	11962
1600	0.27341	0.43501	1.5911	0.26875	8.480	11919
1700	0.27370	0.43572	1.5919	0.26913	8.512	11874
1800	0.27401	0.43645	1.5929	0.26953	8.545	11828
1900	0.27432	0.43722	1.5938	0.26995	8.580	11780
2000	0.27465	0.43801	1.5948	0.27038	8.616	11731
2100	0.27499	0.43883	1.5958	0.27083	8.653	11680
2200	0.27534	0.43969	1.5969	0.27130	8.692	11627
2300	0.27571	0.44058	1.5980	0.27178	8.733	11573
2400	0.27609	0.44150	1.5911	0.27229	8.776	11517
2500	0.27648	0.44246	1.6003	0.27281	8.820	11459
2600	0.27689	0.44345	1.6015	0.27335	8.866	11400
2606	0.27692	0.44351	1.6016	0.27338	8.869	11396

$$d1 = (a^2/3 + c^2/4)^{½} \qquad d2 = a$$

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45 RHODIUM Rh

This review is based on the assessment of Arblaster 1997

Atomic Weight: 102.90549 (2) (Meija 2017)

Structure: Face-centered cubic (cF4)

The freezing point is a secondary fixed point on ITS-90 at 2236 (3) K (Bedford et al. 1996).

45.1 Low temperature region

In the low temperature region the thermal expansion coefficients of White and Pawlowicz 1970 (3-85, 283 K) were combined with the revised value of (8.40 ± 0.10) x 10^{-6} K^{-1} at 283 K obtained by White 1988. Measurements above 29 K were fitted to equation A using specific heat (C_p) values given in Part 45.3:

$$0 - 29\ K: \quad \alpha\ (K^{-1}) = 2.10040 \times 10^{-9}\ T + 9.38048 \times 10^{-13}\ T^{3} + 1.49885 \times 10^{-14}\ T^{5} - 5.37107 \times 10^{-18}\ T^{7} \qquad (45a)$$

$$29 - 293.15\ K: \quad \alpha\ (K^{-1}) = C_p\,(3.34487 \times 10^{-7} + 3.07676 \times 10^{-11} T - 8.09712 \times 10^{-7}/T) \qquad (45b)$$

On the basis 100Δε dilatometric measurements of Erfling 1939 (58-273 K) agree with the selected length change values to within 0.001 while values of Laquer 1952 (0-300 K) reach a maximum deviation of 0.009 high at 80 to 100 K. In this region length change values derived from the lattice parameter measurements of Schröder et al. 1972 (87-1942 K) deviate up to 0.027 low at 87 K before converging towards the selected values. Thermal expansion coefficients of Valentiner and Wallot 1915 (96-287 K) scatter from 5% lower to 6% higher.

45.2 High temperature region

In the high temperature region there is close agreement between the lattice parameter measurements of Ross and Hume-Rothery 1963 (296-2223 K) (but specifically the high precision measurements from 296 to 1168 K) and those of Schröder et al. 1972 (87-1942 K) which were fitted to the following equation which was extrapolated to the melting point:

$$\varepsilon_T = 7.24305 \times 10^{-6}\ T + 2.22307 \times 10^{-9}\ T^{2} - 4.24678 \times 10^{-13}\ T^{3} + 2.43319 \times 10^{-16}\ T^{4} - 2.30544 \times 10^{-3} \qquad (45c)$$

On the basis 100Δε dilatometric measurements of Swanger 1929 (293-773 K) deviate only 0.006 low at 473 K to 0.010 high at 773 K while those of Holzmann 1931 (293-1269 K) trend up to 0.058 low and the measurements of Ebert 1938 (373-1773 K) trend up to 0.040 high. Length change measurements derived from the lattice parameter

measurements of Pawar 1968 (301-860 K) trend to 0.026 high while those of Singh 1968 (303-1138 K) vary only from 0.012 low at 611 K to 0.006 high at 1138 K. Lattice parameter values of Bale 1958 (298-1819 K) were only shown graphically with actual data points being given by Touloukian et al. 1975. These show an extraordinary expansion of the lattice being on average 0.38 high but this is almost certainly due to severe oxygen contamination of the sample surfaces. Additional lattice parameter values also shown only graphically include those of Raub et al. 1959 (293-1473 K) which are estimated to be on average 0.10 high and additional values of Ross and Hume-Rothery 1963 (1323-2223 K) which scatter 0.21 low to 0.009 high. Thermal expansion coefficients of Glazkov 1988 (1200-2000 K) trend from 1% high to 4% low to 1% low. When corrected to length change values the volume ratios obtained by Hüpf et al. 2009 (1400-2236 K) trend from initially 0.31 low to average 0.11 low above 1900 K.

Table 45a. Lattice parameter of rhodium at 293.15 K

References	Original Temperature K	*a* nm
Owen and Iball 1932	289.7	0.38034
Owen and Yates 1933	291	0.38036
Swanson, et al. 1954	298	0.38032
Anderson and Hume-Rothery 1960	293	0.38033
Černohorský 1960	294.7	0.38038
Ross and Hume-Rothery 1963	295.8	0.38033
Pawar 1968	301	0.38034
Singh 1968	303	0.38033
Schröder et al. 1972	299	0.38030
	Selected	0.38034(2)

At 293.15 K: Density 12423 (2) kg m^{-3} Molar volume 8.283 (1) cm^3 mol^{-1}.

45.3 Low temperature specific heat of rhodium

Furukawa, Reilly and Gallagher 1974 give the specific heat only to the nearest 0.01 J mol^{-1} K^{-1} above 70 K in their Table 4 but also gives values to the nearest 0.001 cal mol^{-1} K^{-1} in their Appendix B. These values have been combined to give all values to three decimal places in J mol^{-1} K^{-1}.

Table 45b. Low temperature specific heat values

T K	10	15	20	25	30	35	40	45	50
C_p	0.0629	0.136	0.284	0.577	1.090	1.814	2.740	3.842	5.040
T K	60	70	80	90	100	110	120	130	140
C_p	7.466	9.731	11.770	13.560	15.113	16.443	17.577	18.556	19.393
T K	150	160	170	180	190	200	210	220	230
C_p	20.121	20.753	21.305	21.794	22.230	22.623	22.974	23.292	23.581
T K	240	250	260	270	280	290	293.15	298.15	300
C_p	23.840	24.071	24.280	24.468	24.635	24.790	24.833	24.900	24.925

Table 45c. Low temperature crystallographic properties of rhodium

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	- 0.160	0.37973	0.26851	8.244	12483
10	0.023	- 0.160	0.37973	0.26851	8.244	12483
20	0.091	- 0.160	0.37973	0.26851	8.244	12483
30	0.34	- 0.160	0.37973	0.26851	8.244	12483
40	0.86	- 0.159	0.37973	0.26851	8.244	12483
50	1.61	- 0.158	0.39794	0.26852	8.244	12482
60	2.41	- 0.156	0.37975	0.26852	8.245	12482
70	3.16	- 0.153	0.37976	0.26853	8.245	12481
80	3.85	- 0.150	0.37977	0.26854	8.246	12479
90	4.45	- 0.146	0.37979	0.26855	8.247	12478
100	4.98	- 0.141	0.37980	0.26856	8.248	12476
110	5.43	- 0.136	0.37982	0.26858	8.250	12474
120	5.83	- 0.130	0.37984	0.26859	8.251	12472
130	6.16	- 0.124	0.37987	0.26861	8.253	12470
140	6.46	- 0.118	0.37989	0.26862	8.254	12467
150	6.71	- 0.111	0.37992	0.26864	8.256	12465
160	6.94	- 0.105	0.37994	0.26866	8.257	12462
170	7.14	- 0.098	0.37997	0.26868	8.259	12460
180	7.32	- 0.090	0.38000	0.26870	8.261	12457
190	7.47	- 0.083	0.38002	0.26872	8.263	12454
200	7.61	- 0.075	0.38005	0.26874	8.265	12451
210	7.74	- 0.068	0.38008	0.26876	8.267	12448
220	7.86	- 0.060	0.38011	0.26878	8.268	12446
230	7.97	- 0.052	0.38014	0.26880	8.270	12443
240	8.07	- 0.044	0.38017	0.26882	8.272	12440
250	8.16	- 0.036	0.38020	0.26884	8.274	12437
260	8.24	- 0.028	0.38023	0.26887	8.276	12433
270	8.32	- 0.019	0.38027	0.26889	8.279	12430
280	8.38	- 0.011	0.38030	0.26891	8.281	12427
290	8.44	- 0.002	0.38033	0.26893	8.283	12424
293.15	8.46	0	0.38034	0.26894	8.283	12423

$$d = a/\sqrt{2}$$

Table 45d. High temperature crystallographic properties of rhodium

T K	α x 10^6 K^{-1}	100 ε_T	*a* nm	*d* nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
293.15	8.46	0	0.38034	0.26894	8.283	12423
300	8.48	0.006	0.38036	0.26896	8.285	12421
400	8.87	0.093	0.38069	0.26919	8.306	12389
500	9.25	0.183	0.38104	0.26943	8.329	12355
600	9.64	0.278	0.38140	0.26969	8.353	12320
700	10.03	0.377	0.38177	0.26995	8.377	12284
800	10.43	0.479	0.38216	0.27023	8.403	12446
900	10.86	0.586	0.38257	0.27052	8.430	12207
1000	11.31	0.698	0.38299	0.27082	8.458	12167
1100	11.79	0.814	0.38344	0.27113	8.487	12125
1200	12.31	0.936	0.38390	0.27146	8.518	12081
1300	12.87	1.063	0.38438	0.27180	8.550	12035
1400	13.48	1.196	0.38489	0.27216	8.584	11988
1500	14.14	1.336	0.38542	0.27253	8.620	11938
1600	14.86	1.483	0.38598	0.27293	8.657	11886
1700	15.64	1.638	0.38657	0.27335	8.697	11832
1800	16.50	1.801	0.38719	0.27379	8.739	11775
1900	17.42	1.974	0.38785	0.27425	8.784	11716
2000	18.43	2.157	0.38854	0.27474	8.831	11653
2100	19.52	2.351	0.38928	0.27526	8.881	11587
2200	20.69	2.557	0.39006	0.27582	8.935	11517
2236	21.14	2.634	0.39036	0.27602	8.955	11491

$$d = a/\sqrt{2}$$

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46 PALLADIUM Pd

This review is based on the assessment of Arblaster 2012

Atomic Weight: 106.42 (1) (Meija 2017)

Structure: Face-centered cubic (cF4)

The freezing point is a secondary fixed point on ITS-90 at 1828.0 (1) K (Bedford et al. 1996).

46.1 Low temperature region

In the low temperature region the thermal expansion coefficients of Waterhouse and Yates 1968 and Bailey et al. 1969 (30-270 K) and White and Pawlowicz 1970 (3-85, 283 K) were combined with the revised value of (11.70 ± 0.10) x 10^{-6} K^{-1} at 283 K obtained by White 1988. Measurements above 28 K were fitted to equation A using specific heat (C_p) values given in Part 46.3:

$$0 - 28\ K: \quad \alpha\ (K^{-1}) = 4.15367 \times 10^{-9}\ T + 4.27891 \times 10^{-11}\ T^{3} + 7.05954 \times 10^{-15}\ T^{5} - 9.39675 \times 10^{-18}\ T^{7} \qquad (46a)$$

$$28 - 96\ K: \quad \alpha\ (K^{-1}) = C_p\,(4.30784 \times 10^{-7} + 1.79706 \times 10^{-10} T + 1.63606 \times 10^{-7}/T) \qquad (46b)$$

$$96 - 293.15\ K: \quad \alpha\ (K^{-1}) = C_p\,(3.93325 \times 10^{-7} + 1.69782 \times 10^{-10} T + 3.85873 \times 10^{-6}/T) \qquad (46c)$$

Measurements of Smirnov and Timoshenko 1972 (77-300 K) were only shown graphically with actual data points being given by Touloukian et al. 1975 while the values of Lawson et al. 1992 (15-300 K) were also shown only graphically and length values were estimated. The deviations of other low temperature lattice parameter and dilatometric values are given in Part 46.4.

46.2 High temperature region

Only length changes derived from the lattice parameter values of Owen and Jones 1937 (283-559 K), Dutta and Dayal 1963 (298-1151 K) and Rao and Rao 1964 (296-1063 K) show agreement with the low temperature data. It was found that continuity with the low temperature data could best be achieved if equation 46c was extended to 500 K and length change values obtained by integration were combined with the measurements of Rao and Rao 1964 for the range 873 K to 1063 K. In order to extend beyond this temperature limit it was noted that length change values derived from the lattice parameter values of Filipponi et al. 2000 (1249-1769 K), direct density measurements of Stankus and Tyagel'skii 1992 (293-1827 K) and volume ratio measurements of Hüpf and Pottlacher 2011 (1300-1828 K), although disagreeing with the selected value at 1100 K, converged when approaching the freezing point with estimated values as 100 ε_T of 2.41_2, 2.35 and 2.46 respectively at 1828 K. Because the last two values straddle the lattice parameter value then the latter was selected. However, possibly because of the large

temperature interval between 1100 K and the freezing point, it was found that equation fits with standard polynomials gave unnaturally large increases in the derived thermal expansion coefficient above about 1400 K and that a satisfactory increase in thermal expansion could only be obtained using the non-standard polynomial equation 46d which covers the whole temperature range from 293.15 K to the freezing point:

$$\varepsilon_T = 1.10122 \times 10^{-5} T + 2.69121 \times 10^{-9} T^2 - 2.25680 \times 10^{-13} T^3 + 6.58134 \times 10^{-2} / T - 3.67831 \times 10^{-3} \quad (46d)$$

Because of the procedure adopted values in Table 46b above 1100 K are considered to be tentative.

The density values of Stankus and Tyagel'skii 1992 (293-1827 K) converted to length change values reach a maximum low of 0.099 at 1200 K but are still 0.061 low at the freezing point while when corrected to length change values the volume ratios of Hüpf and Pottlacher 2011 (1300-1828 K) trend from initially 0.25 high to 0.050 high. The deviations of other high temperature lattice parameter and dilatometric values are given in Part 46.4.

Table 46a. Lattice parameter of palladium at 293.15 K

References	Original Temperature K	*a* nm	Notes
Stenzel and Weerts 1931	293	0.38890	
Owen and Yates 1933a, 1933b	291	0.38906	
Owen and Jones 1937	293	0.38906	
Swanson and Tatge 1953	298	0.38898	
Coles 1955-1956	295	0.38909	
Rayne 1960	300	0.38895	
Dutta and Dayal 1963	298	0.38890	
Anderson 1964	293	0.38896	
Goetz and Brophy 1964	RT	0.38891	
Rao and Rao 1964	296, 298	0.38906	
Bidwell and Speiser 1964	298	0.38900	
Maeland and Flanagan	293	0.38898	
Catterall and Barker 1965	295	0.38910	
Rao 1965	RT	0.38908	
Humble 1968	RT	0.38905	
Siller et al. 1969	298	0.38900	
Nagender-Naidu and Houska 1971	298	0.38900	
Schröder et al. 1972	296	0.38903	
King and Manchester 1978	292.7	0.38876	a
Balbaa et al. 1987	296	0.38917	a
Stankus and Tyagel'skii 1992	293	0.38905	b
Filipponi et al. 2000	293	0.38909	
	Selected	0.38902(6)	

Notes for Table 46a

a. Not included in the average

b. Calculated for the direct density measurement 12004 kg m^{-3}

At 293.15 K for Pd: Density 12007 (6) kg m^{-3} Molar volume 8.864 (4) cm^3 mol^{-1}

46.4 Deviations of experimental values from the selected values

Table 46c. Lattice parameter values

References	Temperature Range K	Deviations 100Δε
Owen and Jones 1937	283-559	Agrees with selected values to within 0.002
Dutta and Dayal 1963	298-1151	Trends to a maximum of 0.031 high
Abrahams 1963	4	0.090 high
Bidwell and Speiser 1964	298, 1173	0.029 low at 1173 K
Nagender- Naidu and Houska 1971	80-298	0.014 high at both 80 K and 195 K
Schröder et al. 1972	91-1809	Trends from initially 0.044 low and above room temperature trends to 0.39 low
Smirnov and Timoshenko 1972	77-300	Biases to 0.011 low below 220 K
King and Manchester 1978	6-293	Agrees with selected values to within 0.004
Balbaa et al. 1987	77	0.022 low
Lawson et al. 1992	15-300	Estimated scatter 0.012 to 0.019 high
Filipponi et al. 2000	295, 1249-1769	Trends from 0.11 low at 1250 K to 0.019 low at 1769 K

Table 46d. Dilatometric values

References	Temperature Range K	Deviations 100Δε
Holborn and Day 1901	273-1273	Trends to 0.067 low
Henning 1907	82, 289-1273	0.001 low at 82 K and above room temperature trends to 0.067 low
Scheel 1907	83, 289-373	Agrees with selected values to within 0.002
Holzmann 1931	293-1257	Trends to an average bias of 0.075 low above 1000 K
Nix and MacNair 1941	82-299	Agrees to within 0.002
Krikorian 1960	298-1273	Trends to 0.051 low
Masumoto et al. 1968	318-1184	Trends to 0.084 low
Masumoto and Sawaya 1969	125-1184	Initially 0.084 low. Above room temperature deviates to a maximum of 0.057 high at 877 K
Vest 1971	293-1068	Trends to an average of 0.085 low above 1064 K

46.3 Low temperature specific heat of palladium

This is an extension of the Tables given by Arblaster 1995.

Table 46b. Low temperature specific heat values

T K	10	15	20	25	30	35	40	45	50
C_p	0.196	0.490	0.999	1.768	2.794	3.998	5.388	6.809	8.190
T K	60	70	80	90	100	110	120	130	140
C_p	10.724	12.921	14.803	16.411	17.784	18.949	19.926	20.746	21.443
T K	150	160	170	180	190	200	210	220	230
C_p	22.043	22.561	23.012	23.406	23.752	24.059	24.334	24.582	24.806
T K	240	250	260	270	280	290	293.15	298.15	300
C_p	25.007	25.189	25.352	25.499	25.629	25.751	25.788	25.845	25.866

Table 46e. Crystallographic properties of palladium

T K	α x 10^6 K^{-1}	100 ε_T	*a* nm	*d* nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
0	0	- 0.238	0.38810	0.27442	8.800	12093
10	0.085	- 0.238	0.38810	0.27442	8.800	12093
20	0.44	- 0.238	0.38810	0.27443	8.801	12092
30	1.23	- 0.237	0.38810	0.27443	8.801	12092
40	2.38	- 0.235	0.38811	0.27443	8.801	12092
50	3.63	- 0.232	0.38812	0.27444	8.802	12090
60	4.76	- 0.228	0.38813	0.27445	8.803	12089
70	5.76	- 0.222	0.38815	0.27447	8.804	12087
80	6.63	- 0.216	0.38818	0.27448	8.806	12085
90	7.36	- 0.209	0.38821	0.27450	8.808	12082
100	7.98	- 0.202	0.38824	0.27452	8.810	12079
110	8.47	- 0.194	0.38827	0.27455	8.812	12076
120	8.88	- 0.185	0.38830	0.27457	8.814	12073
130	9.23	- 0.176	0.38834	0.27460	8.817	12070
140	9.53	- 0.166	0.38837	0.27462	8.819	12067
150	9.80	- 0.157	0.38841	0.27465	8.822	12063
160	10.03	- 0.147	0.38845	0.27467	8.825	12060
170	10.24	- 0.137	0.38849	0.27470	8.827	12056
180	10.42	- 0.126	0.38853	0.27473	8.830	12052
190	10.59	- 0.116	0.38857	0.27476	8.833	12048
200	10.74	- 0.105	0.38861	0.27479	8.836	12044
210	10.89	- 0.094	0.38865	0.27482	8.838	12041
220	11.02	- 0.083	0.38870	0.27485	8.841	12037
230	11.14	- 0.072	0.38874	0.27488	8.844	12033
240	11.26	- 0.061	0.38878	0.27491	8.847	12029
250	11.37	- 0.050	0.38883	0.27494	8.850	12025
260	11.47	- 0.039	0.38887	0.27497	8.853	12020
270	11.56	- 0.027	0.38891	0.27500	8.856	12016
280	11.65	- 0.015	0.38896	0.27504	8.859	12012
290	11.74	- 0.004	0.38901	0.27057	8.863	12008
293.15	11.77	0	0.38902	0.27508	8.864	12007
300	11.83	0.008	0.38905	0.27510	8.866	12004
400	12.63	0.131	0.38953	0.27544	8.898	11960
500	13.24	0.260	0.39003	0.27579	8.933	11913
600	13.76	0.396	0.39056	0.27617	8.969	11865
700	14.24	0.537	0.39111	0.27655	9.007	11815
800	14.68	0.682	0.39167	0.27695	9.046	11764
900	15.10	0.832	0.39226	0.27737	9.087	11712
1000	15.50	0.987	0.39286	0.27779	9.128	11658
1100	15.88	1.145	0.39347	0.27823	9.172	11603
1200	16.24	1.308	0.39411	0.27868	9.216	11548
1300	16.58	1.474	0.39475	0.27913	9.261	11491
1400	16.91	1.644	0.39542	0.27960	9.308	11433
1500	17.22	1.818	0.39609	0.28008	9.356	11375
1600	17.52	1.995	0.39678	0.28057	9.405	11316
1700	17.80	2.175	0.39748	0.28106	9.455	11256
1800	18.06	2.358	0.39819	0.25157	9.506	11196
1828.0	18.13	2.410	0.39840	0.28171	9.520	11179

$$d = a/\sqrt{2}$$

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47 SILVER Ag

Atomic weight: 107.8682 (2) (Meija 2017)

Structure: Face-centered cubic (cF4)

The freezing point is a primary fixed point on ITS-90 at 1234.93 K (Preston-Thomas 1990).

47.1 Low temperature

Below 25 K the thermal expansion coefficients of White and Collins 1972 (2-85, 283 K) and McClean et al. 1972 (1-26 K) were averaged. Above this temperature the measurements of White and Collins 1972 were combined with thermal expansion coefficients measured by Waterhouse and Yates 1968 and Bailey et al. 1969 (30-270 K) and thermal expansion coefficients derived from the length change values of Nix and MacNair 1942 (87-298 K), except that for the last two sets of measurements values above 230 K were not used in the evaluation because of a sudden sharp increase in the thermal expansion values. Accepted values were fitted to Equation A using the specific heat (C_p) values calculated from the equation given by Martin 1987 and the thermal expansion equation was extrapolated to 293.15 K:

$$\alpha\ (K^{-1}) = C_p\ (7.19005 \times 10^{-7} + 1.20777 \times 10^{-10} T - 1.04738 \times 10^{-6} / T) \qquad (47a)$$

Thermal expansion coefficients of Kos and Lamarche 1969 (5-15 K) trend to a value of 3.4×10^{-8} K^{-1} lower than the selected values. A comparison between other low temperature lattice and dilatometric measurements and the selected values is given in Part 47.4 except for the dilatometric measurements of Evans and Winstanley 1966 (98-174 K) which were only shown graphically and the lattice parameter measurements of Straumanis and Woodard 1971 (40-180 K) which were also only shown graphically and were not related to room temperature values. The dilatometric measurements of Lallement 1963 and Chistov et al. 1968 were given by Touloukian et al. 1975.

47b. High temperature

Based on sample purity and the precision of the measurements, selected length change values derived from the lattice parameter measurements of Hume-Rothery and Reynolds 1938 (293-1216 K), Owen and Roberts 1939 (291-830 K), Simmons and Balluffi 1960 (293-1223 K), Cockett and Davis 1963 (293-869 K) and Straumanis and Riad 1965 (312-1168 K) were combined with dilatometric measurements of Simmons and Balluffi 1960 (293-1223 K) where the latter were only included up to 1023 K to avoid inclusion of values subject to thermal vacancy effects. The actual measurements of Straumanis and Riad 1965 were given by Touloukian et al. 1975. The derived equation has an overall accuracy on the basis $\pm 100\varepsilon_T$ of ± 0.006:

$$\varepsilon_T = 1.24814 \times 10^{-5} T + 1.63711 \times 10^{-8} T^2 - 1.46370 \times 10^{-11} T^3 + 6.09100 \times 10^{-15} T^4 - 4.74205 \times 10^{-3} \quad (47b)$$

Lattice parameter measurements of Esser et al. 1938 (293-1273 K) were only shown graphically. The deviations of other high temperature measurements from the selected values are given in Part 47.4 where the measurements of Brand and Goldschmidt 1956 and Stuart and Ridley 1966 were originally only shown graphically with actual data points given by Touloukian et al. 1975.

Table 47a. Lattice parameter of silver at 293.15 K

References	Original Temperature K	*a* nm
Stenzel and Weerts 1931	293	0.40858
Owen and Iball 1932	289.7	0.40860
Owen and Yates 1933	291	0.40859
Saini 1933	293	0.40859
Owen and Yates 1934	288	0.40861
Jette and Foote 1935	298	0.40860
Hume-Rothery et al. 1936	297	0.40860
Moeller 1937	293, 298	0.40861
Hume-Rothery and Reynolds 1938	293	0.40859
Owen and Roberts 1939	291	0.40858
Miller and DuMond 1940	298	0.40857
Chiswik and Hultgren 1940	298	0.40863
Foote and Jette 1940,1941	298	0.40860
Owen and Rowlands 1940	291	0.40860
Felipe 1940	291	0.40858
Lipson et al. 1941	293	0.40860
Hume-Rothery and Andrews 1942	297	0.40860
Swenson and Tatge 1953	298	0.40861
Becherer and Ifland 1954	293	0.40857
Owen and Williams 1954	291	0.40861
Smakula and Kalnajs 1955	298	0.40860
Coles 1955-1956	295	0.40857
Hill and Axon 1956-1957	298	0.40858
Spreadborough and Christian 1959	289, 295	0.40860
King and Vassamillet 1961	301	0.40859
Calvert and Henry 1962	294	0.40863
Cockett and Davis 1963	293	0.40858
Rao and Rao 1964	RT	0.40863
Straumanis and Riad 1965	298	0.40861
Swanson et al. 1966	298	0.40862
Swanson et al. 1970	298	0.40861
Nagender Naidu and Houska 1971	298	0.40862
Straumanis 1971	298	0.40861
Seshadri and Downie 1979	294, 300	0.40858
Tang et al. 1998	299	0.40861
	Selected	0.40860 (3)

The assigned accuracy represents the spread of the values.

At 293.15 : Density 10503 (2) kg m^{-3} Molar volume 10.270 (2) cm^3 mol^{-1}.

47.3 Bulk properties of silver

Measurements of Simmons and Balluffi 1960b lead to a value of C_V which is notably lower than later measurements at the freezing point:

Table 47b. Thermal vacancy parameters for silver

References	10^4 C_V	H_V eV	S_V/k
Simmons and Balluffi 1960	1.7 (5)	1.09 (10)	(1.5)
Lüdecke 1981	4.2 (1.4)	1.04 (5)	2.0 (7)
Wolff 1991	5.2 (8)	1.07 (5)	2.5 (8)
Mosig et al. 1992	5.2 (7)	1.05 (4)	2.3 (8)

The values of Mosig et al. 1992 are accepted. The value of H_V can be considered to be in satisfactory agreement with values obtained from positron annihilation lifetime spectroscopy although the values obtained are systematically higher: 1.13 (5) eV (Schmul 1985); 1.13 (5) eV (Lühr-Tanck et al. 1985) and 1.11 (6) eV (Schaefer 1987).

47.4 Deviations of experimental values from the selected values

Table 47c. Lattice parameter values

References	Temperature Range K	Deviations $100\Delta\varepsilon$
Saini 1933	293-573	Trends to 0.034 lower
Owen and Yates 1934	288-873	Trends to 0.017 low
Owen and Williams 1954	79-291	Average bias 0.004 low
Mauer and Bolz 1955	237-1149	Scatters 0.013 low to 0.013 high
Brand and Goldschmidt 1956	273-1173	Trends to maximum 0.065 high at 673 K and then falls to 0.034 low at 1173 K
Spreadborough and Christian 1959	289-1119	Scatters 0.016 low to 0.033 high
Stuart and Ridley 1966	303-1177	Trends to maximum 0.033 high at 581 K and then falls to 0.11 low at 1177 K
Michel 1968	298-1119	Trends to 0.092 low
Nagender Naidu and Houska 1971	80-298	Average bias 0.005 low
Seshadri and Downie 1979	294-917	First run 291 to 917 K scatters 0.006 low to 0.016 high. Second run 300 to 693 K shows average bias of 0.004 high
Suh 1988	293-1228	First run trend to 0.097 low. Second run scatters 0.024 low to 0.068 high
Vesnin and Shubin 1988	293-1234	Trends to 0.093 low

Table 47d. Dilatometric values

References	Temperature Range K	Deviations 100Δε
Holborn and Day 1901	273-1023	Trends to 0.015 low
Dorsey 1907	93-293	Average bias 0.002 low
Buffington and Latimer 1926	87-310	Average bias 0.002 high
Esser and Eusterbrock 1941	273-1173	Trends to 0.073 low
Leksina and Novikova 1963	90-1273	Initially 0.011 high then trends to 0.13 low above 293.15 K
Lallement 1963	10-240	Trends from initially 0.075 low to then agree with the selected values
Fraser and Hollis Hallet 1965	17-100	Average bias 0.005 low
Grove 1967	424-922	Scatters 0.020 low to 0.013 high
Chistov et al. 1968	90-540	Agree to within 0.004 below 293.15 K and show an an average bias of 0.006 low above this temperature
Pathak and Vasavada 1970	300-1200	Trends to 0.030 low as length change values
Vest 1971	293-1067	Trends to 0.22 low
Suh et al. 1988	293-1000	Trends to 0.048 low

Table 47e. Low temperature crystallographic properties of silver

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	- 0.410	0.40693	0.28774	10.145	10633
10	0.12	- 0.410	0.40693	0.28774	10.145	10633
20	1.11	- 0.409	0.40693	0.28774	10.145	10633
30	3.28	- 0.407	0.40694	0.28775	10.145	10632
40	5.83	- 0.403	0.40695	0.28776	10.147	10631
50	8.15	- 0.396	0.40698	0.28778	10.149	10629
60	10.06	- 0.387	0.40702	0.28781	10.152	10626
70	11.58	- 0.376	0.40706	0.28784	10.155	10622
80	12.78	- 0.364	0.40711	0.28787	10.159	10618
90	13.74	- 0.350	0.40717	0.28791	10.163	10614
100	14.50	- 0.336	0.40723	0.28795	10.167	10610
110	15.12	- 0.322	0.40729	0.28799	10.172	10605
120	15.62	- 0.306	0.40735	0.28804	10.176	10600
130	16.05	- 0.290	0.40741	0.28808	10.181	10595
140	16.41	- 0.274	0.40748	0.28813	10.186	10590
150	16.72	- 0.258	0.40755	0.28818	10.191	10584
160	16.99	- 0.241	0.40762	0.28823	10.196	10579
170	17.22	- 0.224	0.40769	0.28828	10.202	10574
180	17.44	- 0.207	0.40776	0.28833	10.207	10568
190	17.62	- 0.189	0.40783	0.28838	10.212	10563
200	17.79	- 0.171	0.40790	0.28843	10.218	10557
210	17.95	- 0.153	0.40797	0.28848	10.223	10551
220	18.10	- 0.135	0.40805	0.28853	10.229	10546
230	18.23	- 0.117	0.40812	0.28858	10.234	10540
240	18.36	- 0.099	0.40820	0.28864	10.240	10534
250	18.48	- 0.081	0.40827	0.28869	10.246	10528
260	18.58	- 0.062	0.40835	0.28874	10.251	10522
270	18.69	- 0.044	0.40842	0.28880	10.257	10517
280	18.79	- 0.025	0.40850	0.28885	10.263	10511
290	18.90	- 0.006	0.40858	0.28891	10.269	10505
293.15	18.92	0	0.40860	0.28892	10.270	10503

$$d = a/\sqrt{2}$$

Table 47f. High temperature crystallographic properties of silver

T K	α x 10^6 K^{-1}	100 ε_T	*a* nm	*d* nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
293.15	18.92	0	0.40860	0.28892	10.270	10503
300	19.01	0.013	0.40865	0.28896	10.274	10499
350	19.59	0.110	0.40905	0.28924	10.304	10468
400	20.07	0.209	0.40945	0.28953	10.335	10437
450	20.48	0.311	0.40987	0.28982	10.366	10406
500	20.83	0.414	0.41029	0.29012	10.399	10373
550	21.15	0.520	0.41072	0.29043	10.431	10341
600	21.45	0.627	0.41116	0.29073	10.465	10308
650	21.74	0.736	0.41161	0.29105	10.499	10274
700	22.05	0.846	0.41206	0.29137	10.533	10241
750	22.40	0.958	0.41251	0.29169	10.568	10207
800	22.80	1.072	0.41298	0.29202	10.604	10172
850	23.27	1.189	0.41346	0.29236	10.641	10137
900	23.83	1.308	0.41394	0.29270	10.679	10101
950	24.50	1.430	0.41444	0.29306	10.717	10065
1000	25.28	1.556	0.41496	0.29342	10.757	10027
1050	26.21	1.687	0.41549	0.29380	10.799	9989
1100	27.30	1.823	0.41605	0.29419	10.842	9949
1150	28.56	1.965	0.41663	0.29460	10.888	9907
1200	30.01	2.115	0.41724	0.29503	10.936	9864
1234.93	31.14	2.224	0.41769	0.29535	10.971	9832

$$d = a/\sqrt{2}$$

Table 47g. Bulk properties of silver

$3\,(\varepsilon_T L - \varepsilon_T a) = \exp(2.3 - 12185/T)$ $\quad \alpha_L - \alpha_a = (4062/T^2)\exp(2.3 - 12185/T)$

T K	α x 10^6 K^{-1}	100 ε_T	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
850	23.27	1.189	10.641	10137
900	23.90	1.308	10.679	10101
950	24.62	1.431	10.718	10065
1000	25.49	1.558	10.758	10027
1050	26.55	1.690	10.800	9988
1100	27.82	1.828	10.844	9947
1150	29.33	1.974	10.801	9905
1200	31.11	2.128	10.940	9860
1234.93	32.53	2.241	10.976	9827

This Table is considered to be identical to Table 47f below 850 K.

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48 CADMIUM Cd

Atomic weight: 112.414 (4) (Meija 2017)

Structure: Hexagonal close packed (hP2)

The freezing point is a secondary fixed point on ITS-90 at 594.219 (1) K (Bedford et al. 1996).

48.1 Crystallographic properties

Above 293.15 K length change values derived from the lattice parameter measurements of Janot and George 1975 (290-588 K) and Feder and Nowick 1972 (296-592 K) and dilatometric measurements of Feder and Nowick 1972 (297-590 K) were combined except that that the dilatometric measurements were not used above 410 K to avoid including values affected by thermal vacancy effects. Experimental values of Feder and Nowick 1972 were only shown graphically with actual data points given by Touloukian et al. 1975. On the basis ± $100\varepsilon_T$ both of the equations given below have overall accuracies of ± 0.002:

$$\varepsilon_T\, a = -2.06504 \times 10^{-5}\, T + 1.38086 \times 10^{-7}\, T^{2} - 2.26805 \times 10^{-10}\, T^{3} + 1.69394 \times 10^{-13}\, T^{4} - 1.35026 \times 10^{-3} \quad (48a)$$

$$\varepsilon_T\, c = 1.62556 \times 10^{-4}\, T - 4.05933 \times 10^{-7}\, T^{2} + 6.83789 \times 10^{-10}\, T^{3} - 4.54684 \times 10^{-13}\, T^{4} - 2.66370 \times 10^{-2} \quad (48b)$$

Up to 85 K the thermal expansion coefficient values of McCammon and White 1965 (3-283 K) were accepted. In the intermediate temperature range 85 K to 293.15 K for the *a* axis the thermal expansion coefficients of McCammon and White 1965 from 65 K to 85 K were combined with the value at 293.15 K derived from equation 48a and fitted to Equation A using the specific heat (C_p) values selected in Part 48.3:

$$\alpha_a\,(K^{-1}) = C_p\,(7.75443 \times 10^{-7} + 1.91272 \times 10^{-10}\, T - 3.04082 \times 10^{-5}/\, T) \quad (48c)$$

For the *c* axis because of the complex behavior of the low temperature thermal expansion coefficient it was found that Equation A could not be applied and instead values were estimated graphically and then smoothed using the equation:

$$\alpha_c\,(K^{-1}) = 6.07889 \times 10^{-10}\, T - 1.91004 \times 10^{-10}\, T^{2} + 9.38655 \times 10^{-13}\, T^{3} - 1.79431 \times 10^{-15}\, T^{4} - 6.12240 \times 10^{-5} \quad (48d)$$

Equations 48a to 48d are considered as showing satisfactory agreement with the experimental values determined by McCammon and White 1965 at 283 K to be $\alpha_a = 19.3 \times 10^{-6}\ K^{-1}$ and $\alpha_c = 54.8 \times 10^{-6}\ K^{-1}$.

In the low temperature region thermal expansion coefficients of Madaiah and Graham 1964 were shown only graphically with actual data points being given by Touloukian et al. 1975. K. Deviations of experimental values are given in Table 48b to 48d.

Table 48a. Lattice parameter measurements of cadmium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Notes
Jenkins and Preston 1931	RT	0.29786	0.56158	
Stenzel and Weerts 1932	293	0.29798	0.56174	a
Jette and Gebert 1933	298	0.29772	0.56147	b
Kossalopow and Trapesnikow 1935	299	0.29789	0.56158	
Jette and Foote 1935	295	0.29790	0.56170	
Owen and Roberts 1936	291	0.29787	0.56162	
Owen et al. 1939	291	0.29788	0.56163	
Lu and Chang 1941	294	0.29789	0.56167	
Edwards et al. 1952	298	0.29793	0.56174	
Swanson et al. 1954	299	0.29791	0.56166	
Feder and Nowick 1972	299	0.29789	0.56164	
Pathak and Desai 1980	293	0.29789	0.56165	c
	Selected	0.29789 (2)	0.56166 (6)	

Notes for Table 48a

a. *a* axis value not included in the average

b. Not included in the average

c. Calculated from equations

At 293.15 K: Density 8649 (2) kg m^{-3} Molar volume 12.997 (2) cm^3 mol^{-1}.

48.2 Bulk properties of cadmium

The following values have been determined for the vacancy concentration parameter (c_V), the enthalpy of vacancy formation (H_V) and the entropy of vacancy formation (S_V/k). The value of McKee et al. 1972 was obtained by positron annihilation and the other two values by equating dilatometric and lattice parameter length change values.

Table 48b. Thermal vacancy parameters for cadmium

Authors	c_V	H_V eV	S_V/k
McKee et al. 1972	-	0.39 (4)	-
Feder and Nowick 1972	5.6×10^{-4}	0.40 (2)	0.3 (4)
Janot and George 1975	$4.5\ (5) \times 10^{-4}$	0.42 (2)	0.5 (1)
Select	5.0×10^{-4}	0.41	0.4

48.2 Deviations of experimental values from the selected values

Table 48c. Thermal expansion values

References	Temperature Range K	Deviations 100Δε
Madaiah and Graham 1964	11-290 (*a* axis) 17-286 (*c* axis)	*a* axis: Above 40 K initially 25% high increasing to 50% high at 80 K before trending to 9% low at 200 K and then to 5% high at 290 K. *c* axis: Between 40 K and 140 K scatters from 12% low to 9% high then trends to an average of 18% low above 200 K
Messer and Weintroub 1965	40-200	3% low along both axes at 100 K and above

Table 48d. Dilatometric and lattice parameter values

References	Temperature Range K	Deviations 100Δε
Grüneisen and Goens 1924	93-373	*a* axis: Average bias only 0.003 low *c* axis: Trends from initially 0.029 to converge to the selected value.
Kossolapow and Trapesnikow 1935	299-462	*a* axis: Average bias 0.027 low *c* axis: Average bias 0.041 low
Owen and Robetrs 1936	291-552	*a* axis: Average bias 0.021 high to 460 K then trending to a maximum of 0.097 high at 552 K *c* axis: Some scatter but average bias 0.027 high
Edwards et al. 1952	298-569	*a* axis: Average bias only 0.002 low above 400 K *c* axi: Trends to 0.064 low
Pathak and Desai 1980	273-583	Average bias only 0.001 high along the *a* axis and 0.002 high along the *c* axis

48.3 Specific heat of cadmium

These are selected or interpolated from the values of Craig et al. 1954 corrected from cal mol^{-1} K^{-1} to J mol^{-1} K^{-1} and for atomic weight 112.411/112.41.

Table 48e. Low temperature specific heat of cadmium

T K	20	25	30	40	50	57.5	60	65	70
C_p	5.188	7.544	9.648	12.213	15.912	17.464	17.920	18.736	19.443
T K	75	80	85	90	100	110	120	130	140
C_p	20.054	20.585	21.075	21.498	22.108	22.648	23.088	23.464	23.782
T K	150	160	170	180	190	200	210	220	230
C_p	24.041	24.263	24.452	24.619	24.778	24.920	25.054	25.180	25.301
T K	240	250	260	270	280	290	293.15	298.15	300
C_p	25.410	25.506	25.602	25.707	25.820	25.945	25.983	26.041	26.062

Table 48f. Crystallographic properties of cadmium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 ε_T *a*	100 ε_T *c*	100 ε_T avr
0	0	0	0	- 0.339	- 1.586	- 0.755
5	- 0.01	0.28	0.09	- 0.339	- 1.586	- 0.755
10	- 1.05	7.20	1.70	- 0.339	- 1.585	- 0.754
15	- 2.93	20.88	5.01	- 0.340	- 1.578	- 0.753
20	- 3.85	34.00	8.17	- 0.342	- 1.564	- 0.749
25	- 3.74	43.59	12.04	- 0.344	- 1.545	- 0.745
30	- 2.95	50.00	14.70	- 0.345	- 1.522	- 0.738
40	1.36	56.70	19.81	- 0.347	- 1.469	- 0.721
50	3.04	59.40	21.83	- 0.344	- 1.411	- 0.700
60	5.05	60.45	23.52	- 0.340	- 1.352	- 0.677
65	6.00	60.60	24.20	- 0.337	- 1.322	- 0.666
70	6.88	60.51	24.76	- 0.334	- 1.292	- 0.654
80	8.46	60.36	25.76	- 0.327	- 1.233	- 0.629
90	9.78	60.19	26.58	- 0.317	- 1.173	- 0.603
100	10.84	60.01	27.23	- 0.307	- 1.114	- 0.576
110	11.78	59.83	27.80	- 0.296	- 1.054	- 0.549
120	12.58	59.65	28.27	- 0.284	- 0.995	- 0.521
130	13.29	59.47	28.68	- 0.271	- 0.936	- 0.493
140	13.91	59.28	29.03	- 0.257	- 0.877	- 0.464
150	14.46	59.09	29.34	- 0.243	- 0.819	- 0.435
160	14.95	58.91	29.60	- 0.228	- 0.760	- 0.406
170	15.38	58.71	29.82	- 0.213	- 0.702	- 0.376
180	15.78	58.52	30.03	- 0.198	- 0.644	- 0.346
190	16.15	58.31	30.20	- 0.182	- 0.585	- 0.316
200	16.49	58.10	30.36	- 0.165	- 0.528	- 0.286
210	16.81	57.88	30.50	- 0.149	- 0.470	- 0.256
220	17.10	57.64	30.61	- 0.132	- 0.412	- 0.225
230	17.39	57.38	30.72	- 0.115	- 0.355	- 0.195
240	17.65	57.10	30.80	- 0.097	- 0.298	- 0.164
250	17.90	56.79	30.86	- 0.079	- 0.241	- 0.133
260	18.13	56.45	30.90	- 0.061	- 0.185	- 0.103
270	18.37	56.08	30.94	- 0.043	- 0.129	- 0.072
280	18.60	55.66	30.95	- 0.025	- 0.073	- 0.041
290	18.84	55.19	30.95	- 0.006	- 0.017	- 0.010
293.15	18.91	55.03	30.95	0	0	0
300	19.26	54.49	31.00	0.013	0.038	0.021
320	20.24	53.15	31.21	0.053	0.145	0.083
340	21.20	52.05	31.48	0.094	0.251	0.146
360	22.17	51.11	31.82	0.137	0.354	0.210
380	23.18	50.24	32.20	0.183	0.456	0.274
400	24.26	49.35	32.63	0.230	0.556	0.339
420	25.45	48.37	33.09	0.280	0.654	0.405
440	26.77	47.20	33.58	0.333	0.750	0.472
460	28.26	45.75	34.09	0.388	0.844	0.540
480	29.95	43.95	34.61	0.446	0.935	0.609
500	31.87	41.70	35.14	0.508	1.021	0.679
520	34.05	38.92	35.67	0.574	1.103	0.751
540	36.53	35.52	36.20	0.645	1.178	0.823
560	39.34	31.43	36.70	0.722	1.246	0.897
580	42.50	26.55	37.18	0.804	1.305	0.971
594.219	44.98	22.56	37.51	0.867	1.341	1.025

Table 48g. Crystallographic properties of cadmium

T K	*a* nm	*c* nm	*c*/*a*	*d*2 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.29688	0.55275	1.8619	0.32521	12.704	8849
5	0.29688	0.55275	1.8619	0.32521	12.704	8849
10	0.29688	0.55276	1.8619	0.32522	12.704	8849
15	0.29688	0.55280	1.8620	0.32523	12.705	8848
20	0.29687	0.55287	1.8623	0.32526	12.706	8847
25	0.29687	0.55298	1.8627	0.32531	12.708	8846
30	0.29686	0.55311	1.8632	0.32536	12.711	8844
40	0.29686	0.55341	1.8642	0.32549	12.717	8839
50	0.29686	0.55373	1.8653	0.32562	12.725	8834
60	0.29688	0.55407	1.8663	0.32577	12.734	8828
65	0.29688	0.55423	1.8668	0.32584	12.739	8825
70	0.29689	0.55440	1.8673	0.32592	12.743	8822
80	0.29691	0.55474	1.8683	0.32607	12.753	8815
90	0.29694	0.55507	1.8693	0.32622	12.763	8808
100	0.29698	0.55541	1.8702	0.32637	12.773	8800
110	0.29701	0.55574	1.8711	0.32652	12.784	8793
120	0.29704	0.55607	1.8720	0.32667	12.795	8786
130	0.29708	0.55640	1.8729	0.32683	12.806	8779
140	0.29712	0.55673	1.8737	0.32698	12.817	8771
150	0.29717	0.55706	1.8746	0.32713	12.828	8763
160	0.29721	0.55739	1.8754	0.32729	12.839	8756
170	0.29725	0.55772	1.8762	0.32744	12.851	8748
180	0.29730	0.55805	1.8770	0.32759	12.862	8740
190	0.29735	0.55837	1.8778	0.32774	12.874	8732
200	0.29740	0.55870	1.8786	0.32790	12.886	8724
210	0.29745	0.55902	1.8794	0.32805	12.897	8716
220	0.29750	0.55934	1.8802	0.32820	12.909	8708
230	0.29755	0.55967	1.8809	0.32836	12.921	8700
240	0.29760	0.55999	1.8817	0.32851	12.933	8692
250	0.29765	0.56030	1.8824	0.32866	12.945	8684
260	0.29771	0.56062	1.8831	0.32881	12.957	8676
270	0.29776	0.56094	1.8838	0.32896	12.969	8668
280	0.29782	0.56125	1.8846	0.32911	12.981	8660
290	0.29787	0.56156	1.8852	0.32926	12.993	8652
293.15	0.29789	0.56166	1.8855	0.32931	12.997	8649
300	0.29793	0.56187	1.8859	0.32941	13.005	8644
320	0.29805	0.56248	1.8872	0.32970	13.029	8627
340	0.29817	0.56307	1.8884	0.32999	13.054	8611
360	0.29830	0.56365	1.8895	0.33028	13.079	8595
380	0.29843	0.56422	1.8906	0.33057	13.104	8579
400	0.29858	0.56478	1.8916	0.33085	13.129	8562
420	0.29872	0.56533	1.8925	0.33113	13.155	8546
440	0.29888	0.56588	1.8933	0.33141	13.182	8528
460	0.29905	0.56640	1.8940	0.33168	13.208	8511
480	0.29922	0.56691	1.8946	0.33195	13.236	8493
500	0.29940	0.56740	1.8951	0.33221	13.263	8476
520	0.29960	0.56785	1.8954	0.33247	13.292	8458
540	0.29981	0.56828	1.8954	0.33271	13.320	8439
560	0.30004	0.56866	1.8953	0.33294	13.349	8421
580	0.30029	0.56899	1.8948	0.33316	13.379	8402
594.219	0.30047	0.56919	1.8942	0.33330	13.400	8389

Interatomic distance calculations for Table 48g: $d1 = a \quad d2 = (a^2/3 + c^2/4)^{½}$

Table 48h. Bulk properties of cadmium

$3\ (\varepsilon_T L - \varepsilon_T \text{avr}) = \exp(0.4 - 4754/T) \quad \alpha_L - \alpha_{avr} = (1584.7/T^2) \exp(0.4 - 4754/T)$

T K	$\alpha \times 10^6$ K^{-1}	$100\varepsilon_T$	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
400	32.63	0.339	13.129	8562
420	33.25	0.406	13.156	8545
440	33.83	0.473	13.182	8528
460	34.46	0.542	13.209	8510
480	35.13	0.612	13.237	8492
500	35.85	0.683	13.265	8475
520	36.62	0.756	13.294	8456
540	37.44	0.831	13.323	8437
560	38.27	0.907	13.354	8418
580	39.14	0.985	13.385	8399
594.219	37.98	1.042	13.407	8385

This Table is assumed to be identical to Tables 48f and 48g below 400 K.

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49 INDIUM In

Atomic weight: 114.818 (1) (Meija 2017)

Structure: Body-centered tetragonal (tI2)

The structure is also described in terms of an equivalent face-centered tetragonal cell such that $a_{FCT} = \sqrt{2}\ a_{BCT}$ and $c_{FCT} = c_{BCT}$. All values have been corrected to conform to the body-centered tetragonal cell.

The freezing point is a primary fixed point on ITS-90 at 429.7485 K (Preston Thomas 1990) while the triple point at 429.7436 (2) K, and superconducting temperature at 3.4145 (25) K are secondary fixed points (Bedford et al. 1996).

The thermal expansion equations given by Touloukian et al. 1975 (100-400 K) which appear to be based on length change values derived form the thermal expansion coefficients of Smith and Schneider 1964 (100-300 K) and lattice parameter measurements of Deshpande and Pawar 1969b (300-379 K) and Straumanis et al. 1971 (283-333 K) have generally been accepted except for a small change to pass through zero at 293.15 K:

$$\varepsilon_T a = 2.76600 \times 10^{-5}\, T - 3.77900 \times 10^{-9}\, T^2 + 1.07600 \times 10^{-10}\, T^3 - 1.04945 \times 10^{-2} \quad (49a)$$

$$\varepsilon_T c = 2.39900 \times 10^{-5}\, T - 1.96900 \times 10^{-8}\, T^2 - 8.60800 \times 10^{-11}\, T^3 - 3.17201 \times 10^{-3} \quad (49b)$$

However, the derived thermal expansion coefficients are not compatible with the low temperature thermal expansion coefficients given by Collins et al. 1967 (2-85, 283 K) when both are extrapolated to 100 K. This problem was overcome by combining the values obtained by Collins et al. 1967 over the range 57.5 to 85 K with the values at 140 to 170 K derived from equations 49a and 49b leading to the following equations to interpolate between 85 and 140 K:

$$\alpha_a\,(K^{-1}) = 5.09303 \times 10^{-7}\, T - 2.70334 \times 10^{-9}\, T^2 + 5.82622 \times 10^{-12}\, T^3 - 1.20512 \times 10^{-6} \quad (49c)$$

$$\alpha_c\,(K^{-1}) = -2.55160 \times 10^{-8}\, T - 5.73382 \times 10^{-10}\, T^2 + 1.16625 \times 10^{-12}\, T^3 + 2.51422 \times 10^{-5} \quad (49d)$$

Below 85 K the thermal expansion coefficients of Collins et al. 1967 were accepted. Touloukian et al. 1975 summarized length change differences between the normal and superconducting states below the superconducting temperature.

Lattice parameter measurements of Graham et al. 1955 (91-408 K) were only shown graphically with actual data points given by Touloukian et al. 1975 while values of Madaiah and Graham 1964 (14-291 K) were only shown graphically and measurements were not carried out along the principal axes. Deviations of experimental values from the selected values are given in Table 49b where for comparison purposes thermal expansion values of Vernon and Weintroub 1953 (303-393 K) and Smith and Schneider 1964 (100-300 K) and were converted to length change values. In comparison with the selected

values mean thermal expansion coefficients of Shinoda 1933 (296-360 K) are 45.0 x 10^{-6} K^{-1} along the *a* axis and 11.7 x 10^{-6} K^{-1} along the *c* axis. Lattice parameter measurements of Wolcyrz et al. 1981 (140-350 K) were only shown in the form of a small graph but room temperature values of 43 x 10^{-6} K^{-1} along the *a* axis and –13 x 10^{-6} K^{-1} along the *c* axis were given. The dilatometric measurements of Collins et al. 1967 at 283 K are given as 51.4 x 10^{-6} K^{-1} along the *a* axis and – 7.7 x 10^{-6} K^{-1} along the *c* axis. Lattice parameter measurements of Barrett 1962 were only determined at 4.2 K and 78 K. At 4.2 K the *a* axis value is only 0.00003 nm lower than the selected value but the *c* axis value is 0.00017 nm lower. At 78 K the differences are 0.00013 nm lower and 0.00018 nm lower respectively.

Table 49a. Lattice parameters of indium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Notes
Betterridge 1938	293	0.32515	0.49460	
Fink et al. 1945	299.5	0.32507	0.49477	
Guttman 1950	297	0.32517	0.49483	
Swanson et al. 1954	299	0.32509	0.49465	
Tyzack and Raynor 1954	293	0.32514	0.49470	
Graham et al. 1955	293	0.32519	049475	a
Graham and Raynor 1957	293	0.32517	0.49472	
Ievinš and Lindinya 1964	298	0.32522	0.49495	
Smith and Schneider 1964	RT	0.32532	0.49458	b
Ridley 1965	298	0.32516	0.49466	
Ridley 1968	298	0.32519	0.49455	
Deshpande and Pawar 1969	300, 301	0.32518	0.49467	
Straumanis et al. 1971	293	0.32515	0.49512	c
Wolcyrz et al. 1981	293	0.32521	0.49467	
	Selected	0.32516 (4)	0.49471 (10)	

Notes for Table 49a

a. Values given by Touloukian et al. 1975

b. Not included in the average

c. *c* axis value not included in the average

Values at 293.15: Density 7290 (2) kg m^{-3} Molar volume 15.749 (4) cm^3 mol^{-1}.

Table 49b. Deviations of experimental values from the selected values

References	Temperature Range K	Deviations 100Δε
Vernon and Weintroub 1953	303-393	Trends to 0.022 low along the *a* axis and 0.041 high along the *c* axis
Graham et al. 1955	91-408	Above 200 K scatter 0.012 low to 0.057 high along the *a* axis and bias 0.060 high along the *c* axis
Swenson et al. 1955	6-303	Dilatometric measurements scattering only 0.003 low to 0.003 high
Smith and Schneider 1964	100-300	Ultra pure metal: Bias 0.005 high along the *a* axis 0.016 low along the *c* axis High purity metal: Bias 0.003 low along the *a* axis and trends 0.021 low to 0.005 high along the *c* axis
Deshpande and Pawar 1969	300-379	Scatter 0.020 low to 0.035 high along the *a* axis and trends to 0.055 low along the *c* axis
Straumanis et al. 1971	283-333	Bias only 0.003 low along the *a* axis and 0.008 high along the *c* axis

Table 49c. Crystallographic properties of indium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
0	0	0	0	- 0.914	- 0.289	- 0.706
5	0.99	- 1.26	0.24	- 0.914	- 0.289	- 0.706
10	0.94	4.01	1.96	- 0.913	- 0.289	- 0.705
15	0.92	12.0	4.61	- 0.913	- 0.285	- 0.704
20	2.36	18.1	7.60	- 0.912	- 0.277	- 0.701
25	4.82	21.4	10.4	- 0.910	- 0.267	- 0.696
30	7.59	23.1	12.8	- 0.907	- 0.256	- 0.690
35	10.3	24.0	14.9	- 0.903	- 0.244	- 0.684
40	12.9	24.1	16.6	- 0.897	- 0.232	- 0.676
45	15.3	23.7	18.1	- 0.890	- 0.220	- 0.667
50	17.5	23.1	19.4	- 0.882	- 0.209	- 0.658
60	20.9	21.8	21.2	- 0.863	- 0.186	- 0.638
70	23.2	20.9	22.4	- 0.841	- 0.165	- 0.616
80	25.2	20.0	23.5	- 0.817	- 0.145	- 0.593
90	27.0	19.0	24.3	- 0.791	- 0.125	- 0.569
100	28.5	18.0	25.0	- 0.763	- 0.107	- 0.545
110	29.9	16.9	25.5	- 0.734	- 0.089	- 0.520
120	31.1	15.8	26.0	- 0.704	- 0.073	- 0.494
130	32.1	14.6	26.3	- 0.673	- 0.058	- 0.468
140	33.1	13.4	26.6	- 0.640	- 0.044	- 0.442
150	34.0	12.3	26.8	- 0.607	- 0.031	- 0.415
160	34.9	11.1	27.0	- 0.572	- 0.019	- 0.388
170	35.9	9.83	27.2	- 0.537	- 0.009	- 0.361
180	36.9	8.53	27.5	- 0.501	0.001	- 0.334
190	38.1	7.18	27.8	- 0.464	0.008	- 0.307
200	39.2	5.78	28.1	- 0.425	0.015	- 0.279
210	40.5	4.33	28.4	- 0.386	0.020	- 0.251
220	41.8	2.83	28.8	- 0.345	0.024	- 0.222
230	43.1	1.27	29.2	- 0.302	0.026	- 0.193
240	44.6	- 0.34	29.6	- 0.259	0.026	- 0.164
250	46.0	- 1.99	30.0	- 0.213	0.025	- 0.134
260	47.6	- 3.71	30.5	- 0.167	0.022	- 0.104
270	49.2	- 5.47	31.0	- 0.118	0.018	- 0.073
280	50.9	- 7.28	31.5	- 0.068	0.011	- 0.042
290	52.6	- 9.15	32.0	- 0.017	0.003	- 0.010
293.15	53.2	- 9.75	32.2	0	0	0
300	54.4	- 11.1	32.6	0.037	- 0.007	0.022
310	56.3	- 13.0	33.2	0.092	- 0.019	0.055
320	58.2	- 15.1	33.8	0.150	- 0.033	0.089
330	60.2	- 17.1	34.4	0.209	- 0.049	0.123
340	62.2	- 19.3	35.1	0.270	- 0.067	0.158
350	64.3	- 21.4	35.7	0.334	- 0.088	0.193
360	66.5	- 23.7	36.4	0.399	- 0.110	0.229
370	68.7	- 26.0	37.2	0.467	- 0.135	0.266
380	71.0	- 28.3	37.9	0.537	- 0.162	0.304
390	73.4	- 30.7	38.7	0.610	- 0.192	0.342
400	75.8	- 33.2	39.5	0.685	- 0.224	0.381
410	78.2	- 35.7	40.3	0.763	- 0.258	0.421
420	80.7	- 38.2	41.1	0.843	- 0.295	0.462
429.7485	83.3	- 40.8	41.9	0.924	- 0.333	0.503

Table 49d. Crystallographic properties of indium

T K	*a* nm	*c* nm	*c*/*a*	*d*2 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.32219	0.49328	1.5310	0.33576	15.418	7447
5	0.32219	0.49328	1.5310	0.33576	15.418	7447
10	0.32219	0.49328	1.5310	0.33576	15.419	7447
15	0.32219	0.49330	1.5311	0.33577	15.419	7446
20	0.32220	0.49334	1.5312	0.33578	15.421	7446
25	0.32220	0.49339	1.5313	0.33580	15.423	7445
30	0.32221	0.49344	1.5314	0.33583	15.425	7443
35	0.32223	0.49350	1.5315	0.33586	15.429	7442
40	0.32224	0.49356	1.5316	0.33589	15.432	7440
45	0.32227	0.49362	1.5317	0.33592	15.436	7438
50	0.32229	0.49368	1.5318	0.33596	15.441	7436
60	0.32236	0.49379	1.5318	0.33603	15.450	7432
70	0.32243	0.49389	1.5318	0.33610	15.460	7427
80	0.32250	0.49400	1.5317	0.33617	15.471	7422
90	0.32259	0.49409	1.5316	0.33625	15.482	7416
100	0.32268	0.49418	1.5315	0.33633	15.493	7411
110	0.32277	0.49427	1.5313	0.33640	15.505	7405
120	0.32287	0.49435	1.5311	0.33648	15.517	7399
130	0.32297	0.49443	1.5309	0.33656	15.529	7394
140	0.32308	0.49449	1.5306	0.33663	15.542	7388
150	0.32319	0.49456	1.5303	0.33671	15.554	7382
160	0.32330	0.49462	1.5299	0.33678	15.567	7376
170	0.32341	0.49467	1.5295	0.33686	15.579	7370
180	0.32353	0.49471	1.5291	0.33693	15.592	7364
190	0.32365	0.49475	1.5286	0.33700	15.605	7358
200	0.32378	0.49478	1.5282	0.33707	15.618	7352
210	0.32391	0.49481	1.5276	0.33714	15.631	7345
220	0.32404	0.49483	1.5271	0.33722	15.645	7339
230	0.32418	0.49484	1.5264	0.33729	15.658	7333
240	0.32432	0.49484	1.5258	0.33735	15.672	7326
250	0.32447	0.49483	1.5251	0.33742	15.686	7320
260	0.32462	0.49482	1.5243	0.33749	15.700	7313
270	0.32478	0.49480	1.5235	0.33756	15.715	7306
280	0.32494	0.49477	1.5226	0.33762	15.730	7299
290	0.32511	0.49472	1.5217	0.33769	15.745	7292
293.15	0.32516	0.49471	1.5214	0.33771	15.749	7290
300	0.32528	0.49467	1.5208	0.33776	15.760	7285
310	0.32546	0.49462	1.5197	0.33782	15.776	7278
320	0.32565	0.49455	1.5187	0.33789	15.791	7271
330	0.32584	0.49447	1.5175	0.33795	15.808	7264
340	0.32604	0.49438	1.5163	0.33801	15.824	7256
350	0.32625	0.49428	1.5150	0.33808	15.841	7248
360	0.32646	0.49416	1.5137	0.33814	15.858	7240
370	0.32668	0.49404	1.5123	0.33820	15.876	7232
380	0.32691	0.49391	1.5108	0.33826	15.893	7224
390	0.32714	0.49376	1.5093	0.33832	15.912	7216
400	0.32739	0.49360	1.5077	0.33838	15.930	7208
410	0.32764	0.49343	1.5060	0.33844	15.949	7199
420	0.32790	0.49325	1.5043	0.33850	15.969	7190
429.7485	0.32816	0.49306	1.5025	0.33856	15.988	7181

Interatomic distance calculations for Table 49d: $d1 = a \quad d2 = (a^2/2 + c^2/4)^{½}$

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50 TIN Sn

Atomic weight: 118.710 (7) (Meija 2017)

Structure: Alpha phase: Cubic (cF8)
Beta phase: Body-centered tetragonal (tI4)

Hultgren et al. 1973 selected 286.2 K for the alpha-beta transition temperature based on the measurements of Raynor and Smith 1958. However, the alpha phase can be retained in a metastable state at room temperature while the beta phase is metastable down to the lowest temperatures. The freezing point is a primary fixed point on ITS-90 at 505.078 K (Preston Thomas 1990).

50.1 Alpha Phase: Cubic (cF8): 0 K to 286.2 K

Thermal expansion coefficients of Novikova 1960 (24-217 K) and lattice parameter measurements of Thewlis and Davey 1954 (143-296 K) are both shown graphically with actual data points being given by Touloukian 1975. Giving preference to the more sensitive thermal expansion coefficients measurements then up to 213 K these can be represented by the equations in which a determination at 209 K was not included in the fit. Equation 50a was extrapolated below 24 K:

$$0 - 80\ \text{K}: \quad \alpha\ (\text{K}^{-1}) = -1.60588 \times 10^{-7}\,T + 3.97886 \times 10^{-9}\,T^{2} - 1.69617 \times 10^{-11}\,T^{3} - 5.53086 \times 10^{-14}\,T^{4} + 9.33032 \times 10^{-7} \qquad (50a)$$

$$80 - 213\ \text{K}: \quad \alpha\ (\text{K}^{-1}) = -9.88703 \times 10^{-8}\,T + 1.86275 \times 10^{-9}\,T^{2} - 1.02093 \times 10^{-11}\,T^{3} + 1.81356 \times 10^{-14}\,T^{4} + 3.07658 \times 10^{-6} \qquad (50b)$$

Above 213 K a constant thermal expansion coefficient of $5.20 \times 10^{-6}\ \text{K}^{-1}$ is selected. The scatter in the length changes derived from the lattice parameter values of Thewlis and Davey 1954 leads to the measurements being best fitted to a straight line with a derived thermal expansion coefficient of $4.7 \times 10^{-6}\ \text{K}^{-1}$ and on the basis 100ε an average deviation from the selected values of 0.005 high at 273 K and below.

Table 50a. Lattice parameter value of alpha tin at 293.15 K

References	Original Temperature K	*a* nm
Brownlee 1950	RT	0.64916
Swanson and Fuyat 1953	298	0.6489
Thewlis and Davey 1954	293	0.64896
	Selected	0.64896 (5)

The measurement of Thewlis and Davey 1954 is selected because of the close agreement with the less accurate value determined by Swanson and Fuyat 1953.

At 293.15 K: Density 5770 (1) kg m^{-3} Molar volume 20.574 (5) $\text{cm}^3\ \text{mol}^{-1}$.

50.2 Beta Phase: Body-centered tetragonal (tI4): 286.2 K to 505.078 K

Above 293.15 K values selected are based on the precision dilatometric measurements of Current 1974 (293-499 K) which were used to represent the thermal expansion from 293.15 K to the freezing point:

$$\varepsilon_T\, a = 1.35708 \times 10^{-5}\, T + 4.66571 \times 10^{-10}\, T^{\,2} + 9.09254 \times 10^{-12}\, T^{\,3} - 4.24744 \times 10^{-3} \quad (50c)$$

$$\varepsilon_T\, c = 3.46390 \times 10^{-5}\, T - 2.03486 \times 10^{-8}\, T^{\,2} + 3.94974 \times 10^{-11}\, T^{\,3} - 9.40076 \times 10^{-3} \quad (50d)$$

Lattice parameter and length change values determined by Balzer and Sigvaldason 1979 (293-497 K) were only shown graphically but indicate that thermal vacancy effects in tin are negligible.

Up to 85 K the thermal expansion coefficient measurements of White 1964 (4-85, 283K) are selected. Between 85 K and 293.15 K the thermal expansion coefficients of White 1964 over the range 30 K to 85 K were combined with the selected values at 293.15 derived from the above equations and fitted to Equation A using the smoothed specific heat (C_p) values as given in Part 50.3 leading to the following equations which represent the thermal expansion from 85 K to 293.15 K:

$$\alpha_a\,(K^{-1}) = C_p\,(6.99278 \times 10^{-7} - 1.41561 \times 10^{-10}\, T - 1.67211 \times 10^{-5} / T) \quad (50e)$$

$$\alpha_c\,(K^{-1}) = C_p\,(9.28682 \times 10^{-7} + 7.19548 \times 10^{-10}\, T + 2.37132 \times 10^{-5} / T) \quad (50f)$$

On the basis $100\Delta\varepsilon$ in the low temperature region, dilatometric measurements of Erfling 1939 (58-293 K) bias only 0.002 high along the *a* axis but trends to 0.095 high along the *c* axis while length change values derived from the lattice parameter values of Rayne and Chandrasekhar 1960 (4.2-298 K) trend from 0.008 high along the *a* axis and 0.010 low along the *c* axis. Thermal expansion coefficients of Childs and Weintroub 1950 (303-493 K) when converted to length change values bias only 0.002 high along the *a* axis but trend to 0.012 low along the *c* axis. Length change values derived from the lattice parameter measurements of Deshpande and Sirdeshmukh 1961 (308-424 K) trend to 0.030 high along the *a* axis and 0.045 high along the *c* axis while the later measurements of Deshpande and Sirdeshmukh 1962 (306-485 K) trend to 0.036 high along the *a* axis and 0.085 high along the *c* axis. Lattice parameter measurements of Wolcyrz et al. 1981 (200-420 K) were only shown in the form of small graphs.

Table 50b. Lattice parameter values of beta tin at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Note
Stenzel and Weerts 1932	293	0.58315	0.31819	a
Jette and Foote 1935	298	0.58311	0.31811	
Ievinš et al. 1938	298	0.58313	0.31810	
Carapella and Hultgren 1941, 1942	298	0.58313	0.31811	
Fink et al. 1945	298	0.58311	0.31811	
Lee and Raynor 1954	298	0.58315	0.31810	
Vogel and Kempter 1959, 1961	298	0.58316	0.31815	
Rayne and Chandrasekhar 1960	300	0.58312	0.31823	a
Deshpande and Sirdeshmukh 1961	308	0.58316	0.31811	
Deshpande and Sirdeshmukh 1962	306	0.58317	0.31809	
King and Massalski 1962	299	0.58311	0.31811	
Helfrich and Dodd 1964	298	0.58311	0.31811	
Wolcyrz et al. 1981	293	0.58309	0.31811	
	Selected	0.58313 (2)	0.31811 (2)	

Note for Table 50b

a. *c* axis value not included in the average

At 293.15 K: Density 7289 (1) kg m^{-3} Molar volume 16.285 (2) cm^3 mol^{-1}.

Table 50c. Comparison of density and molar volume differences at the transition temperature 286.2 K

Phase	Density kg m^{-3}	Molar Volume cm^3 mol^{-1}
Alpha	5771	20.572
Beta	7293	16.278

At the transition the contraction is 4.294 (5) cm^3 mol^{-1} (20.9 %)

50.3 Low temperature specific heat of the beta phase

Smooth values of specific heat (C_p) in J mol^{-1} K^{-1} derived from the experimental values of Naumov et al. 1979 (1.7-331.4 K). Atomic weight correction 118.710/118.69 was applied:

T K	5	10	15	20	25	30	35	40
C_p	0.0670	0.907	2.63	4.62	6.67	8.72	10.67	12.40
T K	45	50	60	65	70	80	85	90
C_p	13.96	15.34	17.58	18.48	19.26	20.50	21.00	21.44
T K	100	110	120	130	140	150	160	170
C_p	22.22	22.80	23.29	23.71	24.10	24.43	24.68	24.89
T K	180	190	200	210	220	230	240	250
C_p	25.11	25.31	25.50	25.68	25.86	26.03	26.19	26.34
T K	260	270	280	286.2	290	293.15	298.15	300
C_p	26.49	26.64	26.78	26.86	26.91	26.95	27.01	27.03

50d. Crystallographic properties of alpha tin

T K	α x 10^6 K^{-1}	100 ε_T	*a* nm	*d*1 nm	*d*2 nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
0	0	- 0.104	0.64829	0.28072	0.45841	20.510	5788
5	- 0.05	- 0.104	0.64829	0.28072	0.45841	20.510	5788
10	- 0.40	- 0.104	0.64829	0.28072	0.45841	20.510	5788
15	- 0.70	- 0.104	0.64829	0.28072	0.45841	20.510	5788
20	- 0.85	- 0.104	0.64828	0.28071	0.45841	20.510	5788
25	- 0.88	- 0.105	0.64828	0.28071	0.45840	20.509	5788
30	- 0.81	- 0.105	0.64828	0.28071	0.45840	20.509	5788
40	-0.35	- 0.106	0.64827	0.28071	0.45840	20.509	5788
50	0.38	- 0.106	0.64827	0.28071	0.45840	20.509	5788
60	1.24	- 0.105	0.64828	0.28071	0.45840	20.509	5788
70	2.00	- 0.103	0.64829	0.28072	0.45841	20.510	5788
80	2.60	- 0.101	0.64830	0.28072	0.45842	20.511	5788
90	3.01	- 0.098	0.64832	0.28073	0.45843	20.513	5787
100	3.42	- 0.095	0.34834	0.28074	0.45845	20.515	5787
110	3.81	- 0.091	0.64837	0.28075	0.45846	20.517	5786
120	4.15	- 0.087	0.64839	0.28076	0.45848	20.520	5786
130	4.45	- 0.083	0.64842	0.28077	0.45850	20.523	5785
140	4.70	- 0.079	0.64845	0.28079	0.45852	20.525	5784
150	4.88	- 0.074	0.64848	0.28080	0.45855	20.528	5784
160	5.01	- 0.069	0.64851	0.28081	0.45857	20.531	5783
170	5.09	- 0.064	0.64855	0.28083	0.45859	20.534	5782
180	5.13	- 0.059	0.64858	0.28084	0.45861	20.538	5781
190	5.15	- 0.054	0.64861	0.28086	0.45864	20.541	5780
200	5.16	- 0.048	0.64865	0.28087	0.45866	20.544	5779
210	5.18	- 0.043	0.64868	0.28089	0.45869	20.547	5778
220	5.20	- 0.038	0.64871	0.28090	0.45871	20.550	5777
230	5.20	- 0.033	0.64875	0.28092	0.45873	20.554	5777
240	5.20	- 0.028	0.64878	0.28093	0.45876	20.557	5776
250	5.20	- 0.022	0.64881	0.28094	0.45878	20.560	5775
260	5.20	- 0.017	0.64885	0.28096	0.45881	20.563	5774
270	5.20	- 0.012	0.64888	0.28097	0.45883	20.566	5773
280	5.20	- 0.007	0.64892	0.28099	0.45885	20.570	5772
286.2	5.20	- 0.004	0.64894	0.28100	0.45887	20.572	5771
290	5.20	- 0.002	0.64895	0.28100	0.45888	20.573	5770
293.15	5.20	0	0.64896	0.28101	0.45888	20.574	5770

$$d1 = \sqrt{3}a/4 \qquad d2 = a/\sqrt{2}$$

Table 50e. Crystallographic properties of beta tin

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 ε_T *a*	100 ε_T *c*	100 ε_T avr
0	0	0	0	- 0.334	- 0.765	- 0.478
5	- 0.02	0.13	0.03	- 0.334	- 0.765	- 0.478
10	- 0.10	1.65	0.48	- 0.334	- 0.765	- 0.477
15	- 0.15	4.75	1.48	- 0.334	- 0.763	- 0.477
20	- 0.04	8.40	2.77	- 0.334	- 0.760	- 0.476
25	0.43	11.70	4.19	- 0.334	- 0.755	- 0.474
30	1.20	15.20	5.87	- 0.333	- 0.748	- 0.472
40	3.42	19.20	8.68	- 0.331	- 0.731	- 0.464
50	5.49	22.03	11.00	- 0.327	- 0.710	- 0.455
60	7.25	23.99	12.83	- 0.320	- 0.687	- 0.443
70	8.68	25.36	14.24	- 0.312	- 0.663	- 0.429
80	9.82	26.30	15.31	- 0.303	- 0.637	- 0.414
90	10.74	26.95	16.14	- 0.293	- 0.611	- 0.399
100	11.51	27.50	16.84	- 0.282	- 0.584	- 0.382
110	12.12	27.89	17.38	- 0.270	- 0.556	- 0.365
120	12.65	28.24	17.85	- 0.258	- 0.528	- 0.348
130	13.09	28.56	18.25	- 0.245	- 0.500	- 0.330
140	13.50	28.89	18.63	- 0.231	- 0.471	- 0.311
150	13.84	29.19	18.96	- 0.218	- 0.442	- 0.293
160	14.12	29.42	19.22	- 0.204	- 0.413	- 0.274
170	14.36	29.63	19.45	- 0.190	- 0.384	- 0.254
180	14.59	29.88	19.69	- 0.175	- 0.354	- 0.235
190	14.79	30.12	19.90	- 0.161	- 0.324	- 0.215
200	14.98	30.37	20.11	- 0.146	- 0.294	- 0.195
210	15.15	30.63	20.31	- 0.131	- 0.264	- 0.175
220	15.31	30.90	20.51	- 0.115	- 0.233	- 0.155
230	15.46	31.17	20.70	- 0.100	- 0.202	- 0.134
240	15.60	31.43	20.88	- 0.085	- 0.171	- 0.113
250	15.73	31.70	21.05	- 0.069	- 0.139	- 0.092
260	15.85	31.97	21.22	- 0.053	- 0.107	- 0.071
270	15.96	32.26	21.39	- 0.037	- 0.075	- 0.050
280	16.07	32.53	21.56	- 0.021	- 0.040	- 0.028
286.2	16.13	32.70	21.65	- 0.011	- 0.023	- 0.015
290	16.16	32.81	21.71	- 0.005	- 0.010	- 0.007
293.15	16.19	32.89	21.76	0	0	0
300	16.30	33.09	21.90	0.011	0.023	0.015
320	16.66	33.72	22.34	0.044	0.089	0.059
340	17.03	34.45	22.83	0.078	0.158	0.104
350	17.22	34.84	23.10	0.095	0.192	0.127
360	17.42	35.27	23.37	0.112	0.227	0.151
380	17.84	36.18	23.95	0.148	0.299	0.198
400	18.27	37.18	24.58	0.184	0.373	0.247
420	18.73	38.28	25.25	0.221	0.448	0.297
440	19.21	39.46	25.96	0.259	0.527	0.348
450	19.46	40.09	26.34	0.278	0.567	0.374
460	19.71	40.74	26.72	0.298	0.607	0.401
480	20.24	42.11	27.53	0.338	0.691	0.455
500	20.78	43.57	28.38	0.379	0.777	0.512
505.078	20.92	43.96	28.60	0.390	0.799	0.526

Table 50f. Crystallographic properties of beta tin

T K	*a* nm	*c* nm	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.58118	0.31568	0.30112	16.053	7395
5	0.58118	0.31568	0.30112	16.053	7395
10	0.58118	0.31568	0.30112	16.053	7395
15	0.58118	0.31568	0.30112	16.053	7395
20	0.58118	0.31569	0.30112	16.054	7394
25	0.58118	0.31571	0.30112	16.055	7394
30	0.58119	0.31573	0.30112	16.056	7394
40	0.58120	0.31579	0.30113	16.059	7392
50	0.58122	0.31585	0.30115	16.064	7390
60	0.58126	0.31592	0.30117	16.070	7387
70	0.58131	0.31600	0.30120	16.077	7384
80	0.58136	0.31608	0.30123	16.084	7381
90	0.58142	0.31617	0.30126	16.091	7377
100	0.58149	0.31625	0.30130	16.099	7374
110	0.58516	0.31634	0.30134	16.108	7370
120	0.58163	0.31643	0.30138	16.116	7366
130	0.58170	0.31652	0.30142	16.125	7362
140	0.58178	0.31661	0.30147	16.134	7358
150	0.58186	0.31670	0.30151	16.143	7354
160	0.58194	0.31680	0.30156	16.152	7350
170	0.58202	0.31689	0.30160	16.161	7345
180	0.58211	0.31698	0.30165	16.171	7341
190	0.58219	0.31708	0.30170	16.181	7337
200	0.58228	0.31717	0.30175	16.190	7332
210	0.58237	0.31727	0.30179	16.200	7328
220	0.58246	0.31737	0.30184	16.210	7323
230	0.58255	0.31747	0.30189	16.220	7319
240	0.28264	0.31757	0.30194	16.230	7314
250	0.58273	0.31767	0.30199	16.240	7310
260	0.58282	0.31777	0.30204	16.251	7305
270	0.58291	0.31787	0.30210	16.261	7300
280	0.58301	0.31797	0.30215	16.272	7296
286.2	0.58306	0.31804	0.30218	16.278	7293
290	0.58310	0.31808	0.30220	16.282	7291
293.15	0.58313	0.31811	0.30222	16.285	7289
300	0.58319	0.31818	0.30225	16.293	7286
320	0.58339	0.31839	0.30236	16.314	7276
340	0.58358	0.31861	0.30247	16.336	7267
350	0.58368	0.31872	0.30252	16.348	7262
360	0.58378	0.31883	0.30258	16.359	7256
380	0.58399	0.31906	0.30269	16.382	7246
400	0.58420	0.31930	0.30281	16.406	7236
420	0.58442	0.31954	0.30293	16.431	7225
440	0.58464	0.31978	0.30305	16.456	7214
450	0.58475	0.31991	0.30312	16.469	7208
460	0.58487	0.32004	0.30318	16.482	7202
480	0.58510	0.32031	0.30331	16.509	7191
500	0.58534	0.32058	0.30345	16.537	7179
505.078	0.58540	0.32065	0.30348	16.544	7175

Interatomic distance calculations for Table 50f: $d1 = (a^2/4 + c^2/16)^{½}$ $d2 = c$

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51 ANTIMONY Sb

Atomic weight: 121.760 (1) (Meija 2017)

Structure: Rhombohedral (hR2)

The freezing point is a secondary fixed point on ITS-90 at 903.778 (1) K (Bedford et al. 1996).

51.1 High Temperature

Although likely to be of higher quality, lattice parameter measurements of Fischer et al. 1978 (5-830 K) were unfortunately shown only in the form of small graphs so that the high temperature selected values above 293.15 K are essentially based only on one set of measurements, the scattered measurements of Klemm et al. 1960 (293-833 K) which were originally only shown graphically with actual data points being given by Touloukian et al. 1975. The selected *a* axis equation leads to a maximum in the derived thermal expansion coefficient at 489 K which is considered to be unnatural behavior even though the scatter in the derived thermal expansion values of Deshpande and Pawar 1969 (301-493 K) also appear to suggest this trend. In order to remove this behavior the equations given by Touloukian et al. 1975 were reduced from cubic to quadratic equations to represent the thermal expansion from 293.15 K to the freezing point:

$$\varepsilon_T a = 7.88283 \times 10^{-6} T + 6.14534 \times 10^{-10} T^2 - 2.36366 \times 10^{-3} \quad (51a)$$

$$\varepsilon_T c = 1.52840 \times 10^{-5} T + 2.28552 \times 10^{-9} T^2 - 4.67692 \times 10^{-3} \quad (51b)$$

The actual *a* axis values of Klemm et al. 1960 can be considered as showing a trend to an average of 0.031 low above 680 K while for the *c* axis the trend is a maximum of 0.089 high at 548 K before falling to 0.10 low at the highest temperature. Length change values derived from the lattice parameter measurements of Deshpande and Pawar 1969 (301-493 K) trend to 0.031 high along the *a* axis and for the c axis show a maximum deviation of 0.038 high at 389 K before trending to 0.024 high. Length change values derived from the direct density measurements of Cahill and Kirshenbaum 1963 (293-904 K) trend to 0.11 high while similar values of Stankus and Khairulin 1988 (293-904 K) trend to 0.057 high. Therefore, the high temperature thermal expansion of antimony can be considered as being poorly determined.

51.2 Low Temperature

Thermal expansion coefficients of White 1972 (2-85, 283 K) were accepted up to 85 K but in the interval from 85 to 293.15 K the *a* axis thermal expansion coefficient values of White 1972 at 65 to 85 K were combined with the value derived from Equation 51a at 293.15 K and fitted to Equation A using the values of specific heat (C_p) selected in Part 51.3:

$$\alpha_a\,(K^{-1}) = C_p\,(3.93391 \times 10^{-7} - 1.0749 \times 10^{-10}\,T - 1.01149 \times 10^{-5}/\,T) \qquad (51c)$$

Because of the relative quality of the interpolated specific heat values, thermal expansion values for the *a* axis were further smoothed from 120 K to 293.15 K by fitting to Equation 51d below. The differences between Equations 51c and 51d do not amount to more than 2 x 10^{-8} K^{-1}. For the *c* axis following the same procedure it was found that a fit to Equation A was unsatisfactory and instead interpolated values 90 to 290 K were estimated graphically and then refined by fitting to Equation 51e to cover the range from 90 to 293.15 K:

$$\alpha_a\,(K^{-1}) = 6.99963 \times 10^{-8}\,T - 2.29336 \times 10^{-10}\,T^{\,2} + 2.26068 \times 10^{-13}\,T^{\,3} + 9.50902 \times 10^{-17}\,T^{\,4} + 1.03200 \times 10^{-6} + \qquad (51d)$$

$$\alpha_c\,(K^{-1}) = 8.93726 \times 10^{-8}\,T - 5.20957 \times 10^{-10}\,T^{\,2} + 1.41640 \times 10^{-12}\,T^{\,3} - 1.43768 \times 10^{-15}\,T^{\,4} + 1.01249 \times 10^{-5} \qquad (51e)$$

Above 40 K the thermal expansion coefficients along the *a* axis of Bunton and Weintroub 1969 (10-200 K) scatter 2% low to 2% high up to 100 K but average 2% low above this temperature while for the *c* axis there is a maximum deviation of 6% high at 60 K before converging to the selected values. On the basis $100\Delta\varepsilon$ the anisotropic dilatometric length change values of Erfling 1939 (58-293 K) show excellent agreement with the selected values with the *a* axis values agreeing to within 0.001, while the *c* axis values scatter only 0.003 low to 0.003 high. Lattice parameter measurements given by Schiferl and Barrett 1969 (4.2 – 298 K), which replace earlier values of Cucka and Barrett 1962 and Barrett et al. 1963, when converted to length change values average only 0.006 low along the *a* axis while the *c* axis trends from 0.041 low.

The positional parameter z

Values of *z* determined by Fischer et al. 1978 (5-838 K) were selected because they virtually covered the whole temperature range. They can be averaged to a single value of 0.2339 (2) which is selected and compares to a value of 0.2336 (1) over the range 4.2 to 298 K as determined by Schiferl and Barrett 1969.

Table 51a. Lattice parameter measurements of antimony at 293.15 K

References	Original Temperature K	Hexagonal		Notes
		a_h nm	c_h nm	
Jette and Foote 1935	298	0.43083	1.17240	
Trzebiatowski and Brytak 1938	RT	0.43093	1.12747	
Lu and Chang 1941	295	0.43082	1.12733	
Klemm et al. 1960	293	0.43031	1.12717	a
Barrett et al. 1963	298	0.43085	1.12737	b
Dismukes at al 1968	298	0.43086	1.12729	
Schiferl and Barrett 1969	298	0.43085	1.12737	
Deshpande and Pawar 1969	301	0.43079	1.12732	
Berger et al. 1982	298	0.43077	1.12759	c
	Selected	0.43084 (5)	1.12736 (7)	

Notes for Table 51a

a. Values given by Touloukian et al. 1975. Not included in the averages

b. Superseded by the measurements of Schiferl and Barrett 1969. Not included in the averages

c. *c* axis value not included in the averages

The selected equivalent rhombohedral cell is a_r 0.45066 (3) nm $\alpha = 57.112\ (18)°$

At 293.15: Density 6694 (2) kg m^{-3} Molar volume 18.190 (4) cm^3 mol^{-1}

51.3 Low temperature specific heat of antimony

Hultgren et al. 1973 selected values of specific heat (C_p) in cal mol^{-1} K^{-1} at irregular temperatures up to 298.15 K. Values at 50 K and below are those selected by Hultgren et al. 1973 after conversion to J mol^{-1} K^{-1}. Values at 60 K and above were generally obtained by interpolation.

Table 51b. Low temperature specific heat values for antimony

T K	5	10	15	20	25	30	40	50
C_p	0.037	0.42	1.50	3.14	4.90	6.69	10.08	13.01
T K	60	65	70	75	80	85	90	100
C_p	15.33	16.27	17.15	17.91	18.63	19.25	19.78	20.59
T K	110	120	130	140	150	160	170	180
C_p	21.39	22.04	22.53	22.89	23.14	23.46	23.73	23.97
T K	190	200	210	220	230	240	250	260
C_p	24.17	24.35	24.49	24.60	24.30	24.78	24.85	24.92
T K	270	280	290	293.15	298.15			
C_p	24.99	25.06	25.15	25.18	25.23			

Table 51c. Crystallographic properties of antimony

T K	α_{ah} x 10^6 K^{-1}	α_{ch} x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
0	0	0	0	- 0.170	- 0.412	- 0.251
5	0	0.05	0.02	- 0.170	- 0.412	- 0.251
10	- 0.02	0.49	0.15	- 0.170	- 0.412	- 0.251
15	- 0.04	1.93	0.62	- 0.170	- 0.411	- 0.251
20	0	4.30	1.43	- 0.170	- 0.410	- 0.250
25	0.16	6.68	2.33	- 0.170	- 0.407	- 0.249
30	0.42	8.65	3.16	- 0.170	- 0.403	- 0.248
40	1.30	11.22	4.61	- 0.169	- 0.393	- 0.244
50	2.35	12.62	5.77	- 0.168	- 0.381	- 0.239
60	3.33	13.49	6.72	- 0.165	- 0.368	- 0.233
70	4.14	14.15	7.48	- 0.161	- 0.354	- 0.225
80	4.81	14.61	8.08	- 0.156	- 0.340	- 0.218
90	5.37	14.89	8.54	- 0.151	- 0.325	- 0.209
100	5.79	15.13	8.90	- 0.146	- 0.310	- 0.201
110	6.19	15.33	9.24	- 0.140	- 0.295	- 0.192
120	6.54	15.50	9.52	- 0.133	- 0.280	- 0.182
130	6.78	15.64	9.74	- 0.127	- 0.264	- 0.173
140	6.99	15.76	9.92	- 0.120	- 0.249	- 0.163
150	7.18	15.86	10.07	- 0.113	- 0.233	- 0.153
160	7.35	15.95	10.22	- 0.106	- 0.217	- 0.143
170	7.49	16.02	10.33	- 0.098	- 0.201	- 0.132
180	7.62	16.08	10.44	- 0.091	- 0.185	- 0.122
190	7.73	16.14	10.52	- 0.083	- 0.169	- 0.112
200	7.82	16.19	10.61	- 0.075	- 0.153	- 0.101
210	7.90	16.24	10.68	- 0.067	- 0.137	- 0.090
220	7.96	16.28	10.73	- 0.059	- 0.120	- 0.080
230	8.02	16.33	10.79	- 0.051	- 0.104	- 0.069
240	8.06	16.38	10.83	- 0.043	- 0.088	- 0.058
250	8.10	16.42	10.87	- 0.035	- 0.071	- 0.047
260	8.14	16.47	10.91	- 0.027	- 0.055	- 0.036
270	8.17	16.52	10.95	- 0.019	- 0.038	- 0.025
280	8.20	16.56	10.99	- 0.011	- 0.022	- 0.014
290	8.23	16.61	11.02	- 0.003	- 0.005	- 0.003
293.15	8.24	16.62	11.04	0	0	0
300	8.25	16.65	11.05	0.006	0.011	0.008
350	8.31	16.87	11.16	0.047	0.095	0.063
400	8.37	17.08	11.27	0.089	0.180	0.119
450	8.42	17.29	11.38	0.131	0.266	0.176
500	8.48	17.51	11.49	0.173	0.354	0.233
550	8.54	17.72	11.60	0.216	0.442	0.291
600	8.60	17.93	11.71	0.259	0.532	0.350
650	8.66	18.14	11.82	0.302	0.622	0.409
700	8.71	18.35	11.93	0.345	0.714	0.468
750	8.77	18.56	12.03	0.389	0.807	0.529
800	8.83	18.77	12.14	0.434	0.901	0.589
850	8.89	18.98	12.25	0.478	0.997	0.651
900	8.94	19.19	12.36	0.523	1.093	0.713
903.778	8.95	19.20	12.37	0.526	1.100	0.718

Table 51d. Crystallographic properties of antimony

T K	a_h nm	c_h nm	a_r nm	α°	$d1$ nm	$d2$ nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.43011	1.12272	0.44913	57.217	0.2906	0.3339	18.053	6745
5	0.43011	1.12272	0.44913	57.217	0.2906	0.3339	18.053	6745
10	0.43011	1.12272	0.44913	57.217	0.2906	0.3339	18.053	6745
15	0.43011	1.12272	0.44913	57.217	0.2906	0.3339	18.053	6745
20	0.43011	1.12274	0.44914	57.216	2.2906	0.3339	18.053	6744
25	0.43011	1.12277	0.44915	57.215	0.2906	0.3339	18.054	6744
30	0.43011	1.12281	0.44916	57.213	0.2906	0.3340	18.055	6744
40	0.43011	1.12293	0.44919	57.209	0.2906	0.3340	18.057	6743
50	0.43012	1.12306	0.44923	57.205	0.2906	0.3340	18.060	6742
60	0.43013	1.12321	0.44928	57.200	0.2907	0.3340	18.063	6741
70	0.43015	1.12337	0.44932	57.196	0.2907	0.3340	18.067	6739
80	0.43017	1.12353	0.44938	57.192	0.2907	0.3341	18.071	6738
90	0.43019	1.12369	0.44943	57.187	0.2907	0.3341	18.076	6736
100	0.43021	1.12384	0.44948	57.183	0.2907	0.3341	18.080	6734
110	0.43024	1.12403	0.44954	57.179	0.2908	0.3342	18.085	6733
120	0.43027	1.12421	0.44960	57.175	0.2908	0.3342	18.090	6731
130	0.43029	1.12438	0.44965	57.171	0.2908	0.3342	18.096	6729
140	0.43032	1.12456	0.44971	57.168	0.2909	0.3343	18.101	6727
150	0.43035	1.12474	0.44977	57.164	0.2909	0.3343	18.106	6725
160	0.43039	1.12491	0.44983	57.160	0.2909	0.3344	18.112	6723
170	0.43042	1.12509	0.44989	57.156	0.2909	0.3344	18.118	6721
180	0.43045	1.12528	0.44995	57.153	0.2910	0.3344	18.123	6718
190	0.43048	1.12546	0.45001	57.149	0.2910	0.3345	18.129	6716
200	0.43052	1.12564	0.45007	57.145	0.2910	0.3345	18.135	6714
210	0.43055	1.12582	0.45013	57.142	0.2911	0.3345	18.140	6712
220	0.43058	1.12600	0.45020	57.138	0.2911	0.3346	17.146	6710
230	0.43062	1.12619	0.45026	57.135	0.2911	0.3346	18.152	6708
240	0.43065	1.12637	0.45032	57.131	0.2911	0.3347	18.158	6706
250	0.43069	1.12656	0.45038	57.127	0.2912	0.3347	18.164	6703
260	0.43072	1.12674	0.45045	57.124	0.2912	0.3347	18.170	6701
270	0.43076	1.12693	0.45051	57.120	0.2912	0.3348	18.176	6699
280	0.43079	1.12711	0.45057	57.116	0.2913	0.3348	18.182	6697
290	0.43082	1.12730	0.45064	57.113	0.2913	0.3349	18.188	6695
293.15	0.43084	1.12736	0.45066	57.112	0.2913	0.3349	18.190	6694
300	0.43086	1.12749	0.45070	57.109	0.2913	0.3349	18.194	6692
350	0.43104	1.12843	0.45102	57.091	0.2915	0.3351	18.224	6681
400	0.43122	1.12939	0.45134	57.072	0.2916	0.3353	18.255	6670
450	0.43140	1.13036	0.45167	57.053	0.2918	0.3355	18.286	6659
500	0.43159	1.13135	0.45200	57.034	0.2919	0.3357	18.317	6647
550	0.43177	1.13234	0.45234	57.014	0.2921	0.3359	18.349	6636
600	0.43195	1.13335	0.45268	56.994	0.2923	0.3362	18.381	6624
650	0.43214	1.13438	0.45302	56.974	0.2924	0.3364	18.414	6613
700	0.43233	1.13541	0.45337	59.953	0.2926	0.3366	18.446	6601
750	0.43252	1.13646	0.45372	56.932	0.2928	0.3368	18.480	6589
800	0.43271	1.13752	0.45408	56.910	0.2929	0.3370	18.513	6577
850	0.43290	1.13860	0.45444	56.889	0.2931	0.3372	18.547	6565
900	0.43309	1.13968	0.45480	56.867	0.2932	0.3373	18.581	6553
903.778	0.43311	1.13976	0.45483	56.865	0.2933	0.3375	18.584	6552

$$d1 = [\ a_h{}^2/\ 3 + c_h{}^2\,(2z - ⅓)^{\,2}\ ]^{\,½} \qquad d2 = [\ a_h{}^2/\ 3 + c_h{}^2\,(2z - ⅔)^{\,2}\ ]^{\,½}$$

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52 TELLURIUM Te

Atomic Weight: 127.60 (3) (Meija 2017)

Structure: Hexagonal (hP3)

The triple point was determined by Tevebaugh and Cairns to be 722.95 (5) K.

Below 293.15 K the thermal expansion coefficients determined by White 1973 (2-85, 283 K) were combined with those of Ibach and Ruin 1970 (2-500 K) with preference given to the latter measurements above 35 K. The measurements of Ibach and Ruin 1970 can be represented by the following equations:

a axis

$$100 - 500 \text{ K: } \alpha_a (K^{-1}) = 2.36477 \times 10^{-8} T - 1.26840 \times 10^{-11} T^2 + 2.38043 \times 10^{-5} \quad (52a)$$

c axis

$$70 - 250 \text{ K: } \alpha_c (K^{-1}) = 1.49811 \times 10^{-7} T - 7.08503 \times 10^{-10} T^2 + 1.10837 \times 10^{-12} T^3 - 1.26695 \times 10^{-5} \quad (52b)$$

$$250 - 450 \text{ K: } \alpha_c (K^{-1}) = -1.36000 \times 10^{-9} T - 1.71429 \times 10^{-12} T^2 - 1.73143 \times 10^{-6} \quad (52c)$$

Above 293.15 K length change values obtained by integrating equations 52a and 52c were combined with length change values derived form the lattice parameter measurements of Bonnier et al. 1964 (298-701 K) and fitted to the following equations to represent the thermal expansion up to the triple point:

$$\varepsilon_T a = 2.47646 \times 10^{-5} T + 8.90402 \times 10^{-9} T^2 - 1.31740 \times 10^{-12} T^3 - 7.99174 \times 10^{-3} \quad (52d)$$

$$\varepsilon_T c = -1.73185 \times 10^{-6} T - 6.81029 \times 10^{-10} T^2 - 5.67477 \times 10^{-13} T^3 + 5.80513 \times 10^{-4} \quad (52e)$$

In the range 57 to 85 K the thermal expansion coefficients of White 1973 are on average 5 % higher than the selected values along the *a* axis but trend 19 to 8 % low along the *c* axis. The measurements of Hortal and Leadbetter 1972 (4.5-200 K) along the *a* axis average 9% low between 12 and 25 K before then trending to 5% high while along the *c* axis the difference is initially 5% low trending to 2% low at 30 K before increasing to 7% low at 150 K, with the value at 200 K being 3% high while the measurements of Ahmed and Weintroub 1972 (6-200 K) along the *a* axis are initially 144% high at 10 K but then trending to an average of 4% low above 40 K, while the *c* axis is initially 115% low at 10 K before trending to 17% high at 200 K.

The values of Novikova 1968 (24-297 K) were only shown graphically with actual data points given by Touloukian et al. 1977. The measurements show some scatter with the *a* axis varying from 10% low to 4% high below 100 K but above this temperature can be considered as averaging 1.6% low.The *c* axis value shows significant scatter varying from 37% low to 12% high.

On the basis 100Δε length change values derived from the lattice parameter measurements of Deshpande and Pawar 1965 (298-474 K) show a trend of up to 0.037 high at 433 K along the *a* axis but the *c* axis values show satisfactory agreement scattering only 0.009 low to 0.010 high. Similar measurements of Stepień-Damm et al. 1991 (12.5-290 K) show a trend along the *a* axis from inially 0.019 high while along the *c* axis there is a trend from initially 0.010 high to a maximum of 0.041 high at 80 K before converging to the selected values. Measurements of Klemm et al. 1960 (293-673 K) were only shown in the form of small graphs.

Calculation of interatomic distances in tellurium

$d1 = [\,(c/3)^2 + 3\,(ua)^2\,]^{1/2}$ $\quad d2 = [\,(c/3)^2 + 3\,(ua)^2 - a^2(3u-1)\,]^{1/2}$

$d3 = [\,(2c/3)^2 + 3\,(ua)^2\,]^{1/2}$ $\quad d4 = a$ $\quad d5 = [\,(2c/3)^2 + 3\,(ua)^2 - a^2(3u-1)\,]^{1/2}$

arc cos (bond angle) = $1 - d3^2 / (\sqrt{2}\, d1)^2$

where u is the positional parameter, $d1$ is the bond length, $d2$ is the interatomic distance between chains and the bond angle is equal to Se-Se-Se

Cherin and Unger 1967 determined $u = 0.2633$ (5) which Ardenis et al. 1989 refined to 0.2636 (1) which is selected and leads to the above values in the room temperature region $d1 = 0.2836$ nm; $d2 = 0.3492$ nm; $d3 = 0.4445$ nm; $d4 = 0.4456$ nm; $d5 = 0.4890$ nm and bond angle = 103.2°.

Table 52a. Lattice parameters of tellurium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Note
Straumanis 1940	293	0.44562	0.59272	
Swanson and Tatge 1953	299	0.44565	0.59294	
Bonnier et al. 1964	298	0.44539	0.59265	a
Deshpande and Pawar 1965	298	0.44561	0.59267	
Stepień-Damm et al. 1991	290	0.44548	0.59276	
	Selected	0.44559 (8)	0.59275 (12)	

Note for Table 52a

a. *a* axis value not included in the average

At 293.15 K: Density 6237 (3) kg m^{-3} Molar Volume 20.460 (8) cm^3 mol^{-1}

Table 52b. Crystallographic properties of tellurium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
0	0	0	0	- 0.729	0.102	- 0.452
5	0.32	- 0.26	0.13	- 0.729	0.102	- 0.452
10	2.49	- 1.86	1.04	- 0.728	0.101	- 0.452
15	6.84	- 4.61	3.02	- 0.726	0.100	- 0.451
20	11.4	- 7.04	5.27	- 0.722	0.097	- 0.449
25	15.7	- 8.48	7.63	- 0.715	0.093	- 0.446
30	18.9	- 9.06	9.59	- 0.706	0.089	- 0.441
40	22.2	- 8.55	12.0	- 0.686	0.080	- 0.430
50	23.6	- 7.12	13.4	- 0.663	0.072	- 0.418
60	24.5	- 6.03	14.3	- 0.639	0.065	- 0.404
70	25.0	- 5.27	14.9	- 0.614	0.060	- 0.390
80	25.4	- 4.66	15.4	- 0.589	0.055	- 0.375
90	25.7	- 4.12	15.8	- 0.564	0.050	- 0.359
100	26.0	- 3.66	16.1	- 0.538	0.046	- 0.343
110	26.3	- 3.29	16.4	- 0.512	0.043	- 0.327
120	26.5	- 2.98	16.6	- 0.486	0.040	- 0.311
130	26.7	- 2.73	16.9	- 0.459	0.037	- 0.294
140	26.9	- 2.54	17.1	- 0.433	0.034	- 0.277
150	27.1	- 2.40	17.2	- 0.406	0.032	- 0.260
160	27.3	- 2.30	17.4	- 0.379	0.029	- 0.243
170	27.5	- 2.23	17.6	- 0.351	0.027	- 0.225
180	27.6	- 2.20	17.7	- 0.324	0.025	- 0.208
190	27.8	- 2.18	17.8	- 0.296	0.023	- 0.190
200	28.0	- 2.17	18.0	- 0.268	0.021	- 0.172
210	28.2	- 2.17	18.1	- 0.240	0.018	- 0.154
220	28.4	- 2.16	18.2	- 0.212	0.016	- 0.136
230	28.6	- 2.16	18.4	- 0.184	0.014	- 0.118
240	28.7	- 2.16	18.4	- 0.155	0.012	- 0.099
250	28.9	- 2.18	18.6	- 0.126	0.010	- 0.081
260	29.1	- 2.20	18.7	- 0.097	0.007	- 0.062
270	29.3	- 2.22	18.8	- 0.068	0.005	- 0.044
280	29.4	- 2.25	18.9	- 0.039	0.003	- 0.025
290	29.6	- 2.27	19.0	- 0.009	0.001	- 0.006
293.15	29.6	- 2.28	19.0	0	0	0
300	29.7	- 2.29	19.1	0.020	- 0.002	0.013
350	30.5	- 2.42	19.5	0.171	- 0.013	0.110
400	31.2	- 2.55	19.9	0.325	- 0.026	0.208
450	31.8	- 2.69	20.3	0.484	- 0.039	0.309
500	32.5	- 2.84	20.7	0.645	- 0.053	0.413
550	33.1	- 3.00	21.1	0.810	- 0.067	0.518
600	33.7	- 3.16	21.4	0.979	- 0.083	0.625
650	34.3	- 3.34	21.7	1.151	- 0.099	0.734
700	34.8	- 3.52	22.0	1.325	- 0.116	0.845
722.95	35.1	- 3.61	22.2	1.407	- 0.124	0.896

Table 52c. Crystallographic properties of tellurium

T K	*a* nm	*c* nm	*c*/*a*	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.44234	0.59335	1.3414	20.183	6322
5	0.44234	0.59335	1.3414	20.183	6322
10	0.44235	0.59335	1.3414	20.183	6322
15	0.44236	0.59334	1.3413	20.184	6322
20	0.44237	0.59332	1.3412	20.185	6322
25	0.44240	0.59330	1.3411	20.187	6321
30	0.44244	0.59328	1.3409	20.190	6320
40	0.44253	0.59322	1.3405	20.196	6318
50	0.44264	0.59318	1.3401	20.204	6316
60	0.44274	0.59314	1.3397	20.212	6313
70	0.44285	0.59311	1.3393	20.222	6310
80	0.44297	0.59308	1.3389	20.231	6307
90	0.44308	0.59305	1.3385	20.240	6304
100	0.44319	0.59302	1.3381	20.250	6301
110	0.44331	0.59300	1.3377	20.260	6298
120	0.44342	0.59299	1.3373	20.270	6295
130	0.44354	0.59297	1.3369	20.280	6292
140	0.44366	0.59295	1.3365	20.290	6289
150	0.44378	0.59294	1.3361	20.301	6286
160	0.44390	0.59292	1.3357	20.311	6282
170	0.44403	0.59291	1.3353	20.322	6279
180	0.44415	0.59290	1.3349	20.333	6276
190	0.44427	0.59289	1.3345	20.344	6272
200	0.44440	0.59287	1.3341	20.355	6269
210	0.44452	0.59286	1.3337	20.365	6266
220	0.44465	0.59284	1.3333	20.376	6262
230	0.44477	0.59283	1.3329	20.387	6259
240	0.44490	0.59282	1.3325	20.399	6255
250	0.44503	0.59281	1.3321	20.410	6252
260	0.44516	0.59279	1.3316	20.422	6248
270	0.44529	0.59278	1.3312	20.433	6245
280	0.44542	0.59277	1.3308	20.445	6241
290	0.44555	0.59275	1.3304	20.456	6238
293.15	0.44559	0.59275	1.3303	20.460	6237
300	0.44568	0.59274	1.3300	20.468	6234
350	0.44635	0.59267	1.3278	20.527	6216
400	0.44706	0.59260	1.3256	20.588	6198
450	0.44775	0.59252	1.3233	20.650	6179
500	0.44846	0.59244	1.3210	20.714	6160
550	0.44920	0.59235	1.3187	20.779	6141
600	0.44995	0.59226	1.3163	20.845	6121
650	0.45072	0.59216	1.3138	20.913	6102
700	0.45149	0.59206	1.3113	20.981	6082
722.95	0.45186	0.59201	1.3102	21.013	6072

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53 IODINE I

Atomic Weight: 126.90447 (3) (Meija 2017)

Structure: Orthorhombic (oS8)

The triple point was determined by Frederick and Hildenbrand 1938 to be 386.75 K.

53.1 Crystallographic properties

Lattice parameters were determined by Ibberson et al. 1992 (5 – 150 K) and by Ibberson 1993 (150 – 340 K) where the latter measurements were unpublished but are given in Part 53.2. Unfortunately, at the cross over temperature at 150 K the two sets of values did not agree with differences of 0.00042 nm for the *a*-axis, 0.00020 nm for the *b*-axis and 0.00052 nm for the *c*-axis. The differences are possibly due to calibration errors because although the measurements were carried out in the same laboratory different diffractometers were used (Ibberson 1994). However, in order to give both sets of data equal merit the values of Ibberson et al. 1992 were considered only up to 70 K and those of Ibberson 1993 at 240 K and above and jointly fitted to Equation B using the enthalpy values selected by Arblaster 2011:

a-axis

$$0 – 50\ \text{K}: \quad \ln(L_a) = (H_T - H_0)(1.96942 \times 10^{-6} – 4.48587 \times 10^{-9}\,T + 6.31331 \times 10^{-6}/T) – 1.932015 \times 10^{-2} \tag{53a}$$

$$50 – 250\ \text{K}: \ln(L_a) = (H_T - H_0)(8.70579 \times 10^{-7} + 1.42177 \times 10^{-9}\,T + 7.43494 \times 10^{-5}/T) – 1.984225 \times 10^{-2} \tag{53b}$$

$$250 – 386.75\ \text{K}: \varepsilon_T a = 5.57514 \times 10^{-5}\,T + 3.83679 \times 10^{-8}\,T^2 – 2.23144 \times 10^{-2} \tag{53c}$$

b-axis

$$0 – 50\ \text{K}: \quad \ln(L_b) = (H_T - H_0)(2.38504 \times 10^{-6} – 2.95700 \times 10^{-9}\,T – 1.21030 \times 10^{-5}/T) – 2.602020 \times 10^{-2} \tag{53d}$$

$$50 – 250: \ln(L_b) = (H_T - H_0)(1.33692 \times 10^{-6} + 1.75253 \times 10^{-9}\,T + 6.03261 \times 10^{-5}/T) – 2.661470 \times 10^{-2} \tag{53e}$$

$$250 – 386.75\ \text{K}: \varepsilon_T b = 5.28885 \times 10^{-5}\,T + 1.24702 \times 10^{-7}\,T^2 – 2.62207 \times 10^{-2} \tag{53f}$$

c-axis

$$0 - 50\ \text{K}: \quad \ln(L_c) = (H_T - H_0)(-2.37417 \times 10^{-8} + 1.58705 \times 10^{-9}\,T + 7.42626 \times 10^{-6}/T) - 2.869147 \times 10^{-3} \qquad (53g)$$

$$50 - 250\ \text{K}: \ln(L_c) = (H_T - H_0)(2.08926 \times 10^{-7} + 9.21738 \times 10^{-11}\,T - 5.07245 \times 10^{-6}/T) - 2.782453 \times 10^{-3} \qquad (53h)$$

$$250 - 386.75\ \text{K}: \varepsilon_T c = 1.44607 \times 10^{-5}\,T - 3.68094 \times 10^{-9}\,T^2 - 3.92283 \times 10^{-3} \qquad (53i)$$

Although all measurements at 240 K and above were involved in fitting to equation B, because of the large extrapolations from the experimental limit of 340 K, equations 53c, 53f and 53i where fitted to quadratic equations rather than Equation B because of possible uncertainties in the enthalpy measurements of Frederick and Hildenbrand 1938 which were selected by Arblaster 2011 to represent the high temperature enthalpy values of iodine.

Lattice parameter values determined by Van Bolhuis et al. 1967 at 110 K are respectively 0.0022 nm, 0.0005 nm and 0.0018 nm lower than the selected values along the *a*, *b* and *c* axes. Similarly, values determined by Cheesman and Hawes 1959 at 249.7 K are respectively 0.0012 nm, 0.0005 nm and 0.0029 nm lower than the selected values.

Lattice parameter measurements of Straumanis and Sauka 1943 over the range 283 K to 314 K lead to average thermal expansion coefficients of 95 x 10^{-6} K^{-1} along the *a*-axis, 133.4 x 10^{-6} K^{-1} along the *b*-axis and 35.1 x 10^{-6} K^{-1} along the *c*-axis. The values along the *a* and *b* axes show a reasonable agreement with the room temperature values given in Table 53b but the *c* value is about three times higher.

Positional Parameters

Positional parameters given by Ibberson et al. 1992 show discrepant values for the *y* parameter at 110 K and for the *z* parameter at 30 K and 150 K. With these values rejected the following equations are considered as representing the variation of these parameters up to 150 K:

y parameter:

$$0 \text{ to } 25\ \text{K}: \quad y = 1.8 \times 10^{-5}\,T - 1.5 \times 10^{-7}\,T^2 + 0.154764 \qquad (53j)$$

$$25 \text{ to } 70\ \text{K}: \quad y = -5.4241 \times 10^{-6}\,T - 2.3730 \times 10^{-7}\,T^2 + 0.155403 \qquad (53k)$$

$$70 \text{ to } 110\ \text{K}: \quad y = -1.8638 \times 10^{-4}\,T + 1.4350 \times 10^{-6}\,T^2 - 3.6166 \times 10^{-9}\,T^3 + 0.161116 \qquad (53l)$$

$$110 \text{ to } 150\ \text{K}: \quad y = 0.1532 \qquad (53m)$$

z parameter:

0 to 25 K: $z = -2.0 \times 10^{-6} T + 2.5 \times 10^{-7} T^2 + 0.117504$ (53n)

25 to 110 K: $z = -1.3802 \times 10^{-6} T - 6.4161 \times 10^{-9} T^2 + 0.117653$ (53o)

110 to 150 K: $z = 0.1174$ (53p)

A *y* parameter determined at 110 K by Van Bolhuis et al. 1967 agrees with the rejected value of Ibberson et al. 1992 while the *z* value agrees with the selected value. Approximate positional parameters in the room temperature region were given by both Harris et al. 1928 and Kitaigorodskii et al. 1953. Equations for calculating inter-atomic distances in iodine are given below.

Table 53a. Lattice parameters of iodine at 293.15 K

References	Original Temperature K	*a* nm	*b* nm	*c* nm	Note
Ferrari 1927	RT	0.7179	0.4770	0.9803	
Harris et al. 1928	RT	0.7270	0.4805	0.9800	
Neuburger and Schiebold 1936	RT	0.7263	0.4801	0.9791	
Straumanis and Sauka 1943	293	0.72666	0.47873	0.97921	a
Swanson et al. 1954	299	0.7268	0.4789	0.9803	
Ibberson 1993	293	0.72579	0.47828	0.98238	
	Selected	0.72579	0.47828	0.98238	

Note for Table 53a

a. Derived from fit 283 to 314 K

At 293.15 K: Density 4944 (3) kg m^{-3} Molar Volume 51.341 (27) cm^3 mol^{-1}.

The neutron diffraction measurements of Ibberson 1993 were selected because of the much higher resolution at short *d* spacings in what normally would be a region of heavy peak overlap (Ibberson et al. 1992). However, although these values have a high internal accuracy, because of the failure to overlap with the measurements of Ibberson et al. 1992 at 150 K then the absolute accuracies of the measurements are uncertain although nominal values of ± 0.0002 nm at 293.15 K have been applied to reflect the discepancy.

Calculation of interatomic distances for iodine

I (1) – I (2) = $d1 = [\ (2yb)^{2} + (2zc)^{2}\ ]^{½}$ (Bond length r_e)

I (1) – I (3) = $d2 = [\ b^{2}/4 + (0.5 - 2z)^{2} c^{2}\ ]^{½}$

I (1) – I (4) = $d3 = [\ (1 - 2y)^{2} b^{2} + (2zc)^{2}\ ]^{½}$

I (1) – I (5) = $d4 = [\ a^{2}/4 + b^{2}/4\ ]^{½}$

I (1) – I (6) = $d5 = [\ a^{2}/4 + (0.5 - 2y)^{2} b^{2} + (2zc)^{2}\ ]^{½}$

I (1) – I (7) = $d6 = [\ a^{2}/4 + (0.5 - 2z)^{2} c^{2}\ ]^{½}$

53.2 Lattice parameter measurements of Ibberson 1993

Unpublished measurements reproduced by permission of the author.

T K	*a* Å	*b* Å	*c* Å
150	7.17601 (9)	4.70516 (6)	9.80510 (12)
175	7.18798 (10)	4.71846 (6)	9.80819 (13)
200	7.20155 (11)	4.73065 (7)	9.81160 (13)
220	7.21314 (11)	7.47156(7)	9.81467 (14)
240	7.22521 (12)	4.75242 (8)	8.81721 (15)
260	7.23735 (13)	4.76368 (8)	9.81984 (15)
280	7.24981 (14)	4.77492 (8)	9.82205 (16)
300	7.26225 (14)	4.78706 (9)	9.82468 (17)
320	7.27466 (15)	4.79934 (9)	9.82695 (18)
340	7.28799 (20)	4.81244 (9)	9.82937 (17)

Table 53b. Crystallographic properties of iodine

T K	α_a x 10^6 K^{-1}	α_b x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}
0	0	0	0	0
5	1.68	0.32	0.64	0.88
10	9.56	5.90	2.17	5.88
15	22.3	18.1	3.63	14.7
20	33.2	30.9	4.23	22.8
25	42.4	42.7	4.60	29.9
30	49.0	52.2	4.82	35.3
40	56.4	65.0	5.24	42.2
50	60.4	73.0	6.04	46.5
60	60.6	75.7	7.07	47.8
70	61.1	78.4	7.96	49.2
80	61.2	80.1	8.53	49.9
90	61.8	82.1	9.06	51.0
100	62.5	84.0	9.51	52.0
110	63.5	86.0	9.90	53.1
120	64.6	88.1	10.3	54.3
130	65.9	90.2	10.6	55.6
140	67.0	92.1	10.8	56.6
150	68.3	94.2	11.1	57.9
160	69.6	96.3	11.3	59.1
170	71.1	98.4	11.6	60.4
180	72.6	101	11.8	61.6
190	74.1	103	12.0	62.9
200	75.6	105	12.2	64.2
210	77.2	107	12.4	65.6
220	78.8	109	12.6	66.9
230	80.4	111	12.7	68.2
240	82.1	114	12.7	69.4
250	83.7	116	12.6	70.7
260	84.4	118	12.6	71.7
270	85.0	121	12.5	72.7
280	85.7	123	12.4	73.7
290	86.3	125	12.3	74.6
293.15	86.5	126	12.3	74.9
300	86.9	128	12.3	75.6
310	87.6	130	12.2	76.6
320	88.2	132	12.1	77.5
330	88.8	135	12.0	78.5
340	89.4	137	12.0	79.4
350	90.1	139	11.9	80.4
360	90.7	141	11.8	81.3
370	91.3	144	11.7	82.2
380	91.9	146	11.7	83.2
386.75	92.4	147	11.6	83.8

Table 53c. Crystallographic properties of iodine

T K	100 ε_T *a*	100 ε_T *b*	100 ε_T *c*	100 ε_T avr
0	- 1.913	- 2.568	- 0.286	- 1.594
5	- 1.913	- 2.568	- 0.286	- 1.594
10	- 1.911	- 2.567	- 0.286	- 1.593
15	- 1.903	- 2.562	- 0.284	- 1.588
20	- 1.889	- 2.550	- 0.282	- 1.578
25	- 1.871	- 2.532	- 0.281	- 1.566
30	- 1.848	- 2.508	- 0.278	- 1.549
40	- 1.795	- 2.450	- 0.273	- 1.510
50	- 1.738	- 2.382	- 0.267	- 1.466
60	- 1.678	- 2.309	- 0.261	- 1.420
70	- 1.619	- 2.234	- 0.253	- 1.372
80	- 1.559	- 2.156	- 0.245	- 1.323
90	- 1.499	- 2.077	- 0.236	- 1.274
100	- 1.438	- 1.996	- 0.227	- 1.223
110	- 1.376	- 1.913	- 0.217	- 1.171
120	- 1.313	- 1.827	- 0.207	- 1.118
130	- 1.249	- 1.740	- 0.197	- 1.064
140	- 1.184	- 1.650	- 0.186	- 1.009
150	- 1.117	- 1.559	- 0.175	- 0.952
160	- 1.049	- 1.465	- 0.164	- 0.894
170	- 0.980	- 1.369	- 0.153	- 0.835
180	- 0.909	- 1.271	- 0.141	- 0.775
190	- 0.836	-1.170	- 0.125	- 0.711
200	- 0.762	- 1.068	- 0.117	- 0.650
210	- 0.687	- 0.963	- 0.105	- 0.586
220	- 0.609	- 0.856	- 0.092	- 0.520
230	- 0.530	- 0.746	- 0.079	- 0.452
240	- 0.450	- 0.634	- 0.067	- 0.384
250	- 0.367	- 0.520	- 0.054	- 0.314
260	- 0.283	- 0.404	- 0.041	- 0.243
270	- 0.198	- 0.285	- 0.029	- 0.171
280	- 0.113	- 0.164	- 0.016	- 0.098
290	- 0.027	- 0.040	- 0.004	- 0.024
293.15	0	0	0	0
300	0.060	0.087	0.008	0.052
310	0.147	0.216	0.021	0.128
320	0.235	0.347	0.033	0.205
330	0.324	0.481	0.045	0.283
340	0.413	0.618	0.057	0.362
350	0.503	0.757	0.069	0.443
360	0.594	0.898	0.089	0.526
370	0.686	1.042	0.092	0.606
380	0.778	1.188	0.104	0.689
386.75	0.841	1.289	0.112	0.746

Table 53d. Crystallographic properties of iodine

T K	*a* nm	*b* nm	*c* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.71190	0.46600	0.97956	48.925	5188
5	0.71190	0.46600	0.97956	48.925	5188
10	0.71192	0.46601	0.97957	48.927	5187
15	0.71198	0.46603	0.97959	45.935	5187
20	0.71208	0.46609	0.97960	48.948	5185
25	0.71221	0.46618	0.97963	48.968	5183
30	0.71238	0.41129	0.97965	48.992	5181
40	0.71276	0.46657	0.97970	49.050	5174
50	0.71318	0.46689	0.97975	49.115	5168
60	0.71361	0.46724	0.97982	49.185	5160
70	0.71404	0.46760	0.97989	49.257	5153
80	0.71447	0.46797	0.97997	49.330	5145
90	0.71491	0.46835	0.98006	49.404	5137
100	0.71535	0.46874	0.98015	49.480	5129
110	0.71580	0.46914	0.98024	49.558	5121
120	0.71626	0.46954	0.98034	49.638	5113
130	0.71672	0.46996	0.98044	49.720	5105
140	0.71720	0.47039	0.98055	48.803	5096
150	0.71768	0.47083	0.98066	49.889	5088
160	0.71817	0.47128	0.98077	49.976	5079
170	0.71868	0.47174	0.98088	50.066	5070
180	0.71919	0.47221	0.98099	50.157	5060
190	0.71972	0.47269	0.98111	50.251	5051
200	0.72026	0.47318	0.98123	50.347	5041
210	0.72080	0.47368	0.98135	50.445	5031
220	0.72137	0.43419	0.98147	50.545	5021
230	0.72194	0.41471	0.98160	50.647	5011
240	0.72253	0.47525	0.98172	50.752	5001
250	0.72313	0.47579	0.98185	50.859	4990
260	0.72374	0.47635	0.98197	50.968	4980
270	0.72434	0.47692	0.98210	51.079	4969
280	0.72497	0.47750	0.98222	51.191	4958
290	0.72559	0.47809	0.98234	51.305	4947
293.15	0.72579	0.47828	0.98238	51.341	4944
300	0.72622	0.47870	0.98246	51.421	4936
310	0.72685	0.47932	0.98258	51.538	4925
320	0.72749	0.47995	0.98270	51.558	4913
330	0.72814	0.48059	0.98282	51.778	4902
340	0.72879	0.48124	0.98294	51.901	4890
350	0.72944	0.48190	0.98305	52.026	4879
360	0.73010	0.48258	0.98317	52.152	4867
370	0.73076	0.48327	0.98329	52.280	4855
380	0.73143	0.48397	0.98340	52.410	4843
386.75	0.73189	0.48445	0.98348	52.498	4835

Table 53e. Inter-atomic distances for iodine

T K	*y*	*z*	*d*1 nm	*d*2 nm	*d*3 nm	*d*4 nm	*d*5 nm	*d*6 nm
0	0.1548	0.1175	0.2717	0.3488	0.3956	0.4254	0.4331	0.4405
5	0.1548	0.1175	0.2717	0.3488	0.3956	0.4254	0.4331	0.4405
10	0.1549	0.1175	0.2718	0.3488	0.3955	0.4254	0.4331	0.4405
15	0.1550	0.1175	0.2718	0.3488	0.3955	0.4255	0.4331	0.4405
20	0.1551	0.1176	0.2719	0.3488	0.3955	0.4255	0.4332	0.4406
25	0.1551	0.1176	0.2720	0.3487	0.3956	0.2456	0.4333	0.4406
30	0.1550	0.1176	0.2720	0.3488	0.3957	0.4257	0.4334	0.4406
40	0.1548	0.1176	0.2719	0.3489	0.3960	0.4259	0.4336	0.4408
50	0.1545	0.1176	0.2718	0.3490	0.3964	0.4262	0.4338	0.4410
60	0.1542	0.1176	0.2717	0.3492	0.3968	0.4265	0.4340	0.4412
70	0.1539	0.1175	0.2716	0.3494	0.3973	0.4268	0.4343	0.4414
80	0.1535	0.1175	0.2715	0.3495	0.3977	0.4270	0.4345	0.4416
90	0.1533	0.1175	0.2714	0.3497	0.3981	0.4273	0.4348	0.4419
100	0.1532	0.1175	0.2714	0.3499	0.3984	0.4276	0.4350	0.4421
110	0.1532	0.1174	0.2714	0.3501	0.3986	0.4279	0.4352	0.4423
120	0.1532	0.1174	0.2714	0.3503	0.3988	0.4282	0.4353	0.4425
130	0.1532	0.1174	0.2715	0.3505	0.3991	0.4285	0.4355	0.4428
140	0.1532	0.1174	0.2716	0.3506	0.3993	0.4288	0.4358	0.4430
150	0.1532	0.1174	0.2716	0.3509	0.3996	0.4292	0.4360	0.4432

*d*1 is the bond length (r_e).

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54 XENON Xe

Atomic weight: 131.293 (6) (Meija 2017)

Structure: Face-centered cubic (cF4)

The triple point is a secondary fixed point on ITS-90 at 161.405 (1) K (Bedford et al. 1996).

54.1 Crystallographic properties

Lattice parameter values were determined by Granfors et al. 1981 along the sublimation line, 78.2 to 160.7 K, and fitted to a cubic equation. Smooth dilatometric measurements of Tilford and Swenson 1972 (1-105 K) were unscaled and expected to be in error by several percent. However, instead it was found that in the high temperature region that the volume thermal expansion coefficients were in excellent agreement with those derived from the measurements of Granfors et al. 1981 with a smooth transition between 100 and 110 K. The selected values are therefore based on these two sets of measurements. At 110 K and above the lattice parameter measurements along the sublimation line were represented by the equation:

$$a \text{ (nm)} = 6.63637 \times 10^{-5} T + 4.57640 \times 10^{-7} T^{2} + 0.6122049 \quad (54a)$$

Granfors et al. 1981 also determined the lattice parameter along the melting line, 161.7 to 216.0 K, but the reason why this leads to an extrapolated value 0.00006 nm higher at the triple point was not satisfactorily explained. Neutron diffraction measurements on single crystals by Lurie et al. 1974 lead to lattice parameters which exactly agree with the selected value at 10 K, agrees to within 0.0001 nm at 111 K but is 0.0055 nm higher at 159.6 K. Earlier lattice parameter measurements show unsatisfactory agreement with the selected values. Those of Cheesman and Soane 1957 (58-89 K) on commercial purity material average 0.002 nm high. Measurements of Eatwell and Smith 1961 (20-120 K), also on commercial purity material, were only shown graphically with actual lattice parameter values being calculated from length change values given by Touloukian et al. 1977. These average 0.0003 nm high while lattice parameter measurements of Sears and Klug 1962 (5-75 K), which were carried out on samples solidified on gold-plated copper substrates, also averaged 0.0003 nm high. However, these latter measurements are suspect because of a sudden sharp rise in the derived volume thermal expansion coefficient which is 16% greater than the selected value at 75 K. A single determination of the lattice parameter at 85 K by Syassen and Holzapfel 1978 leads to a value 0.0006 nm high.

54.2 Bulk properties of xenon

Based on an initial slope of the melting curve of 2.547 MPa K^{-1} from the modified Simons equation given by Crawford 1977 and an enthalpy of fusion selected as 2297 (8) J mol^{-1} by Hultgren et al. 1973, then from the Clausius-Clapeyron equation the derived

molar volume difference at the triple point is 5.588 (20) $cm^3\ mol^{-1}$. Selecting the molar volume of the liquid as determined by Terry et al. 1969 to be 44.312 (12) $cm^3\ mol^{-1}$ then the molar volume of the solid at the triple point is 38.724 (23) $cm^3\ mol^{-1}$, equivalent to a length change value of $100\ \varepsilon_0 = 3.779$. Using the difference between this value and the value of 3.596 calculated for the crystallographic data and assuming that the difference is "negligible" at 100 K, i.e. $\Delta\varepsilon_0 = 5 \times 10^{-6}$, then this leads to thermal vacancy parameters of and $H_V/k = 1551$ K and $S_V/k = 4.40$ which were used to generate the values in Table 54b.

Manzhelii et al. 1969 (90-157 K) obtained dilatometric volume thermal expansion coefficients which, if extrapolated to the triple point, are considered to be equal to the crystallographic value at 85 K, can be used to derive length change values by three-point integration which, at the triple point, leads to $100\varepsilon_0 = 3.892$ and a derived molar volume of 38.851 $cm^3\ mol^{-1}$ which is much higher than the value obtained from the Clausius-Clapeyron equation. Compared to the selected values these thermal expansion coefficients vary from initially 1% high, reach a maximum deviation of 7% high at 125 K and then converge to only 3% high at 157 K. Based on their own measurements and the dilatometric measurements of Manzhelii et al. 1969, Granfors et al. 1981 arrived at thermal vacancy parameters of $H_V/k = 1100$ K and $S_V/k = 2.2$ but these values lead to $100\varepsilon_0 = 3.926$ at the triple point and an even higher value of the molar volume of 38.889 $cm^3\ mol^{-1}$. Because both of these molar volume values greatly exceed that obtained from the Clausius-Clapeyron equation then they are not considered for evaluating the bulk properties. Volume thermal expansion coefficients of Manzhelii et al. 1967 (21.5-90 K) were initially 12% low and then trended to coincide with the selected values above 70 K. Earlier direct density measurements of Gavrilko and Manzhelii 1964 (120-160 K) trend from 1 $kg\ m^{-3}$ lower to 10 $kg\ m^{-3}$ higher than the selected values. Molar volume values of Anderson and Swenson 1975 (4-159 K) drift from 0.09 $cm^3\ mol^{-1}$ high to 0.07 $cm^3\ mol^{-1}$ low.

Table 54a. Crystallographic properties of xenon

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_0$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	0	0.61280	0.43332	34.646	3789.5
1	0.051	< 0.0001	0.61280	0.43332	34.646	3789.5
2	0.430	< 0.0001	0.61280	0.43332	34.646	3789.5
3	1.60	0.0001	0.61280	0.43332	34.646	3789.5
4	4.26	0.0004	0.61281	0.43332	34.647	3789.5
5	8.80	0.0010	0.61281	0.43332	34.647	3789.4
6	15.38	0.0022	0.61282	0.43333	34.649	3789.3
7	23.63	0.0042	0.61283	0.43334	34.651	3789.1
8	32.87	0.0070	0.61285	0.43335	34.654	3788.7
9	42.70	0.0108	0.61288	0.43336	34.657	3788.3
10	52.57	0.0155	0.61290	0.43339	34.662	3787.8
11	62.20	0.0213	0.61293	0.43341	34.668	3787.1
12	71.30	0.0280	0.61298	0.43344	34.675	3786.4
13	79.83	0.0355	0.61302	0.43347	34.683	3785.5
14	87.87	0.0439	0.61307	0.43351	34.692	3784.5
15	95.33	0.0530	0.61313	0.43355	34.701	3783.5
16	102.3	0.0629	0.61319	0.43359	34.712	3782.4
18	114.6	0.0846	0.61332	0.43368	34.734	3779.9
20	124.6	0.109	0.61347	0.43379	34.759	3777.2
25	144.7	0.176	0.61388	0.43408	34.830	3769.6
30	158.3	0.252	0.61435	0.43441	34.909	3761.0
35	169.3	0.334	0.61485	0.43477	34.995	3751.8
40	178.0	0.421	0.61539	0.43514	35.086	3742.0
45	185.7	0.513	0.61595	0.43554	35.182	3731.8
50	192.3	0.608	0.61653	0.43595	35.282	3721.2
55	198.7	0.706	0.61713	0.43638	35.385	3710.4
60	205.0	0.808	0.61776	0.43682	35.493	3699.1
65	211.0	0.912	0.61839	0.43727	35.603	3687.7
70	216.7	1.020	0.61905	0.43774	35.717	3675.9
75	222.0	1.131	0.61973	0.43822	35.835	3663.8
80	227.7	1.245	0.62043	0.43871	35.956	3651.4
85	233.7	1.361	0.62114	0.43922	36.080	3638.9
90	240.0	1.481	0.62188	0.43974	36.208	3626.0
95	246.7	1.605	0.62264	0.44027	36.341	3612.8
100	253.7	1.732	0.62342	044082	36.478	3599.3
105	260.5	1.863	0.62422	0.44139	36.619	3585.4
110	267.3	1.997	0.62504	0.44197	36.764	3571.3
115	274.2	2.135	0.62589	0.44257	36.913	3556.8
120	281.1	2.277	0.62676	0.44319	37.067	3542.0
125	288.0	2.423	0.62765	0.44382	37.226	3526.9
130	294.9	2.572	0.62857	0.44446	37.389	3511.5
135	301.7	2.725	0.62950	0.44513	37.557	3495.9
140	308.5	2.882	0.63047	0.44581	37.729	3479.9
145	315.3	3.043	0.63145	0.44650	37.906	3463.7
150	322.0	3.207	0.63246	0.44721	38.088	3447.1
155	328.7	3.375	0.63349	0.44794	38.274	3430.4
160	335.4	3.547	0.63454	0.44869	38.465	3413.3
161.405	337.2	3.596	0.63484	0.44890	38.520	3408.5

$$d = a/\sqrt{2}$$

Table 54b. Bulk properties of xenon

$3\ (\varepsilon_T L - \varepsilon_T a) = \exp\ (4.4 - 1551/\ T)$ $\quad \alpha_L - \alpha_a = (517.0/\ T^{\ 2})\ \exp\ (4.4 - 1551/\ T)$

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_0$	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
100	253.7	1.732	36.478	3599.3
105	262.0	1.864	36.620	3585.3
110	269.9	1.999	36.766	3571.1
115	278.6	2.139	36.917	3556.4
120	288.2	2.284	37.075	3541.3
125	299.0	2.434	37.228	3525.8
130	311.3	2.590	37.409	3509.7
135	325.4	2.753	37.587	3493.0
140	341.7	2.924	37.775	3475.6
145	360.6	3.104	37.974	3457.5
150	382.5	3.295	38.185	3438.4
155	407.8	3.498	38.410	3418.2
160	436.8	3.714	38.652	3396.8
161.405	445.7	3.779	38.724	3390.5

This Table is considered to be identical to Table 54a below 100 K.

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55 CESIUM Cs

Atomic weight: 132.90545196 (6) (Meija 2017)

Structure: Body-centered cubic (cI2)

Alcock et al. 1994 select 301.6 (1) K for the melting point.

55.1 Thermal expansion

There have been a number of determinations of the lattice parameter but because these generally show a fair degree of scatter then the thermal expansion over the whole temperature range were based on the volume ratios of Anderson and Swenson 1985 (4-290 K) which below 110 K were combined with enthalpy values selected by Alcock et al. 1994 and fitted to Equation B. However, because equation 55b showed derived negative thermal expansion coefficients below 10 K the thermal expansion below 12 K was derived as shown in part 55.3:

$$0 – 12\ \text{K}: \quad \alpha\ (\text{K}^{-1}) = 5.74 \times 10^{-9}\, T + 8.06 \times 10^{-9}\, T^{3} \tag{55a}$$

$$12 – 110\ \text{K}: \quad \ln (L_T) = (H_T – H_0)\,(2.64300 \times 10^{-6} + 2.13118 \times 10^{-10}\, T – 3.22761 \times 10^{-5}/\, T) – 1.96126 \times 10^{-2} \tag{55b}$$

$$110 – 230\ \text{K}: \quad \ln (L_T) = 4.37552 \times 10^{-5}\, T + 2.53508 \times 10^{-7}\, T^{2} – 1.15946 \times 10^{-9}\, T^{3} + 2.08955 \times 10^{-12}\, T^{4} – 2.05555 \times 10^{-2} \tag{55c}$$

$$230 – 301.6\ \text{K}: \quad \ln (L_T) = 8.21374 \times 10^{-5}\, T – 1.08264 \times 10^{-7}\, T^{2} + 2.86805 \times 10^{-10}\, T^{3} – 2.20000 \times 10^{-2} \tag{55d}$$

The mean thermal expansion coefficient over the range from 293.15 K to the melting point derived from equation 55d at 93.9 x 10^{-6} K^{-1} is in excellent agreement with the values of 93.7 x 10^{-6} K^{-1} derived from the density values of Basin 1972 (286.8–301.4 K). The degree of self-consistency in the data is shown by the fact that a lattice parameter at 2 K derived from de Haas – van Alphen measurements by Gaertner and Templeton 1977 agrees with the selected value to within 0.0001 nm. Earlier measurements by Barrett 1956 at 5 K and 78 K are both 0.0003 nm high while a single measurement by Brauer 1947 at 173 K is 0.0012 low. The molar volume measurements of Anderson et al. 1969 (0-300 K) were initially 0.1 $cm^3\ mol^{-1}$ high but were 0.1 to 0.2 $cm^3\ mol^{-1}$ low at 100 K and above.

55.2 The lattice parameter of cesium at 293.15 K

Measurements of the density of the high purity solid by Basin 1972 (286.8-301.4 K) were referenced to a liquid density of 1841.65 kg m^{-3} at 308.15 K which leads to a solid density of 1896.3 kg m^{-3} at 293.15 K and a lattice parameter of 0.6151 nm. However, the reference density value appears to be far too high when compared to a consensus value of 1832.0 kg m^{-3} at 308.15 K calculated from the equation given by Shpil'rain et al. 1985

which was based on a large number of liquid density measurements, including those of Basin 1972. The corrected density at 293.15 K would then be 1886.4 kg m^{-3} and the equivalent lattice parameter 0.6162 nm. The use of this value would then mean density values for the solid and liquid are self-consistent. Density measurements on a more commercial quality metal by Basin et al. 1969 (285.9 – 301.5 K) lead to a density of 1888 kg m^{-3} at 293.15 K and lattice parameter of 0.6160 nm. Lattice parameter measurements of Simon et al. 1976 (108-228 K), but more specifically 138 K to 228 K, are systematically 0.0002 nm higher than the selected values but this is equivalent to a value of 0.6164 nm if extrapolated to 293.15 K and therefore these three determinations of the lattice parameter are in satisfactory agreement. An indirect measurement of the lattice parameter by Hall et al. 1964 in which the lattice parameters of the cesium high pressure face-centered cubic phases Cs II and Cs III were used to obtain a molar volume ratio with the body-centered cubic room temperature phase leads to an average lattice parameter of 0.6176 nm at 300 K.

Table 55a. Lattice parameter of cesium at 293.15 K

References	Original Temperature K	*a* nm	Notes
Hall et al. 1964	300	0.6172	
Weir et al. 1971	RT	0.6141	
McWhan, et al. 1974	298	0.618	
Basin et al. 1969	293	0.6160	a
Basin 1972	293	0.6162	b
Simon et al. 1976	293	0.6164	c
	Selected	0.6162 (10)	

Notes for Table 55a

a. Based on interpolated density value 1888 kg m^{-3}

b. Based on corrected interpolated density value 1886.4 kg m^{-3}

c. Lattice parameter measurements extrapolated from 138 to 228 K

At 293.15 K: Density: 1886 (9) kg m^{-3} Molar Volume: 70.45 (34) cm^3 mol^{-1}.

55.3: Very low temperature thermal expansion of cesium

Equation 55b leads to negative thermal expansion coefficients below 10 K which is considered to be unnatural behavior. Therefore, values below 12 K were fitted to a Debye function $\alpha = A\,T + B\,T^3$ where $A = \gamma_e\,C_e / 3\,B_T\,V_m$:

γ_e = Gruneisen parameter for an ideal electron gas = ⅔

C_e = electronic specific heat coefficient = 3.60 mJ mol^{-1} K^{-1} (Alcock et al. 1994)

B_T = bulk modulus = 2.10 GPa (Anderson and Swenson 1985)

V_m = molar volume = 66.42 c m^3 mol^{-1} (present evaluation)

Hence A = 8.74 x 10^{-9} K^{-2} and B = 8.06 x 10^{-9} K^{-4} results as an average from fits to derived thermal expansion coefficients obtained from equation 55b at 11, 12 and 13 K. Averaging then the length change values below 12 K are calculated as L_T:

$$L_T = 2.87000 \times 10^{-9} T^2 + 2.01500 \times 10^{-9} T^4 + 0.980533 \quad (55e)$$

Table 55b. Crystallographic properties of cesium

T K	α x 10^6 K^{-1}	100 ε_T	*a* nm	*d* nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
0	0	- 1.947	0.6042	0.5233	66.42	2001
5	1.0	- 1.947	0.6042	0.5233	66.42	2001
10	8.1	- 1.945	0.6042	0.5233	66.42	2001
15	24.1	- 1.937	0.6043	0.5233	66.44	2000
20	36.4	- 1.922	0.6044	0.5234	66.47	2000
25	44.7	- 1.902	0.6045	0.5235	66.51	1998
30	50.2	- 1.878	0.6046	0.5236	66.56	1997
40	56.9	- 1.825	0.6050	0.5239	66.66	1994
50	60.6	- 1.768	0.6053	0.5242	66.78	1990
60	62.9	- 1.707	0.6057	0.5245	66.90	1986
70	64.6	- 1.644	0.6061	0.5249	67.03	1983
80	66.2	- 1.580	0.6065	0.5252	67.16	1979
90	67.0	- 1.514	0.6069	0.5256	67.30	1975
100	67.9	- 1.448	0.6073	0.5259	67.43	1971
110	68.6	- 1.381	0.6077	0.5263	67.57	1967
120	69.0	- 1.314	0.6081	0.5266	67.71	1963
130	69.2	- 1.246	0.6085	0.5270	67.85	1959
140	69.5	- 1.177	0.6089	0.5274	67.99	1955
150	69.8	- 1.108	0.6094	0.5277	68.13	1951
160	70.1	- 1.039	0.6098	0.5281	68.28	1947
170	70.5	- 0.969	0.6102	0.5285	68.42	1942
180	71.1	- 0.899	0.6107	0.5288	68.57	1938
190	71.8	- 0.829	0.6111	0.5292	68.71	1934
200	72.9	- 0.757	0.6115	0.5296	68.86	1930
210	74.2	- 0.684	0.6120	0.5300	69.02	1926
220	75.9	- 0.609	0.6124	0.5304	69.17	1921
230	77.9	- 0.533	0.6129	0.5308	69.33	1917
240	79.7	- 0.455	0.6134	0.5312	69.49	1912
250	81.8	- 0.374	0.6139	0.5316	69.66	1908
260	84.0	- 0.292	0.6144	0.5321	69.84	1903
270	86.4	- 0.207	0.6149	0.5325	70.01	1898
280	89.0	- 0.119	0.6155	0.5330	70.20	1893
290	91.7	- 0.029	0.6160	0.5335	70.39	1888
293.15	92.6	0	0.6162	0.5336	70.45	1886
295	93.1	0.017	0.6163	0.5337	70.49	1886
300	94.6	0.064	0.6166	0.5340	70.59	1883
301.6	95.1	0.079	0.6167	0.5341	70.62	1882

$$d = \sqrt{3}a/2$$

Referernces for Cesium

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56 BARIUM Ba

Atomic Weight: 137.327 (7) (Meija 2017)

Structure: Body-centered cubic (cI2)

Alcock et al. 1993 select 1000 (3) K for the melting point. Rinck 1932 suggested a transformation at 648 K but electrical resistivity and thermopower measurements of Cook and Laubitz 1976 on high purity barium established that there was no evidence of allotropic transformations.

Unlike strontium, where there was satisfactory agreement, the thermal expansion coefficients of White 1972 (3-85, 283 K) and the direct density measurements of Stankus and Tyagel'skii 1992 (293-1000 K) show relatively poor agreement and cannot be directly reconciled. This may be due to purity because the metal used by White 1972 contained 1% Sr while the metal used by Stankus and Tyagel'skii 1992 was stated as being only 99.6% pure. In order to overcome this problem it was first assumed that the measurements of White 1972 were correct to 293.15 K. Values up to 8 K were fitted to a Debye equation and from 26 K to 283 K to Equation A using the specific heat values selected by Alcock et al. 1993:

$$0 - 8: \quad \alpha\,(K^{-1}) = 7.27865 \times 10^{-9}\,T + 7.53196 \times 10^{-10}\,T^{3} + 3.71838 \times 10^{-11}\,T^{5} - 3.21523 \times 10^{-13}\,T^{7} \qquad (56a)$$

$$26 - 283\ K: \quad \alpha\,(K^{-1}) = C_p\,(7.39920 \times 10^{-7} - 1.83164 \times 10^{-11}\,T - 1.10378 \times 10^{-6}\,/\,T) \qquad (56b)$$

Equation 56a has an accuracy of $2.9 \times 10^{-9}\ K^{-1}$ and equation 56b $4.3 \times 10^{-8}\ K^{-1}$. Values in the range 8 K to 26 K were those selected by White 1972 while equation 56b was extrapolated to 293.15 K.

The lattice parameter determined by Barrett 1956 at 5 K agrees exactly with the selected value. Length change values derived from the volume ratios given by Anderson et al. 1990 (4-295 K) show a maximum deviation of 0.027 high at 100 K.

In the high temperature region the selected thermal expansion coefficient and its derivative at 293.15 K were combined with the length change value of $\varepsilon_T = 0.01967_5$ at 1000 K derived from the direct density values of Stankus and Tyagel'skii 1992 and the combination was fitted to the equation:

$$\varepsilon_T = 1.71120 \times 10^{-5}\,T + 3.91514 \times 10^{-9}\,T^{2} + 4.10411 \times 10^{-12}\,T^{3} - 5.45622 \times 10^{-3} \qquad (56c)$$

The measurements of Stankus and Tyagel'skii 1992 reduced to length change values then on the basis $100\Delta\varepsilon$ show a maximum deviation of 0.13 high at 700 K.

Table 56a. Lattice parameter of barium at 293.15 K

References	Original Temperature K	*a* nm	Notes
King and Clarke 1929	RT	0.5025	a
Klemm and Mika 1941	RT	0.5019	a
Swanson et al. 1955	299	0.5025	
Hirst et al. 1956	298	0.5023	
King 1956	298	0.5022	
Keller et al. 1958	298	0.5026	
Kanda et al. 1965	295	0.5026	
Rashid and Kayser 1971	298	0.5027	
Bruzzone 1971	RT	0.5019	a
Evers et al. 1992	298	0.5028	
Stankus and Tyagel'skii 1992	293	0.5018	a, b
	Selected	0.5025 (3)	

Notes for Table 56a

a. Not included in the average

b. From direct density value 3608.9 kg m^{-3}

At 293.15 K: Density: 3594 (6) kg m^{-3} Molar Volume: 38.21 (7) cm^3 mol^{-1}.

Table 56b. Crystallographic properties of barium

T K	α x 10^6 K^{-1}	100 ε_T	*a* nm	*d* nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
0	0	- 0.491	0.5000	0.4330	37.65	3648
10	1.73	- 0.491	0.5000	0.4330	37.65	3648
20	6.58	- 0.487	0.5001	0.4331	37.65	3647
30	10.55	- 0.478	0.5001	0.4331	37.66	3646
40	13.21	- 0.466	0.5002	0.4331	37.67	3645
50	14.80	- 0.452	0.5002	0.4332	37.69	3644
60	15.79	- 0.437	0.5003	0.4333	37.71	3642
70	16.48	- 0.421	0.5004	0.4333	37.72	3640
80	16.96	- 0.404	0.5005	0.4334	37.74	3638
90	17.35	- 0.387	0.5006	0.4335	37.76	3636
100	17.65	- 0.370	0.5006	0.4336	37.78	3635
110	17.90	- 0.352	0.5007	0.4336	37.80	3633
120	18.11	- 0.334	0.5008	0.4337	37.82	3631
130	18.30	- 0.316	0.5009	0.4338	37.84	3629
140	18.47	- 0.298	0.5010	0.4339	37.86	3627
150	18.62	- 0.279	0.5011	0.4340	37.89	3625
160	18.76	- 0.261	0.5012	0.4340	37.91	3623
170	18.89	- 0.242	0.5013	0.4341	37.93	3621
180	19.02	- 0.223	0.5014	0.4342	37.95	3619
190	19.15	- 0.204	0.5015	0.4343	37.97	3616
200	19.27	- 0.185	0.5016	0.4344	37.99	3614
210	19.39	- 0.165	0.5017	0.4345	38.02	3612
220	19.50	- 0.146	0.5018	0.4345	38.04	3610
230	19.63	- 0.126	0.5019	0.4346	38.06	3608
240	19.75	- 0.107	0.5020	0.4347	38.08	3606
250	19.87	- 0.087	0.5021	0.4348	38.11	3604
260	20.00	- 0.067	0.5022	0.4349	38.13	3602
270	20.13	- 0.047	0.5023	0.4350	38.15	3599
280	20.27	- 0.027	0.5024	0.4351	38.17	3597
290	20.42	- 0.006	0.5025	0.4352	38.20	3595
293.15	20.47	0	0.5025	0.4352	38.21	3594
300	20.57	0.014	0.5026	0.4352	38.22	3593
350	21.33	0.119	0.5031	0.4357	38.34	3582
400	22.16	0.228	0.5036	0.4362	38.47	3570
450	23.05	0.341	0.5042	0.4367	38.60	3558
500	24.00	0.459	0.5048	0.4372	38.73	3545
550	25.00	0.582	0.5054	0.4377	38.88	3532
600	26.06	0.711	0.5061	0.4383	39.03	3519
650	27.17	0.845	0.5067	0.4389	39.18	3505
700	28.35	0.985	0.5074	0.4395	39.35	3490
750	29.58	1.131	0.5082	0.4401	39.52	3475
800	30.86	1.284	0.5090	0.4408	39.70	3459
850	32.20	1.434	0.5098	0.4415	39.88	3443
900	33.59	1.611	0.5106	0.4422	40.08	3426
950	35.04	1.785	0.5115	0.4429	40.29	3409
1000	36.54	1.968	0.5124	0.4437	40.51	3390

$$d = \sqrt{3}a/2$$

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57 LANTHANUM La

Atomic Weight: 138.90547 (7) (Meija 2017)

Allotropy: Alpha phase: Double hexagonal close-packed (hP4)
Beta phase: Face-centered cubic (cF4)
Gamma phase: Body-centered cubic (cI2)

For the alpha-beta transformation Gschneidner 1990 indicated significant hysteris varying between 583 K on heating and 533 K on cooling. Therefore, a specific value of 566 K determined by Spedding et al. 1961 from X-ray diffraction was accepted. Gschneidner 1990 selected 1138 K for the beta-gamma transformation and 1191 K for the melting point.

57.1 Alpha Phase: Double hexagonal close-packed (hP4): 0 K to 566 K

For the bulk thermal expansion Touloukian et al. 1975 combined the low temperature dilatometric measurements of Barson et al. 1953 (98-321 K) and the high temperature dilatometric measurements of Barson et al. 1957 (300-1137 K) as two equations. Both sets of measurements were only shown graphically with actual data points given by Touloukian et al. 1975. The equation covering the range from 100 K to the transition temperature is accepted which after correction to the reference temperature of 293.15 K is given by:

$$\varepsilon_T \text{ avr} = 2.78600 \times 10^{-6} T + 4.09400 \times 10^{-9} T^2 - 4.48100 \times 10^{-13} T^3 - 1.15725 \times 10^{-3} \quad (57a)$$

This equation was differentiated and derived thermal expansion coefficients over the range 120 K to 210 K were combined with specific heat (C_p) values selected by Arblaster 2013 and fitted to equation A:

$$\alpha\ (K^{-1}) = C_p\ (1.25070 \times 10^{-7} + 1.88214 \times 10^{-10} T + 6.74037 \times 10^{-7} / T) \quad (57b)$$

This equation was extrapolated below 120 K. The superconducting transition temperature at 5.12 K (Legvold et al. 1976) was not considered.

In the high temperature region length change values derived by Touloukian et al. from the lattice parameter measurements of Spedding et al. 1961 (293-566 K in the alpha range) showed considerable scatter and in agreement with Touloukian et al. 1975 the values for the *c* axis were rejected. Selecting values for the *a* axis is highly subjective but after rejection of data points at 323 K and 462 K the remaining four data points were fitted to the linear equation 57c with the *c* axis values being obtained by the difference between equations 57a and 57c:

$$\varepsilon_T a = 2.89617 \times 10^{-6} T - 8.49012 \times 10^{-4} \quad (57c)$$

$$\varepsilon_T c = 3.25769 \times 10^{-6} T + 1.05858 \times 10^{-8} T^2 - 1.86470 \times 10^{-3} \quad (57d)$$

On the basis 100Δε then over the range 366 K to 557 K the actual *c* axis values of Spedding et al. 1961 scatter 0.20 to 0.46 high. Length change values derived from the lattice parameter measurements of Eliseev et al. 1964 (293-603 K in the alpha range) scatter 0.32 to 1.05 high along the *a* axis and 0.63 to 1.01 high along the *c* axis. Length change values derived from the direct density measurements of Khairulin and Stankus 1987 (293-605 K in the alpha range), as given in analytical form by Stankus and Khairulin 1991, trend to 0.017 low.

Table 57a: Lattice parameters of alpha lanthanum at 293.15 K

Only the measurements of Beaudry and Palmer 1974 on electropolished wires were considered to be of sufficient accuracy to include in the evaluation. In agreement with Gschneidner 1990 these values, determined at 297 K, were selected and corrected to 293.15 K as *a* 0.37742 (3) nm *c* 1.2171 (1) nm. The derived density is 6145 (1) kg m^{-3} and the derived molar volume 22.605 (3) cm^3 mol^{-1}.

57.2 Beta Phase: Face-centered cubic (cF4): 566 K to 1138 K

Although the beta phase is easily obtained in a metastable condition down to the lowest temperatures, Legvold et al. 1977 have shown that for pure samples the phase cannot be retained below the transformation temperature. Dilatometric measurements of Barson et al. 1957 (588-1098 K in the beta range) were shown only graphically with actual data points given by Touloukian et al. 1975. These were fitted to the following equations based on both the reference state at 293.15 K and to the face-centered cubic base line:

$$\varepsilon_{T\,REF} = 6.39870 \times 10^{-6}\,T + 2.43891 \times 10^{-9}\,T^{2} - 3.77632 \times 10^{-3} \quad (57e)$$

$$\varepsilon_{T\,FCC} = 6.39870 \times 10^{-6}\,T + 2.43891 \times 10^{-9}\,T^{2} - 2.08537 \times 10^{-3} \quad (57f)$$

At the alpha-beta transition there is a molar volume contraction of 0.071 cm^3 mol^{-1} (0.31%).

On the basis 100Δε length change values derived by Touloukian et al. 1975 from the lattice parameter measurements of Spedding et al. 1961 (294-871 K) scatter 0.024 to 0.15 low while values derived from the lattice parameter measurements of Eliseev et al. 1964 (293-713 K) scatter 0.11 to 1.36 low.

Length change values derived from the direct density measurements of Khairulin and Stankus 1987 (605-1130 K in the beta region), as given in analytical form by Stankus and Khairulin 1991, trend from 0.045 low to 0.040 high in this range.

Table 57a. Lattice parameter of beta lanthanum at 293.15 K

References	Original Temperature K	*a* nm
Evans et al. 1960	298	0.53059
Evans and Raynor 1962	298	0.53058
Harris and Raynor 1964	298	0.53059
Norman et al. 1967	295	0.53059
Hill and Ellinger 1971	RT	0.53061
	Selected	0.53060 (4)

At 293.15 K: Density 6176 (1) kg m^{-3} Molar volume 22.490 (5) cm^3 mol^{-1}.

57.3 Gamma Phase: Body-centered cubic (cI2): 1138 K to 1191 K

In order to be consistent with the beta phase the direct density measurements of Khairulin and Stankus 1987 at 1130 K and 1187 K when derived as length change values were on the basis $100\varepsilon_T$ reduced by 0.040 and fitted to the following equations to represent lattice parameters and length change values relative to 293.15 K:

$$a \text{ (nm)} = 7.12079 \times 10^{-6} T + 0.417267 \quad (57g)$$

$$\varepsilon_T = 1.68799 \times 10^{-5} T - 1.08663 \times 10^{-2} \quad (57h)$$

The average thermal expansion coefficient is 16.7 x 10^{-6} K^{-1}. At the beta-gamma transition there is a molar volume expansion of 0.12 (3) cm^3 mol^{-1} (0.51%). Jayaraman 1965 determined the initial slope of the pressure curve to be a value of 0.05 K MPa^{-1} which together with an entropy of transition of 2.755 J mol^{-1} K^{-1} selected by Arblaster 2013 leads to a molar volume expansion of 0.14 cm^3 mol^{-1} in satisfactory agreement with the value determined from density differences.

The selected lattice parameter at 1160 K at 0.4255 nm is in excellent agreement with the measured value of 0.426 nm determined by Spedding et al. 1961.

Table 57b. Low temperature bulk properties of alpha lanthanum

T K	$\alpha \times 10^6$ K^{-1}	100 ε_T	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	- 0.107	22.532	6165
10	0.2	- 0.107	22.532	6165
20	1.0	- 0.106	22.533	6165
30	1.8	- 0.105	22.524	6164
40	2.3	- 0.102	22.535	6164
50	2.7	- 0.100	22.537	6163
60	3.0	- 0.097	22.539	6163
70	3.2	- 0.094	22.541	6162
80	3.3	- 0.091	22.543	6162
90	3.4	- 0.087	22.545	6161
100	3.6	- 0.084	22.547	6160
110	3.7	- 0.080	22.550	6160
120	3.8	- 0.076	22.553	6159
130	3.8	- 0.073	22.555	6158
140	3.9	- 0.069	22.558	6158
150	4.0	- 0.065	22.561	6157
160	4.1	- 0.061	22.563	6156
170	4.1	- 0.057	22.566	6155
180	4.2	- 0.053	22.569	6155
190	4.3	- 0.048	22.572	6154
200	4.4	- 0.044	22.575	6153
210	4.4	- 0.040	22.578	6152
220	4.5	- 0.035	22.581	6151
230	4.6	- 0.031	22.584	6151
240	4.7	- 0.026	22.587	6150
250	4.7	- 0.021	22.590	6149
260	4.8	- 0.016	22.594	6148
270	4.9	- 0.012	22.597	6147
280	5.0	- 0.007	22.600	6146
290	5.0	- 0.002	22.604	6145
293.15	5.1	0	22.605	6145

Table 57c. High temperature crystallographic properties of alpha lanthanum

T K	$\alpha_a \times 10^6$ K^{-1}	$\alpha_c \times 10^6$ K^{-1}	$\alpha_{avr} \times 10^6$ K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
293.15	2.9	9.5	5.1	0	0	0
300	2.9	9.6	5.2	0.002	0.007	0.004
350	2.9	10.7	5.5	0.016	0.057	0.030
400	2.9	11.7	5.8	0.031	0.113	0.058
450	2.9	12.8	6.2	0.045	0.174	0.088
500	2.9	13.8	6.5	0.060	0.241	0.120
550	2.9	14.9	6.9	0.074	0.313	0.154
566	2.9	15.2	7.0	0.079	0.337	0.165

Table 57d. High temperature crystallographic properties of alpha lanthanum

T K	*a* nm	*c* nm	*c*/2*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
293.15	0.37742	1.2171	1.6124	0.37425	22.605	6145
300	0.37743	1.2712	1.6125	0.37427	22.607	6144
350	0.37748	1.2178	1.6131	0.37442	22.625	6139
400	0.37754	1.2185	1.6137	0.37457	22.644	6134
450	0.37759	1.2192	1.6145	0.37474	22.665	6129
500	0.37765	1.2200	1.6153	0.37493	22.686	6123
550	0.37770	1.2209	1.6162	0.37512	22.709	6117
566	0.37772	1.2212	1.6166	0.37519	22.717	6115

$$d1 = (a^2/3 + c^2/16)^{1/2} \qquad d2 = a$$

Table 57e. Crystallographic properies of beta lanthanum

T K	$\alpha \times 10^6\ K^{-1}$	$100\ \varepsilon_{T\ REF}$	$100\ \varepsilon_{T\ FCC}$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
293.15	7.8	- 0.169	0	0.53060	0.37519	22.490	6176
300	7.9	- 0.164	0.005	0.53063	0.37521	22.494	6175
350	8.1	- 0.124	0.045	0.53084	0.37536	22.521	6168
400	8.4	- 0.083	0.086	0.53106	0.37552	22.549	6160
450	8.6	- 0.040	0.129	0.53128	0.37567	22.577	6152
500	8.8	0.003	0.172	0.53151	0.37584	22.607	6144
550	9.1	0.048	0.217	0.53175	0.37601	22.637	6136
566	9.2	0.063	0.232	0.53183	0.37606	22.647	6134
600	9.3	0.094	0.263	0.53200	0.37618	22.669	6128
650	9.6	0.141	0.310	0.53225	0.37636	22.701	6119
700	9.8	0.190	0.359	0.53250	0.37654	22.733	6110
750	10.0	0.239	0.409	0.53277	0.37672	22.767	6101
800	10.3	0.290	0.459	0.53304	0.37691	22.802	6092
850	10.5	0.342	0.512	0.53331	0.37711	22.837	6082
900	10.7	0.396	0.565	0.53360	0.37731	22.874	6073
950	11.0	0.450	0.619	0.53389	0.37751	22.911	6063
1000	11.2	0.506	0.675	0.53418	0.37772	22.948	6053
1050	11.5	0.563	0.732	0.53449	0.37794	22.988	6043
1100	11.7	0.621	0.790	0.53479	0.37816	23.027	6032
1138	11.9	0.666	0.835	0.53503	0.37833	23.058	6024

$$d = a/\sqrt{2}$$

Table 57f. Crystallographic properties of gamma lanthanum

T K	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1138	0.834	0.4254	0.3684	23.18	5994
1150	0.855	0.4255	0.3685	23.19	5990
1170	0.888	0.4256	0.3686	23.21	5984
1191	0.924	0.4257	0.3687	23.24	5978

$$d = \sqrt{3}a/2$$

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58 **CERIUM** **Ce**

Atomic Weight: 140.116 (1) (Meija 2017)

Allotropy: Alpha phase: Collapsed face-centered cubic (cF4)
Beta phase: Double hexagonal close-packed (hP4)
Gamma phase: Face-centered cubic (cF4)
Delta phase: Body-centered cubic (cI2)

The lower temperature transitions show considerable hysteris but Koskenmaki and Gschneidner 1978 select 96 K for the equilibrium alpha-beta transformation and Gschneidner et al. 1996 have determined the beta-gamma transition to be at 283 K. Gschneidner 1990 selected 999 K for the gamma-delta transition and 1071 K for the melting point.

58.1 Alpha Phase: Collapsed face-centered cubic (cF4): 0 K to 96 K

Increasing temperature thermal expansion coefficients over the range 60 K to 110 K determined by Smith and Morrice 1963 (4-293 K) were fitted to the equation:

$$\alpha\ (K^{-1}) = 2.14053 \times 10^{-7}\, T + 1.45049 \times 10^{-11}\, T^{3} \qquad (58a)$$

Length change values of Smith and Morrice 1963 below 50 K average to the value of $100\varepsilon = -4.24$ equivalent to a lattice parameter of 0.4942 nm while Gschneidner et al. 1962 obtain $100\varepsilon = -4.36$ between 20 K and room temperature, equivalent to 0.4936 nm in satisfactory agreement. However, both values are 0.01 nm higher than an average directly determined lattice parameter value of 0.484 (2) nm at 87 K, equivalent to the value $100\varepsilon = -6.22$, as an average of the closely agreeing values of Schuch and Sturdivant 1950, McHargue and Yakel 1960 and Waber et al. 1964. Because it is unlikely that these three independent determinations of the lattice parameter would contain a similar systematic error then it is considered that the dilatometric measurements may not have fully detected the very large shrinkage involved in the structure collapse. However, equation 58a was retained and combined with the lattice parameter value at 87 K to give the variation in lattice parameters and length change values over the range up to 96 K:

$$a\ (nm) = 5.52388 \times 10^{-8}\, T^{2} + 1.87100 \times 10^{-12}\, T^{4} + 0.483475 \qquad (58b)$$

$$\varepsilon_T = 1.07027 \times 10^{-7}\, T^{2} + 3.62512 \times 10^{-12}\, T^{4} - 6.32514 \times 10^{-2} \qquad (58c)$$

Although the selected lattice parameter was only determined to three significant figures values have been expanded to four significant figures in Table 58c for interpolation purposes.

58.2 Beta Phase: Double hexagonal close-packed (hP4): 96 K to 283 K

The hysteris of the alpha-beta transformation is such that it occurs as low as 45 K on cooling and 125 K on heating (Gschneidner 1990). Lattice parameter values of Beaudry and Palmer 1974 were determined at a temperature of 297 K according to Gschneidner 1990. Because there are no anisotropic thermal expansion values for the beta phase then it is assumed that the room temperature thermal expansion coefficient for the gamma phase can also be applied to the beta phase and it is further assumed that the *c*/*a* ratio remains the same over the narrow temperature range from 297 to 293.15 K. The derived lattice parameters at 293.15 K are therefore a = 0.36811 (6) nm c = 1.1857 (1) nm. The derived density value is 6689 (2) kg m^{-3} and the molar volume 20.948 (7) cm^3 mol^{-1}.

Dilatometric measurements of Trombe and Foex 1943 (77-679 K) and Rashid and Altstetter 1966 (82-557 K), as given as length change values by Touloukian et al. 1975, show large variations possibly due to difficulties arising from the marked hysteris in the transformation temperatures. These measurements could not be considered analytically and therefore the procedure adopted by Touloukian et al. 1975 is accepted in that the high temperature equation 58d is extended into the low temperature region down to the alpha-beta transformation temperature. Because of the procedure used the molar volume difference between the alpha and beta phases at 3.79 cm^3 mol^{-1} at the transformation temperature probably represents a maximum.

58.3 Gamma Phase: Face-centered cubic (cF4): 283 K to 999 K

The dilatometric measurements of Barson et al. 1957 (294-996 K), as given as length change values by Touloukian et al. 1975, were fitted to the following equation with an accuracy on the basis $\pm 100\varepsilon_T$ as ± 0.004:

$$\varepsilon_T = 5.32166 \times 10^{-6} T + 1.36609 \times 10^{-9} T^2 - 1.67744 \times 10^{-3} \quad (58d)$$

Selected values of Touloukian et al. 1975 were based on a cubic equation but it was found in the present evaluation that such an equation always led to a minimum in the derived thermal expansion equation at about 500 K which was considered to be unnatural behavior. On the basis $100\Delta\varepsilon$ the selected length change values of Touloukian et al. 1975 trend from 0.013 low at 700 K rising to 0.011 high at 1000 K.

On the same basis length change values derived by Touloukian et al. 1975 from the lattice parameter measurements of Pavlov and Finkel' 1967 (114-299 K) initially show scatter from 0.14 to 0.25 low but above 120 K trended from 0.21 low. Similarly length change values derived by Touloukian et al. 1975 from the lattice parameter values of Spedding et al. 1961 (286-892 K) scatter 0.026 low to 0.014 high. Length change values derived from direct density measurements of Stankus and Basin 1983 (293-1850 K) as reviewed by Stankus and Khairulin 1991 trend to 0.081 high at 999 K. Direct density measurements of Perkins et al. 1965 (273-787 K) were only shown graphically.

Table 58a. Lattice parameter of gamma cerium at 293.15 K

References	Original Temperature K	*a* nm	Note
Spedding et al. 1956	RT	0.51615	
Weiner and Raynor 1959	RT	0.51609	
Gschneidner et al. 1962	296	0.51603	
Evans and Raynor 1962	298	0.51611	
Gschneidner and Waber 1964	RT	0.51603	
Harris and Raynor 1964	298	0.51614	
Waber et al. 1964	RT	0.51615	
Harris et al. 1966	298	0.51614	
Norman et al. 1967a	298	0.51614	
Norman et al. 1967b	295	0.51615	
Speight et al. 1968	299	0.51615	
Beaudry and Palmer 1974	297	0.51612	a
	Selected	0.51612 (3)	

Note for Table 58b

a. Temperature of measurement given by Gschneidner 1990

In agreement with Gschneidner 1990 the values determined by Beaudry and Palmer 1974 for electropolished wires were selected. However, the average for all values in Table 58b is 0.51612 (5) nm in agreement

At 293.15 K: Density 6769 (1) kg m^{-3} Molar volume 20.699 (4) cm^3 mol^{-1}.

58.4 Delta Phase: Body-centered cubic (cI2): 999 K to 1071 K

Jayaraman 1965 determined the initial slope of the pressure curve to be – 0.014 K MPa^{-1} which together with an entropy of transition of 2.931 J mol^{-1} K^{-1} selected by Arblaster 2013 leads to a molar volume contraction of 0.041 cm^3 mol^{-1} and fixes the molar volume of the delta phase as 20.970 cm^3 mol^{-1} at the transition temperature. A thermal expansion coefficient a value of 18 x 10^{-6} K^{-1} is selected which is an average of the values obtained for gamma lanthanum and beta praseodymium:

$$a \text{ (nm)} = 7.40567 \times 10^{-6} T + 0.404028 \quad (58e)$$

$$\varepsilon_T = 1.80783 \times 10^{-5} T - 1.37121 \times 10^{-2} \quad (58f)$$

The calculated lattice parameter at 1015 K as 0.4115 nm is in excellent agreement with the directly determined value of 0.411 nm by Spedding et al. 1961. On the basis $100\Delta\varepsilon$ length change values derived from the direct density measurements of Stankus and Basin 1983 (293-1850 K) as reviewed by Stankus and Khairulin 1991 trend to 0.12 high at 1042 K.

Table 58b. Crystallographic properties of alpha cerium

T K	α x 10^6 K^{-1}	100 ε_T	*a* nm	*d* nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
0	0	- 6.325	0.4835	0.3419	17.01	8235
10	2	- 6.324	0.4835	0.3419	17.01	8235
20	4	- 6.321	0.4835	0.3419	17.02	8234
30	7	- 6.315	0.4835	0.3419	17.02	8233
40	9	- 6.309	0.4836	0.3419	17.02	8230
50	13	- 6.296	0.4836	0.3420	17.03	8228
60	16	- 6.282	0.4837	0.3420	17.04	8224
70	20	- 6.265	0.4838	0.3421	17.05	8219
80	25	- 6.243	0.4839	0.3422	17.06	8213
90	30	- 6.217	0.4840	0.3422	17.07	8206
96	33	- 6.199	0.4841	0.3423	17.08	8201

$$d = a/\sqrt{2}$$

Table 58c. Bulk properties of beta cerium

T K	α x 10^6 K^{-1}	100 ε_T	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
96	5.6	- 0.115	20.876	6712
100	5.6	- 0.113	20.877	6711
110	5.6	- 0.108	20.881	6710
120	5.7	- 0.102	20.884	6709
130	5.7	- 0.096	20.888	6708
140	5.7	- 0.091	20.892	6707
150	5.7	- 0.085	20.895	6706
160	5.8	- 0.079	20.899	6705
170	5.8	- 0.073	20.902	6703
180	5.8	- 0.068	20.906	6702
190	5.8	- 0.062	20.910	6701
200	5.9	- 0.056	20.913	6700
210	5.9	- 0.050	20.917	6699
220	5.9	- 0.044	20.921	6697
230	6.0	- 0.038	20.924	6696
240	6.0	- 0.032	20.928	6695
250	6.0	- 0.026	20.932	6694
260	6.0	- 0.020	20.936	6693
270	6.1	- 0.014	20.940	6691
280	6.1	- 0.008	20.943	6690
283	6.1	- 0.006	20.945	6690
290	6.1	- 0.002	20.947	6689
293.15	6.1	0	20.948	6689

Table 58d. Crystallographic properties of beta cerium

T K	*a* nm	*c* nm	*c*/ 2*a*	d1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
293.15	0.36811	1.1857	1.6105	0.36474	20.948	6689

$$d1 = (a^2/3 + c^2/16)^{½} \quad d2 = a$$

Table 58e. Crystallographic properties of gamma cerium

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
283	6.1	- 0.006	0.51609	0.36493	20.695	6771
290	6.1	- 0.002	0.51611	0.36494	20.698	6770
293.15	6.1	0	0.51612	0.36495	20.699	6769
300	6.1	0.004	0.51614	0.36497	20.701	6768
350	6.3	0.035	0.51630	0.36508	20.721	6762
400	6.4	0.067	0.51647	0.36520	20.740	6756
450	6.5	0.099	0.51663	0.36531	20.760	6749
500	6.7	0.132	0.51680	0.36544	20.781	6742
550	6.8	0.166	0.51698	0.36556	20.802	6736
600	6.9	0.201	0.51716	0.36568	20.824	6729
650	7.1	0.236	0.51734	0.36581	20.846	6722
700	7.2	0.272	0.51752	0.36594	20.868	6714
750	7.3	0.308	0.51771	0.36608	20.891	6707
800	7.5	0.345	0.51790	0.36621	20.914	6700
850	7.6	0.383	0.51810	0.36635	20.938	6692
900	7.7	0.422	0.51830	0.36649	20.962	6684
950	7.9	0.461	0.51850	0.36663	20.986	6677
999	8.0	0.500	0.51870	0.36678	21.011	6669

$$d = a/\sqrt{2}$$

Table 58f. Crystallographic properties of delta cerium

T K	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
999	0.435	0.4114	0.3563	20.97	6682
1000	0.437	0.4114	0.3563	20.97	6682
1020	0.473	0.4116	0.3564	20.99	6674
1040	0.509	0.4117	0.3565	21.02	6667
1060	0.545	0.4119	0.3567	21.04	6660
1071	0.565	0.4120	0.3568	21.05	6656

$$d = \sqrt{3}a/2$$

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59 PRASEODYMIUM Pr

Atomic Weight: 140.90766 (2) (Meija 2017)

Allotropy: Alpha phase: Double hexagonal close-packed (hP4)
Beta phase: Body-centered cubic (cI2)

Gschneidner 1990 selects 1068 K for the alpha-beta transformation temperature and 1204 K for the melting point. In the low temperature region Colclough 1986 determined a second order Néel transformation with ordering on hexagonal sites at 0.039 K.

59.1 Alpha phase: Double hexagonal close-packed (hP4): 0 K to 1068 K

Lattice parameter measurements of Bulatov and Dolzhenko 1988 (4.2-250 K) were only shown graphically with selected values estimated from the graphs. However, in the range 150 K to 250 K for the *a* axis the derived thermal expansion coefficient shows a peculiar sinusoidal behavior which is probably due to difficulties in reading the graphs. Therefore, above 150 K this coefficient is adjusted to coincide with a value of 1.4 x 10^{-6} K^{-1} at 293.15 K. For the *c* axis the thermal expansion coefficient is decreasing continuously above 30 K whereas the high temperature measurements suggest a continuous increase. In order to cause a minimum distortion away from the experimental values it was assumed that an abrupt change occurred when the high and low thermal expansion curves were interpolated and extrapolated respectively to the intercept temperature at 270 K at which point the thermal expansion coefficient has a minimum value of 10.3 x 10^{-6} K^{-1}. Therefore, the high temperature thermal expansion equation was used above this temperature.

Thermal expansion coefficient values are considered to be accurate to ± 0.5 x 10^{-6} K^{-1} below 10 x 10^{-6} K^{-1} and to ± 5% above while lattice parameters are at best considered to be accurate to ± 0.00007 nm along the *a* axis and to ± 0.0001 nm along the *c* axis.

Dilatometric measurements on single crystals by Ott 1975 (0.5-25 K) were shown only graphically but suggest an *a* axis thermal expansion coefficient trending to a negative value – 40 x 10^{-6} K^{-1} at 16 K before increasing to – 25 x 10^{-6} K^{-1} at 20 K, which is slightly contrary to the measurements of Bulatov and Dolzhenko 1988 which suggested a trend to – 30 x 10^{-6} K^{-1} at 20 K before increasing. For the *c* axis Ott 1975 suggested a rise to a value of 90 x 10^{-6} K^{-1} at 20 K compared to the selected value of 72 x 10^{-6} K^{-1} at this temperature. These differences may be partially due to the difficulties in deriving values from graphical interpretations.

In the high temperature region lattice parameter measurements of Smirnov and Prokhorov 1974 (73-973 K) were only shown graphically. Along the *a* axis there was a marked anomaly between 513 K and 673 K which was considered to be impurity induced and was not included in the evaluation. In spite of difficulties in reading the graphs for the *a* axis a thermal expansion coefficient of 1.4 (5) x 10^{-6} K^{-1} was selected at 293.15 K.

Between 473 and 953 K the *a* axis behavior is linear and can be represented by the following equation which was extrapolated to the transition temperature:

$$\varepsilon_T a = 6.72693 \times 10^{-6} T - 2.79507 \times 10^{-3} \quad (59a)$$

Between 293.15 and 473 K it was difficult to interpret the behavior because the thermal expansion coefficient had to increase from 1.4 x 10^{-6} K^{-1} to 6.7 x 10^{-6} K^{-1} in an interval of only 180 K and was also restrained by the fixed length change value at 473 K. Therefore, it was found necessary to evaluate the data graphically rather than analytically. For the *c* axis there was only a very minor effect on the thermal expansion at 625 K which was ignored and estimated length change values 273 K to 953 K were fitted to the following equation which was extrapolated to the transition temperature:

$$\varepsilon_T c = 4.03616 \times 10^{-6} T + 1.35743 \times 10^{-8} T^2 - 4.66381 \times 10^{-12} T^3 - 2.23224 \times 10^{-3} \quad (59b)$$

The tabulated values are considered to have the same accuracy as assigned to the low temperature values. Because of difficulties in reading the graphical representations then the measurements of Bulatov and Dolzhenko 1988 below 250 K were preferred to those of Smirnov and Prokhorov 1974.

Touloukian et al. 1975 selected length change values derived from the lattice parameter measurements of Spedding et al. 1961 (295-722K) and on the basis 100Δε showed major differences from the selected values, along the *a* axis trending to 0.060 low at 800 K and along the *c* axis trending to 0.18 low at 800 K. The reason for the large difference is uncertain but could possibly be due to impurities because in both cases only commercial grade materials were used.

Length change values derived from the direct density measurements of Khairulin and Stankus 1987 (293-1680 K), as given in analytical form by Stankus and Khairulin 1991, trend to 0.074 low at 800 K but then converges to only 0.028 lower at the transition temperature.

Table 59a. Lattice parameters of alpha praseodymium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Note
Spedding et al. 1956	RT	0.36727	1.18361	
Lundin et al. 1965	298	0.36717	1.18354	
Norman et al. 1966	295	0.36716	1.18315	
Harris et al. 1966	298	0.36716	1.18311	
Beaudry and Palmer 1974	297	0.36723	1.18328	a
	Selected	0.36723 (5)	1.18328 (6)	

Note for Table 59a

a. Temperature of measurement given by Gschneidner 1990

In agreement with Gschneidner 1990 the values determined by Beaudry and Palmer 1974 for electropolished wires were selected.

At 293.15 K for Pr: Density 6773 (2) kg m^{-3} Molar volume 20.806 (6) cm^3 mol^{-1}.

59.2 Beta Phase: Body-centered cubic (cI2): 1068 K to 1204 K

In order to obtain continuity with the alpha phase, direct density measurements of Khairulin and Stankus 1987 (1069 to 1207 K in the beta range) were converted to length change values which on the basis $100\varepsilon_T$ were increased by 0.028. This increase leads to the following values for the lattice parameters and length changes relative to 293.15 K:

$$a \text{ (nm)} = 7.97468 \times 10^{-6} T + 0.404665 \quad (59c)$$

$$\varepsilon_T = 1.94338 \times 10^{-5} T - 1.38553 \times 10^{-2} \quad (59d)$$

The average thermal expansion coefficient is 19.2 x 10^{-6} K^{-1}. The direct density measurements suggest that the molar volume difference between the alpha and beta phases at the transition temperature is negligible. However, Jayaraman 1965 obtained an initial slope of the pressure curve to be approximately 0.02 K MPa^{-1} which together with the entropy of transition of 2.981 J mol^{-1} K^{-1} selected by Arblaster 2013, would lead to a molar volume expansion of 0.06 cm^3 mol^{-1}. This does perhaps indicate the limitations on the sensitivity of the direct density measurements.

The selected lattice parameter at 1094 K at 0.4134 nm is in excellent agreement with the measured value of 0.413 nm determined by Spedding et al. 1961.

Table 59b. Low temperature crystallographic properties of alpha praseodymium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
0	0	0	0	0.160	- 0.840	- 0.173
1	- 14.8	0.8	- 9.6	0.159	- 0.840	- 0.174
2	- 16.3	2.0	- 10.2	0.158	- 0.840	- 0.175
3	- 17.8	4.5	- 10.4	0.156	- 0.840	- 0.176
4	- 19.2	7.5	- 10.3	0.154	- 0.840	- 0.177
5	- 20.5	11.5	- 9.8	0.152	- 0.839	- 0.178
6	- 21.6	17.9	- 8.5	0.150	- 0.837	- 0.179
7	- 22.7	23.3	- 7.4	0.148	- 0.835	- 0.180
8	- 23.7	28.5	- 6.3	0.145	- 0.832	- 0.181
9	- 24.7	33	- 5.3	0.143	- 0.829	- 0.181
10	- 25.5	38	- 4.3	0.141	- 0.826	- 0.182
15	- 28.6	58	- 0.3	0.127	- 0.802	- 0.183
20	- 29.9	72	4.1	0.112	- 0.769	- 0.182
25	- 29.8	82	7.3	0.097	- 0.730	- 0.179
30	- 28.3	86	10.0	0.080	- 0.689	- 0.176
40	- 21.4	86	14.3	0.055	- 0.602	- 0.164
50	- 16.0	75	14.4	0.037	- 0.522	- 0.149
60	- 12.0	60	11.9	0.023	- 0.455	- 0.136
70	- 8.9	46	9.5	0.013	- 0.405	- 0.127
80	- 6.8	38	8.1	0.005	- 0.363	- 0.118
90	- 5.0	32	7.2	- 0.001	- 0.328	- 0.110
100	- 3.6	27.0	6.6	- 0.006	- 0.299	- 0.104
110	- 2.4	23.7	6.3	- 0.009	- 0.274	- 0.097
120	- 1.6	21.6	6.2	- 0.011	- 0.252	- 0.091
130	- 0.9	20.2	6.1	- 0.012	- 0.231	- 0.085
140	- 0.4	18.4	5.8	- 0.012	- 0.211	- 0.079
150	- 0.1	16.9	5.6	- 0.013	- 0.194	- 0.073
160	0.1	15.9	5.4	- 0.013	- 0.177	- 0.068
170	0.3	15.2	5.3	- 0.012	- 0.162	- 0.062
180	0.5	14.8	5.3	- 0.012	- 0.147	- 0.057
190	0.6	14.6	5.3	- 0.012	- 0.132	- 0.052
200	0.8	14.4	5.3	- 0.011	- 0.118	- 0.046
210	0.9	14.3	5.4	- 0.010	- 0.103	- 0.041
220	1.0	14.2	5.4	- 0.009	- 0.089	- 0.036
230	1.1	14.0	5.4	- 0.008	- 0.075	- 0.030
240	1.1	13.5	5.3	- 0.007	- 0.061	- 0.025
250	1.2	12.8	5.1	- 0.006	- 0.048	- 0.020
260	1.3	11.8	4.8	- 0.004	- 0.036	- 0.015
270	1.3	10.3	4.3	- 0.003	- 0.024	- 0.010
280	1.3	10.5	4.4	- 0.002	- 0.014	- 0.006
290	1.4	10.7	4.5	- 0.001	- 0.003	- 0.001
293.15	1.4	10.8	4.5	0	0	0

Table 59c. Low temperature crystallographic properties of alpha praseodymium

T K	*a* nm	*c* nm	*c*/2*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.36782	1.17334	1.5950	0.36214	20.697	6808
5	0.36779	1.17336	1.5952	0.36213	20.694	6809
10	0.36775	1.17351	1.5955	0.36215	20.692	6810
15	0.36770	1.17379	1.5961	0.36219	20.691	6810
20	0.36764	1.17418	1.5969	0.36225	20.692	6810
25	0.36759	1.17463	1.5978	0.36232	20.694	6809
30	0.36752	1.17513	1.5987	0.36740	20.696	6809
40	0.36743	1.17615	1.6005	0.36258	20.703	6806
50	0.36736	1.17711	1.6021	0.36275	20.713	6803
60	0.36731	1.17790	1.6034	0.36289	20.721	6800
70	0.36728	1.17849	1.6044	0.36300	20.727	6798
80	0.36725	1.17899	1.6052	0.36309	20.732	6797
90	0.36723	1.17939	1.6058	0.36316	20.737	6795
100	0.36721	1.17974	1.6064	0.36324	20.741	6794
110	0.36720	1.18004	1.6068	0.36328	20.745	6792
120	0.36719	1.18030	1.6072	0.36333	20.749	6791
130	0.36719	1.18055	1.6076	0.36338	20.753	6790
140	0.36718	1.18078	1.6079	0.36343	20.757	6789
150	0.36718	1.18099	1.6082	0.36347	20.760	6787
160	0.36718	1.18118	1.6084	0.36351	20.764	6786
170	0.36718	1.18137	1.6087	0.36355	20.767	6785
180	0.36719	1.18154	1.6089	0.36359	20.770	6784
190	0.36719	1.18172	1.6091	0.36362	20.774	6783
200	0.36719	1.18189	1.6094	0.36366	20.777	6782
210	0.36719	1.18206	1.6096	0.36369	20.780	6781
220	0.36720	1.18223	1.6098	0.36373	20.784	6780
230	0.36720	1.18239	1.6100	0.36376	20.787	6779
240	0.36720	1.18256	1.6102	0.36380	20.790	6778
250	0.36721	1.18271	1.6104	0.36383	20.793	6777
260	0.36721	1.18286	1.6106	0.36386	20.797	6776
270	0.36722	1.18299	1.6107	0.36389	20.799	6775
280	0.36722	1.18311	1.6109	0.36392	20.802	6774
290	0.36722	1.18324	1.6111	0.36394	20.805	6773
293.15	0.36723	1.18328	1.6111	0.36395	20.806	6773

$$d1 = (a^2/3 + c^2/16)^{½} \quad d2 = a$$

Table 59d. High temperature crystallographic properties of alpha praseodymium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 ε_T *a*	100 ε_T *c*	100 ε_T avr
293.15	1.4	10.8	4.5	0	0	0
300	1.4	10.9	4.6	0.001	0.007	0.003
350	1.5	11.8	4.9	0.008	0.064	0.027
400	2.1	12.6	5.6	0.019	0.126	0.056
450	4.0	13.4	7.1	0.030	0.191	0.084
500	6.7	14.1	9.2	0.057	0.260	0.124
600	6.7	15.2	9.6	0.124	0.407	0.218
700	6.7	16.1	9.8	0.191	0.564	0.316
800	6.7	16.7	10.0	0.259	0.730	0.416
900	6.7	17.0	10.1	0.326	0.900	0.517
1000	6.7	17.0	10.1	0.393	1.071	0.619
1068	6.7	17.0	10.1	0.439	1.188	0.689

Table 59e. High temperature crystallographic properties of alpha praseodymium

T K	*a* nm	*c* nm	*c*/2*a*	*d*1 nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
293.15	0.36723	1.18328	1.6111	0.36395	20.806	6773
300	0.36723	1.18337	1.6112	0.36397	20.808	6772
350	0.36726	1.18404	1.6120	0.36412	20.823	6767
400	0.36730	1.18477	1.6128	0.36428	20.840	6761
450	0.36734	1.18554	1.6137	0.36445	20.858	6756
500	0.36744	1.18635	1.6144	0.36465	20.884	6747
600	0.36769	1.18809	1.6156	0.36509	20.942	6728
700	0.36793	1.18996	1.6171	0.36555	21.003	6709
800	0.36818	1.19191	1.6187	0.36603	21.066	6689
900	0.36843	1.19392	1.6203	0.36652	21.130	6669
1000	0.36867	1.19596	1.6220	0.36702	21.194	6648
1068	0.36884	1.19734	1.6231	0.36735	21.238	6635

$$d1 = (a^2/3 + c^2/16)^{1/2} \qquad d2 = a$$

Table 59f. Crystallographic properties of beta praseodymium

T K	100 ε_T	*a* nm	*d* nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
1068	0.690	0.4132	0.3578	21.24	6634
1100	0.752	0.4134	0.3580	21.28	6622
1150	0.849	0.4138	0.3584	21.34	6603
1200	0.947	0.4142	0.3587	21.40	6584
1204	0.954	0.4143	0.3588	21.41	6582

$$d = \sqrt{3}a/2$$

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60 NEODYMIUM Nd

Atomic Weight: 144.242 (3) (Meija 2017)

Allotropy: Alpha phase: Double hexagonal close-packed (hP4)
Beta phase: Body-centered cubic (cI2)

Gschneidner and Beaudry 1991 determined the alpha-beta transformation temperature to be 1135 K and the melting point 1295 K. Values selected by Gschneidner 1990 based on earlier determinations agree with the newer values to within 1 K.

60.1 Alpha phase: Double hexagonal close-packed (hP4): 0 K to 1135 K

In the low temperature region specific heat measurements of Forgan et al. 1979 determined the second order Néel transition with ordering on cubic sites to be 8.3 K with a first order transition at 6.3 K, which is considered as being due to hexagonal satellites splitting into different components. Bulatov and Dolzhenko 1989 (4.2-300 K) determined the temperatures to be 7.8 K and 6.5 K from lattice parameter measurements and because these represent the thermal expansion then these values are chosen in Tables 60b and 60c. The measurements of Bulatov and Dolzhenko 1989 were only shown graphically but the first order transition at 6.5 K was reported as being due to a slight increase in the *c* axis lattice parameter. From thermal expansion measurements Zochowski and McEwen 1986 determined the Néel transition with ordering on hexagonal sites at 20.0 K and a second transition at 19.1 K described as being due to magnetic satellites split transversely as the modulation wavevectors tilt away from the <100> direction. Sensitive dilatometric measurements by Zochowski and McEwen 1986 suggested that both transitions were weakly first order but the lattice parameter measurements of Bulatov and Dolzhenko 1989 did not detect a first order behavior.

The *a* axis lattice parameter measurements of Bulatov and Dolzhenko 1989 suggested a constant derived thermal expansion coefficient of 4.3 x 10^{-6} K^{-1} above 120 K but values above 210 K were adjusted in order to match up to the selected thermal expansion coefficient of 4.8 x 10^{-6} K^{-1} at 293.15 K. For the *c* axis there is a problem in that the low temperature measurements indicated a continual decrease in the thermal expansion coefficient above 80 K whereas the high temperature data showed a continual increase. In order to cause a minimum distortion away from the experimental values it was assumed that an abrupt change occurred when the high and low thermal expansion curves were interpolated and extrapolated respectively to the intercept temperature at 254 K at which point the thermal expansion coefficient has a minimum value of 10.0 x 10^{-6} K^{-1}. Therefore, the high temperature thermal expansion equations were used above this temperature. The derived thermal expansion values are considered to be accurate to ± 0.5 x 10^{-6} K^{-1} below 10 x 10^{-6} K^{-1} and to ± 5% above while lattice parameters are considered at best to be accurate to ± 0.00007 nm along the *a* axis and to ± 0.0001 nm along the *c* axis.

In the high temperature region lattice parameter measurements of Smirnov and Prokhorov 1974 (73-1073 K) were only shown graphically. Along the *a* axis there was a marked anomaly between 573 K and 833 K which was considered to be impurity induced and was not included in deriving the thermal expansion which was evaluated over the range 273 K to 1073 K. For the *c* axis the thermal expansion appeared to be virtually unaffected by anomalies and was evaluated over the same temperature range. Because of difficulties in reading the graphical representations then the measurements of Bulatov and Dolzhenko 1989 below 273 K were preferred to those of Smirnov and Prokhorov 1974, but above 254 K, and up to the transition temperature, the thermal expansion is represented by:

$$\varepsilon_T a = -1.84943 \times 10^{-6} T + 1.34924 \times 10^{-8} T^2 - 4.78896 \times 10^{-12} T^3 - 4.96691 \times 10^{-4} \quad (60a)$$

$$\varepsilon_T c = 7.34596 \times 10^{-6} T + 5.30081 \times 10^{-9} T^2 - 2.60900 \times 10^{-3} \quad (60b)$$

The tabulated values are considered to have the same accuracy as assigned to the low temperature values.

Touloukian et al. 1975 selected length change values derived from the lattice parameter measurements of Spedding et al. 1961 (293-969 K) and on the basis $100\Delta\varepsilon$ showed major trends differing from the selected values and at 1000 K they were 0.16 low along the *a* axis and 0.11 low along the *c* axis. The reason for the large difference is uncertain but could possibly be due to impurities because in both cases only commercial grade materials were used. Dilatometric measurements of Barson et al. 1957 (295-1158 K), which were given as length change values by Touloukian et al. 1975, could be subject to anisotropic effects but at 1000 K the length change values of 0.591 agrees closely with the average value selected by Touloukian et al. 1975 at 0.614. Length change values derived from direct density measurements of Khairulin and Stankus 1987 (293-1670 K), as given in analytical form by Stankus and Khairulin 1991, are on the basis 100ε, 0.040 lower than the selected value at the transition temperature.

Table 60a. Lattice parameter of alpha neodymium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Note
Spedding et al. 1956	RT	0.36581	1.17999	
Lundin et al. 1965	298	0.36567	1.17984	
Beaudry and Palmer 1974	297	0.36583	1.17968	a
	Selected	0.36583 (3)	1.17968 (6)	

Note for Table 60a

a. Temperature of measurement given by Gschneidner 1990

In agreement with Gschneidner 1990 the values determined by Beaudry and Palmer 1974 for electropolished wires were selected.

At 293.15 K: Density 7007 (1) kg m^{-3} Molar volume 20.585 (4) cm^3 mol^{-1}.

60.2 Beta Phase: Body-centered cubic (cI2): 1135 K to 1295 K

In order to obtain continuity with the alpha phase, length change values on the basis $100\varepsilon_T$ derived from the direct density measurements of Khairulin and Stankus 1987 (1123 to 1292 K in the beta range) were increased by 0.040. This leads to the following equations representing the lattice parameters and length changes relative to 293.15 K:

$$a \text{ (nm)} = 7.91454 \times 10^{-6} T + 0.403755 \quad (60d)$$

$$\varepsilon_T = 1.93561 \times 10^{-5} T - 1.25620 \times 10^{-2} \quad (60e)$$

The average thermal expansion coefficient is 19.1×10^{-6} K^{-1}. The direct density measurements suggest that the molar volume difference between the alpha and beta phases at the transition temperature is negligible. However, Jayaraman 1965 obtained an initial slope of the pressure curve to be approximately 0.02 K MPa^{-1}, which together with the entropy of transition of 2.674 J mol^{-1} K^{-1} selected by Arblaster 2013, would lead to a molar volume expansion of 0.05 cm^3 mol^{-1}. This does perhaps indicate the limitations on the sensitivity of the direct density measurements.

The selected lattice parameter at 1156 K at 0.4129 nm is in excellent agreement with the measured value of 0.413 nm by Spedding et al. 1961.

Table 60b. Crystallographic properties of alpha neodymium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
0	0	0	0	- 0.131	- 0.297	- 0.186
5.0	- 2.6	1.5	- 1.2	- 0.131	- 0.297	- 0.186
6.5	- 17.2	3.6	- 10.3	- 0.132	- 0.296	- 0.186
6.5	- 17.2	2.0	- 10.8	- 0.132	- 0.295	- 0.186
7.0	- 12.9	2.0	- 7.9	- 0.133	- 0.295	- 0.186
7.8	0	0	0	- 0.134	- 0.295	- 0.187
8.0	1.0	- 1.5	0.2	- 0.134	- 0.295	- 0.187
9.0	2.0	- 2.9	0.4	- 0.133	- 0.294	- 0.186
10	4.1	- 5.8	0.8	- 0.133	- 0.295	- 0.186
15	4.1	- 5.8	0.8	- 0.131	- 0.298	- 0.186
20	4.1	- 5.8	0.8	- 0.129	- 0.301	- 0.186
20	0	0	0	- 0.129	- 0.301	- 0.186
25	1.0	1.0	1.0	- 0.128	- 0.301	- 0.186
30	3.6	2.5	3.2	- 0.127	- 0.300	- 0.185
40	6.3	6.7	6.4	- 0.122	- 0.295	- 0.180
50	7.4	10.2	8.3	- 0.115	- 0.287	- 0.172
60	7.5	12.6	9.2	- 0.107	- 0.275	- 0.163
70	6.5	13.6	8.9	- 0.100	- 0.262	- 0.155
80	5.7	13.9	8.4	- 0.093	- 0.248	- 0.145
90	4.9	13.7	7.8	- 0.088	- 0.234	- 0.137
100	4.5	13.5	7.5	- 0.083	- 0.221	- 0.129
110	4.4	13.2	7.3	- 0.079	- 0.207	- 0.122
120	4.3	13.0	7.2	- 0.075	- 0.194	- 0.115
130	4.3	12.8	7.1	- 0.071	- 0.181	- 0.108
140	4.3	12.6	7.1	- 0.067	- 0.169	- 0.101
150	4.3	12.3	7.0	- 0.063	- 0.156	- 0.094
160	4.3	12.1	6.9	- 0.058	- 0.144	- 0.087
170	4.3	11.9	6.8	- 0.054	- 0.132	- 0.080
180	4.3	11.7	6.8	- 0.050	- 0.120	- 0.073
190	4.3	11.5	6.7	- 0.045	- 0.109	- 0.066
200	4.3	11.2	6.6	- 0.041	- 0.098	- 0.060
210	4.3	11.0	6.5	- 0.037	- 0.086	- 0.053
220	4.3	10.8	6.5	- 0.033	- 0.075	- 0.047
230	4.4	10.6	6.4	- 0.029	- 0.065	- 0.041
240	4.4	10.4	6.4	- 0.024	- 0.054	- 0.034
250	4.4	10.1	6.3	- 0.020	- 0.044	- 0.028
260	4.5	10.1	6.4	- 0.015	- 0.034	- 0.021
270	4.5	10.2	6.4	- 0.011	- 0.024	- 0.015
280	4.6	10.3	6.5	- 0.006	- 0.014	- 0.009
290	4.7	10.4	6.6	- 0.002	- 0.003	- 0.002
293.15	4.8	10.5	6.7	0	0	0
300	5.0	10.5	6.8	0.003	0.007	0.005
400	6.6	11.6	8.3	0.062	0.118	0.083
500	8.0	12.6	9.6	0.135	0.239	0.170
600	9.1	13.7	10.7	0.222	0.371	0.271
700	10.0	14.7	11.5	0.318	0.513	0.383
800	10.5	15.7	12.2	0.421	0.666	0.502
900	10.7	16.7	12.7	0.528	0.830	0.628
1000	10.7	17.8	13.1	0.636	1.004	0.758
1100	10.4	18.8	13.2	0.742	1.189	0.891
1135	10.2	19.1	13.2	0.778	1.256	0.937

Table 60c. Crystallographic properties of alpha neodymium

T K	*a* nm	*c* nm	*c*/2*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.36535	1.17618	1.6097	0.36188	20.470	7047
5.0	0.36535	1.17618	1.6097	0.36188	20.470	7047
6.5	0.36535	1.17619	1.6097	0.36188	20.470	7047
6.5	0.36535	1.17620	1.6097	0.36188	20.470	7047
7.8	0.36534	1.17620	1.6097	0.36188	20.470	7047
10	0.36534	1.17620	1.6097	0.36188	20.470	7047
15	0.36535	1.17616	1.6096	0.36188	20.470	7047
20	0.36536	1.17613	1.6096	0.36187	20.470	7047
25	0.36536	1.17613	1.6095	0.36187	20.470	7046
30	0.36537	1.17614	1.6095	0.36188	20.471	7046
40	0.36538	1.17620	1.6095	0.36189	20.474	7045
50	0.36541	1.17629	1.6096	0.36192	20.478	7044
60	0.36544	1.17644	1.6096	0.36196	20.484	7042
70	0.36546	1.17659	1.6097	0.36200	20.490	7040
80	0.36549	1.17675	1.6098	0.36204	20.495	7038
90	0.36551	1.17692	1.6100	0.36208	20.500	7036
100	0.36553	1.17707	1.6101	0.36212	20.505	7034
110	0.36554	1.17723	1.6103	0.36216	20.509	7033
120	0.36556	1.17739	1.6104	0.36219	20.514	7031
130	0.36557	1.17754	1.6105	0.36223	20.518	7030
140	0.36558	1.17769	1.6107	0.36226	20.522	7029
150	0.36560	1.17783	1.6108	0.36230	20.527	7027
160	0.36562	1.17798	1.6109	0.36233	20.531	7026
170	0.36563	1.17812	1.6111	0.36237	20.535	7024
180	0.36565	1.17826	1.6112	0.36240	20.539	7023
190	0.36567	1.17839	1.6113	0.36243	20.544	7021
200	0.36568	1.17853	1.6114	0.36247	20.548	7020
210	0.36569	1.17866	1.6115	0.36250	20.552	7018
220	0.36571	1.17879	1.6116	0.36253	20.556	7017
230	0.36573	1.17892	1.6118	0.36256	20.559	7016
240	0.36574	1.17904	1.6118	0.36259	20.564	7014
250	0.36576	1.17916	1.6119	0.36262	20.567	7013
260	0.36577	1.17928	1.6120	0.36265	20.571	7012
270	0.36579	1.17940	1.6121	0.36268	20.575	7010
280	0.36581	1.17952	1.6122	0.36271	20.579	7009
290	0.36582	1.17964	1.6123	0.36274	20.583	7008
293.15	0.36583	1.17968	1.6123	0.36275	20.585	7007
300	0.36584	1.17976	1.6124	0.36277	20.588	7006
400	0.36606	1.18107	1.6132	0.36311	20.634	6990
500	0.36632	1.18250	1.6140	0.36349	20.690	6972
600	0.36664	1.18405	1.6147	0.36391	20.753	6951
700	0.36699	1.18573	1.6155	0.36437	20.822	6927
800	0.36737	1.18754	1.6163	0.36487	20.897	6903
900	0.36776	1.18947	1.6172	0.36539	20.975	6877
1000	0.36816	1.19152	1.6182	0.36594	21.057	6850
1100	0.36854	1.19370	1.6195	0.36651	21.140	6823
1135	0.36868	1.19449	1.6200	0.36672	21.169	6814

$$d1 = (a^2/3 + c^2/16)^{½} \quad d2 = a$$

Table 60d. Crystallographic properties of beta neodymium

T K	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1135	0.941	0.4127	0.3574	21.17	6813
1150	0.970	0.4129	0.3575	21.19	6807
1200	1.067	0.4133	0.3579	21.25	6788
1250	1.163	0.4136	0.3582	21.31	6769
1295	1.250	0.4140	0.3585	21.37	6751

$$d = \sqrt{3}a/2$$

References for Neodymium

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61 PROMETHIUM Pm

Atomic mass ^{145}Pm: 144.912756(3) (Wang et al. 2017)
Atomic mass ^{147}Pm: 146.9151446 (19) (Wang et al. 2017)

Although ^{145}Pm has the longest half life at 17.7 y, ^{147}Pm is the "most useful" isotope with a half life of 2.6234 y (Audi et al. 2017).

Allotropy: Alpha phase: Double hexagonal close-packed (hP4)
Beta phase: Body-centered cubic (cI2)

The structure of the beta phase has not been determined but is considered to be the same as that obtained for neighboring elements. Gschneidner 1990 selected 1163 K for the alpha-beta transformation temperature and 1315 K for the melting point.

61.1 Alpha Phase: Double hexagonal close-packed (hP4): 0 K to 1163 K

Pallmer and Chikalla 1971 measured low accuracy lattice parameter values in order to determine the structure. It is considered that higher accuracy values can be estimated by assuming that promethium occurs at a 50/50 at% mixture of neodymium and samarium. The double hexagonal close packed structure is a high pressure phase of samarium but has been obtained in a high purity state at ambient pressure by Shi and Fort 1985, 1987 and the determined lattice parameters are in excellent agreement with those obtained by Harris and Speight 1985 by extrapolating Nd-Sm alloy lattice parameters to 100% Sm.

Table 61a. Room temperature lattice parameters of double hexagonal close-packed samarium

References	*a* nm	*c* nm	Note
Shi and Fort 1985, 1987	0.36201	1.1681	
Harris and Speight 1985	0.36205	1.1682	a
Selected	0.36203 (5)	1.1681 (2)	

Notes for Table 61a

a. Values given originally as being in nm appeared to be in Å units divided by 10 and have therefore been corrected accordingly

Combining the above values with the those selected for neodymium at 293.15 K selected as a = 0.36583 (3) nm c = 1.17968 (6) nm then the lattice parameter values for alpha promethium at a 50/50 at% mixture would be a = 0.36393 (10) nm c = 1.1739 (5) nm. The equivalent molar volume is 20.272 (14) cm^3 mol^{-1} and the density values 7149 (5) kg m^{-3} for ^{145}Pm and 7247 (5) kg m^{-3} for ^{147}Pm.

In order to estimate thermal expansion data for alpha promethium the value estimated for the molar volume of the beta phase at the transition temperature, 21.05 (5) cm^3 mol^{-1}, is also applied to the alpha phase on the grounds that for praseodymium and neodymium the volume difference at the transition is negligible. Using neodymium as a model, then the

change of the *c*/*a* ratio with temperature as determined for neodymium when applied to promethium leads to:

$$c/a = 3.22248 + 8.89527 \times 10^{-6} T + 6.14975 \times 10^{-9} T^{2} \quad (61a)$$

Combining the *c*/*a* ratio with the selected molar volumes at 293.15 K and the transition temperature and a further molar volume of 20.605 cm^3 mol^{-1} at 700 K based on the molar volume behavior of neodymium then anisotropic length change values can be represented by the following tentative equations:

$$\varepsilon_T a = 1.00000 \times 10^{-5} T + 1.83176 \times 10^{-9} T^{2} - 3.08892 \times 10^{-3} \quad (61b)$$

$$\varepsilon_T c = 1.27849 \times 10^{-5} T + 3.76094 \times 10^{-9} T^{2} - 4.07110 \times 10^{-3} \quad (61c)$$

61.2 Beta Phase: Body-centered cubic (cI2): 1163 K to 1315 K

The molar volume at the transition temperature is obtained from periodic trends based on neighboring element molar volumes of the body-centered cubic structure at their transition temperatures. Based on atomic number, extrapolating Pr-Nd leads to 21.11 cm^3 mol^{-1}, interpolating Nd-Sm leads to 21.01 cm^3 mol^{-1} and fitting Pr, Nd and Sm to a quadratic leads to 21.04 cm^3 mol^{-1}. The average of these three different approaches was averaged to 21.05 (5) cm^3 mol^{-1} at 1163 K which was selected. Selecting a thermal expansion coefficient of 19 x 10^{-6} K^{-1} which is the value obtained for the beta phases of both praseodymium and neodymium, leads to the following values for lattice parameters and length change values:

$$a \text{ (nm)} = 7.82704 \times 10^{-6} T + 0.402846 \quad (61d)$$

$$\varepsilon_T = 1.92401 \times 10^{-5} T + 9.73743 \times 10^{-3} \quad (61e)$$

Table 61b. Estimated crystallographic properties of alpha promethium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
293.15	11.1	15.0	12.4	0	0	0
300	11.1	15.0	12.4	0.008	0.010	0.008
400	11.5	15.8	12.9	0.120	0.184	0.135
500	11.8	16.5	13.4	0.237	0.326	0.267
600	12.2	17.2	13.8	0.357	0.495	0.403
700	12.5	17.9	14.3	0.481	0.672	0.545
800	12.9	18.6	14.8	0.608	0.856	0.691
900	13.2	19.4	15.3	0.739	1.048	0.842
1000	13.5	20.1	15.7	0.874	1.247	0.999
1100	13.9	20.8	16.2	1.013	1.454	1.160
1163	14.1	21.2	16.5	1.102	1.588	1.264

Table 61c. Estimated crystallographic properties of alpha promethium

T K	*a* nm	*c* nm	*c*/2*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density kg m^{-3} ^{145}Pm	Density kg m^{-3} ^{147}Pm
293.15	0.36393	1.1739	1.6128	0.36094	20.272	7149	7247
300	0.36396	1.1740	1.6129	0.36097	20.277	7147	7245
400	0.36437	1.1758	1.6135	0.36148	20.354	7120	7218
500	0.36479	1.1777	1.6142	0.36201	20.434	7092	7190
600	0.36523	1.1797	1.6150	0.36256	20.518	7063	7160
700	0.36568	1.1818	1.6159	0.36313	20.605	7033	7130
800	0.36614	1.1840	1.6168	0.36373	20.695	7002	7099
900	0.36662	1.1862	1.6178	0.36434	20.788	6971	7067
1000	0.36711	1.1885	1.6188	0.36498	20.885	6939	7034
1100	0.36762	1.1910	1.6199	0.36565	20.985	6906	7001
1163	0.36794	1.1925	1.6206	0.36608	21.050	6884	6979

$$d1 = (a^2/3 + c^2/16)^{1/2} \qquad d2 = a$$

Table 61d. Estimated crystallographic properties of beta promethium

T K	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density kg m^{-3} ^{145}Pm	Density kg m^{-3} ^{147}Pm
1163	1.264	0.4119	0.3568	21.05	6,884	6979
1200	1.375	0.4122	0.3570	21.09	6,870	6965
1250	1.431	0.4126	0.3573	21.15	6,850	6949
1300	1.527	0.4130	0.3577	21.21	6,836	6925
1315	1.556	0.4130	0.3578	21.23	6,825	6919

$$d = \sqrt{3}a/2$$

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62 SAMARIUM Sm

Atomic Weight: 150.36 (2) (Meija 2017)

Allotropy: Alpha phase: Rhombohedral (hR3)
Beta phase: Hexagonal close-packed (hP2)
Gamma phase: Body-centered cubic (cI2)

Beaudry and Gschneidner 1978 selected 1004 K for the equilibrium alpha-beta transformation temperature while Gschneidner 1990 selected 1195 K for the beta-gamma transformation temperature and 1347 K for the melting point. For the alpha phase second order Néel temperatures of 13.25 K for ordering on cubic sites and 105.2 K for ordering on hexagonal sites are selected (Arblaster 2013).

62.1 Alpha Phase: Rhombohedral (hR3): 0 K to 1004 K

All lattice parameters are given in terms of the equivalent hexagonal cell. In the low temperature region lattice parameter measurements of Bulatov and Dolzhenko 1978 (4.2-300 K) were shown only graphically with values being estimated from these graphs. Both Néel transitions were observed and although the lower transition resulted in sudden changes in the lattice parameter values the transition was still described as being second order. Values read from the graphs were smoothed by fitting to polynomial equations.

In the high temperature region the lattice parameter measurements of Smirnov and Prokhorov 1974 (80-970 K) were selected. These were also only shown graphically with values being estimated from the graphs. The values below 273 K were not considered with preference being given to the low temperature measurements of Bulatov and Dolzhenko 1978. The *a* axis values showed a marked anomaly between 273 K and 473 K which is considered to be likely due to impurity effects and was therefore not considered in the evaluation. Similarly, a sudden very sharp increase in the thermal expansion coefficient above 873 K was considered as possibly also being due to impurities and were not included with values above 873 K being obtained by extrapolation. For the *c* axis there was a small anomaly between 273 K and 473 K but otherwise the expansion behaved normally. It was found that the high temperature *a* axis data could be joined smoothly with the low temperature data but for the *c* axis there is a problem in that the low temperature measurements indicated a continual decrease in the thermal expansion coefficient while the high temperature data showed a continual increase. In order to cause a minimum distortion away from the experimental values it was assumed that an abrupt change occurred when the high and low thermal expansion curves were extrapolated and interpolated respectively to the intercept temperature at 323 K where the thermal expansion coefficient has a minimum value of 14.7×10^{-6} K^{-1}. Therefore, the following equations were used to represent the thermal expansion from 293.15 K to the transition temperature for the *a* axis and from 323 K to the transition temperature for the *c* axis:

$$\varepsilon_T a = 1.00129 \times 10^{-6} T + 1.46901 \times 10^{-8} T^2 - 1.83343 \times 10^{-11} T^3 + 1.00493 \times 10^{-14} T^4 - 1.16828 \times 10^{-3} \quad (62a)$$

$\varepsilon_T c = 1.03387 \times 10^{-5} T + 6.82029 \times 10^{-9} T^2 - 3.59133 \times 10^{-3}$ (62b)

Thermal expansion values given in Table 62b are probably accurate to ± 0.5 x 10^{-6} K^{-1} below 10 x 10^{-6} K^{-1} and to ± 5% above while lattice parameters given in Table 62c can probably be considered at best to be accurate to ± 0.00007 nm along the *a* axis and to ± 0.001 nm along the *c* axis.

Lattice parameter measurements of Mardon and Koch 1970 (293-683 K) show a major change in the *a* axis slope at 573 K which possibly associated with marked impurity effects, although the *c* axis thermal expansion is not affected. The results are shown graphically but derived thermal expansion values along the *a* axis between 273 K and 573 K and along the *c* axis between 273 K and 673 K, when corrected to length change values at a common temperature of 573 K are on the basis 100Δε 0.076 high along the *a* axis and 0.092 high along the *c* axis.

Direct density measurements of Stankus and Tyagel'skii 2002 (293-1920 K), which are considered as superceding earlier measurements of Stankus and Basin 1982 (293-1800 K), were made on samples with a high purity of 99.935% although the very important elements oxygen and hydrogen were not reported. Although alpha phase values were only given to 963 K extrapolation of the alpha phase values to the transition temperasture at 1004 K indicate on a length change basis 100Δε a value 0.064 lower than the selected average value.

Table 62a. Lattice parameter of alpha samarium at 293.15 K

References	Original Temperature K	a_h nm	c_h nm	Note
Speight et al. 1968	295	0.36283	2.6232	
Beaudry and Palmer 1974	297	0.36291	2.6207	a
Shi and Fort 1985,1987	RT	0.36292	2.6214	
	Selected	0.36291 (5)	2.6207 (6)	

Note for Table 62a

a. Temperature of measurement given by Gschneidner 1990

The equivalent rhombohedral cell has a_r = 0.89834 (20) nm α = 23.307 (9) °

In agreement with Gschneidner 1990 the values determined by Beaudry and Palmer 1974 for electropolished wires were selected.

At 293.15 K: Density 7518 (3) kg m^{-3} Molar volume 20.001 (7) cm^3 mol^{-1}.

62.2 Beta Phase: Hexagonal close-packed (hp2): 1004 K to 1195 K

To be consistent with the alpha phase, length change values derived from the density measurements of Stankus and Tyagel'skii 2002 (963 to 1220 K in the beta range) were on the basis $100\varepsilon_T$ increased by 0.064 and can be represented by the revised equation:

$$\varepsilon_T = 1.82916 \times 10^{-5}\,T - 7.54868 \times 10^{-3} \quad (62c)$$

The average thermal expansion coefficient is $18.1 \times 10^{-6}\,K^{-1}$

Smirnov and Prokhorov 1974 determined the lattice parameters at 980 K leading to a density value of 7389 kg/m^3 which is 100 kg/m^3 higher than the revised value of Stankus and Tyagel'skii 2002. Although confirming that the structure was hexagonal close-packed the measurements of Smirnov and Prokhorov 1974 appear to be systematically too low although the *c*/*a* ratio at 1.6125 (26) was retained and in the absence of other criteria was assumed to be constant for the whole beta range.This leads to a tentative estimate of the following anisotropic length change values and lattice parameters relative to 293.15 K:

$$\varepsilon_T\, a = 1.51903 \times 10^{-5}\,T - 6.26880 \times 10^{-3} \quad (62d)$$

$$\varepsilon_T\, c = 2.44943 \times 10^{-5}\,T - 1.01084 \times 10^{-2} \quad (62e)$$

$$a\ (\text{nm}) = 6.63229 \times 10^{-6}\,T + 0.359587 \quad (62f)$$

$$c\ (\text{nm}) = 1.06909 \times 10^{-5}\,T + 0.579838 \quad (62g)$$

62.3 Gamma Phase: Body-centered cubic (cI2): 1195 K to 1347 K

To be consistent with the beta phase length change values derived from the density measurements of Stankus and Tyagel'skii 2002 (1220 to 1360 K in the gamma range) were on the basis $100\varepsilon_T$ increased by 0.064 and can be represented by the revised equations relative to 293.15 K:

$$\varepsilon_T = 2.62967 \times 10^{-5}\,T - 1.75418 \times 10^{-2} \quad (62h)$$

$$a\ (\text{nm}) = 1.06510 \times 10^{-5}\,T + 0.397885 \quad (62i)$$

The average thermal expansion coefficient is $25.9 \times 10^{-6}\,K^{-1}$. At the transition temperature the direct density measurements suggested a slight molar volume contraction of 0.03 (2) cm^3 mol^{-1} (0.12%). However, Jayaraman 1965 obtained an initial slope of the pressure curve to be approximately 0.03 K MPa^{-1}, which together with the entropy of transition of 2.590 J mol^{-1} K^{-1} selected by Arblaster 2013, would lead to a molar volume expansion of 0.08 cm^3 mol^{-1}. This does perhaps indicate the limitations on the sensitivity of the direct density measurements. However, because of the quality of material available to Jayaraman 1965 at that time it is uncertain as to the actual nature of the transition

observed whereas Stankus and Tyagel'skii 2002 used materials of fairly high purity and definitely obtained an increase in density at the transition.

Table 62b. Crystallographic properties of alpha samarium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
0	0	0	0	0.169	- 0.786	- 0.149
13.25	- 4.5	22.8	4.6	0.163	- 0.756	- 0.143
13.25	- 1.0	12.1	3.4	0.103	- 0.686	- 0.160
15	- 1.9	13.0	3.0	0.102	- 0.684	- 0.160
20	- 4.5	15.3	2.1	0.101	- 0.677	- 0.158
30	- 9.0	19.9	0.6	0.094	- 0.659	- 0.157
40	- 12.7	24.6	- 0.3	0.083	- 0.637	- 0.157
50	- 15.7	29.2	- 0.7	0.069	- 0.611	- 0.158
60	- 17.8	33.8	- 0.6	0.052	- 0.579	- 0.158
70	- 19.1	38.4	0.1	0.033	- 0.543	- 0.159
80	- 19.6	43.1	1.3	0.014	- 0.503	- 0.159
90	- 30.4	47.7	- 4.4	- 0.011	- 0.458	- 0.160
100	- 41.3	52.8	- 9.9	- 0.047	- 0.408	- 0.167
105.2	- 46.9	54.7	- 13.0	- 0.070	- 0.380	- 0.173
105.2	1.5	24.3	9.1	- 0.070	- 0.380	- 0.173
110	1.6	24.2	9.1	- 0.069	- 0.367	- 0.168
120	1.9	23.7	9.2	- 0.067	- 0.343	- 0.159
130	2.1	23.3	9.2	- 0.065	- 0.320	- 0.150
140	2.3	22.8	9.2	- 0.063	- 0.297	- 0.141
150	2.6	22.4	9.2	- 0.061	- 0.275	- 0.132
160	2.8	21.9	9.2	- 0.058	- 0.252	- 0.123
170	3.0	21.5	9.2	- 0.055	- 0.231	- 0.114
180	3.3	21.0	9.2	- 0.052	- 0.210	- 0.104
190	3.5	20.6	9.2	- 0.048	- 0.189	- 0.095
200	3.7	20.2	9.2	- 0.045	- 0.168	- 0.086
210	4.0	19.7	9.2	- 0.041	- 0.149	- 0.077
220	4.2	19.3	9.2	- 0.037	- 0.129	- 0.068
230	4.4	18.8	9.2	- 0.033	- 0.110	- 0.058
240	4.7	18.4	9.2	- 0.028	- 0.091	- 0.049
250	4.9	17.9	9.2	- 0.023	- 0.074	- 0.046
260	5.1	17.5	9.3	- 0.018	- 0.056	- 0.031
270	5.4	17.1	9.3	- 0.013	- 0.038	- 0.021
280	5.6	16.6	9.3	- 0.008	- 0.021	- 0.012
290	5.8	16.2	9.3	- 0.002	- 0.005	- 0.003
293.15	5.9	16.0	9.3	0	0	0
300	6.0	15.7	9.3	0.004	0.011	0.006
350	6.3	15.1	9.2	0.035	0.086	0.052
400	6.5	15.8	9.6	0.067	0.164	0.099
450	6.7	16.4	10.0	0.100	0.244	0.148
500	7.0	17.1	10.3	0.136	0.328	0.200
600	7.5	18.4	11.1	0.206	0.506	0.306
700	8.4	19.7	12.2	0.285	0.699	0.423
800	9.8	21.1	13.6	0.376	0.904	0.552
900	12.1	22.4	15.6	0.486	1.124	0.699
1000	15.5	23.7	18.2	0.624	1.357	0.868
1004	15.6	23.7	18.3	0.630	1.366	0.876

Table 62c. Crystallographic properties of alpha samarium

T K	a_h nm	c_h nm	$c_h/4.5a_h$	a_r nm	α°	$d1$ nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.36352	2.6001	1.5894	0.89175	23.522	0.35709	19.911	7552
13.25	0.36350	2.6009	1.5900	0.89200	23.513	0.35715	19.915	7550
13.25	0.36328	2.6027	1.5921	0.89257	23.484	0.35724	19.905	7554
15	0.36328	2.6028	1.5921	0.89258	23.483	0.35725	19.905	7552
20	0.36328	2.6030	1.5923	0.89264	23.481	0.35726	19.906	7554
30	0.36325	2.6034	1.5927	0.89279	23.476	0.35730	19.907	7553
40	0.36321	2.6040	1.5932	0.89297	23.468	0.35733	19.907	7553
50	0.36316	2.6047	1.5938	0.89319	23.459	0.35738	19.906	7553
60	0.36310	2.6055	1.5946	0.89345	23.448	0.35743	19.906	7554
70	0.36303	2.6065	1.5955	0.89374	23.436	0.35749	19.906	7554
80	0.36296	2.6075	1.5965	0.89408	23.423	0.35757	19.606	7554
90	0.36287	2.6087	1.5976	0.89445	23.407	0.35764	19.905	7554
100	0.36274	2.6100	1.5989	0.89486	23.388	0.35772	19.901	7555
105.2	0.36266	2.6108	1.5998	0.89508	23.376	0.35775	19.897	7557
110	0.36266	2.6111	1.6000	0.89519	23.373	0.35778	19.900	7556
120	0.36267	2.6117	1.6003	0.89539	23.368	0.35784	19.906	7554
130	0.36267	2.6123	1.6007	0.89559	23.364	0.35790	19.911	7552
140	0.36268	2.6129	1.6010	0.89579	23.359	0.35796	19.917	7549
150	0.36269	2.6135	1.6013	0.89598	23.354	0.35801	19.922	7547
160	0.36270	2.6141	1.6016	0.89617	23.350	0.35807	19.928	7545
170	0.36271	2.6147	1.6019	0.89636	23.346	0.35812	19.933	7543
180	0.36272	2.6152	1.6022	0.89654	23.342	0.35818	19.939	7541
190	0.36273	2.6158	1.6025	0.89672	23.338	0.35823	19.944	7539
200	0.36275	2.6163	1.6028	0.89689	23.334	0.35828	19.950	7537
210	0.36276	2.6168	1.6030	0.89706	23.331	0.35834	19.955	7535
220	0.36278	2.6173	1.6033	0.89723	23.327	0.35839	19.961	7533
230	0.36279	2.6178	1.6035	0.89739	23.324	0.35844	19.966	7531
240	0.36281	2.6183	1.6037	0.89755	23.321	0.35849	19.972	7529
250	0.36283	2.6188	1.6039	0.89771	23.318	0.35853	19.977	7527
260	0.36284	2.6192	1.6041	0.89786	23.315	0.35858	19.983	7525
270	0.36286	2.6197	1.6043	0.89801	23.312	0.35863	19.988	7522
280	0.36288	2.6201	1.6045	0.89816	23.310	0.35868	19.994	7520
290	0.36290	2.6206	1.6047	0.89830	23.307	0.35872	19.999	7518
293.15	0.36291	2.6207	1.6047	0.89834	23.307	0.35874	20.001	7518
300	0.36292	2.6210	1.6049	0.89844	23.305	0.35877	20.005	7516
350	0.36304	2.6230	1.6053	0.89909	23.295	0.35898	20.032	7506
400	0.36315	2.6250	1.6063	0.89977	23.285	0.35921	20.061	7495
450	0.36327	2.6271	1.6071	0.90047	23.274	0.35943	20.090	7484
500	0.36340	2.6293	1.6078	0.90120	23.264	0.35968	20.121	7473
600	0.36366	2.6340	1.6096	0.90275	23.240	0.36019	20.185	7449
700	0.36394	2.6390	1.6114	0.90442	23.215	0.36074	20.256	7423
800	0.36428	2.6444	1.6132	0.90621	23.190	0.36134	20.334	7394
900	0.36467	2.6502	1.6149	0.90813	23.166	0.36199	20.423	7362
1000	0.36517	2.6563	1.6164	0.91017	23.145	0.36271	20.526	7325
1004	0.36520	2.6565	1.6165	0.91026	23.145	0.36274	20.531	7324

$$d1 = (a_h^2/3 + c_h^2/81)^{1/2} \qquad d2 = a_h$$

Table 62d. Crystallographic properties of beta samarium

T K	100 ε_T	a nm	c nm	$d1$ nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1004	1.082	0.3662	0.5906	0.3632	20.66	7279
1050	1.166	0.3666	0.5911	0.3635	20.71	7261
1100	1.257	0.3669	0.5916	0.3638	20.77	7241
1150	1.349	0.3672	0.5921	0.3641	20.82	7221
1195	1.431	0.3675	0.5926	0.3644	20.87	7204

$$d1 = (a^2/3 + c^2/4)^{1/2} \quad d2 = a$$

Table 62e. Crystallographic properties of gamma samarium

T K	100 ε_T	a nm	d nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1195	1.388	0.4106	0.3556	20.85	7213
1200	1.401	0.4107	0.3556	20.85	7210
1250	1.533	0.4112	0.3561	20.94	7182
1300	1.664	0.4117	0.3566	21.02	7154
1347	1.788	0.4122	0.3570	21.09	7128

$$d = \sqrt{3}a/2$$

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63 EUROPIUM Eu

Atomic Weight: 151.964 (1) (Meija 2017)

Allotropy: Alpha phase: Body-centered tetragonal (tI2)
Beta phase: Body-centered cubic (cI2)

Gschneidner 1990 selects 90.4 K for the Néel transition temperature which coincides with the alpha-beta transition and 1095 K for the melting point.

63.1 Alpha Phase: Body-centered tetragonal (tI2): 0 K to 90.4 K

The first order nature of the Néel transition was confirmed not only by the distortion to a tetragonal structure but also by actual measurement of the enthalpy of transition by Åstrom et al. 1992. Measurements of the lattice parameters by Bulatov and Kovalev 1988 (12-87.5 K in the alpha region) were only shown graphically and although values derived from the graph were further refined by fitting to polynomial equations the values in Table 63b cannot be considered to be more accurate than four significant figures and were also considered to be too insensitive to quote derived thermal expansion coefficient values. It is noted that the tetragonality appears to vanish below 35 K which Bulatov and Kovalev suggested was due to the formation of a domain structure below this temperature. Barrett 1956 indexed the structure as being body-centered cubic at 5 K with the determined lattice parameter at 0.4551 (3) nm agreeing satisfactorily with the selected value. However, Barrett 1956 also suggested that the structure was body-centered cubic at 78 K whereas Bulatov and Kovalev 1988 showed that it was tetragonal at this temperature.

63.2 Beta phase: Body-centered cubic (cI2): 90.4 K to 1095 K

Lattice parameter measurements of Bulatov and Kovalev 1988 (87.5 to 240 K in the beta phase region) were again only shown graphically but derived values appear to suggest that the thermal expansion varied linearly with temperature over the range 87.5 to 220 K with a thermal expansion coefficient of 24.5 x 10^{-6} K^{-1}. However, above 142 K values were adjusted until the thermal expansion coefficient coincided with the selected value of 26.3 x 10^{-6} K^{-1} at 293.15 K obtained from equation 63a. At 90.4 K the molar volume decrease at the alpha-beta transition is 0.028 cm^3 mol^{-1} (0.10%).

In the high temperature region Touloukian et al. 1975 fitted length change values derived from the lattice parameter values of Spedding et al. 1961 (293-625 K) to an equation which appeared to follow the scatter in the lattice parameter measurements and was therefore considered to show highly unnatural behavior. It was found that the values could only be satisfactorily correlated by means of a linear equation which gave a derived thermal expansion coefficient in agreement with the mean value of 26 (4) x 10^{-6} K^{-1} determined by Spedding et al. 1958 to cover the range from 293 to 1053 K. Therefore, the value of $100\varepsilon = 1.976$ at 1053 K was combined with the measurements of Spedding et

al. 1961 to derive equation 63a to cover the range from 293.15 K to the melting point. However, on the basis ± 100ε_T, equation 63a has an accuracy of ± 0.062:

$$\varepsilon_T = 2.62773 \times 10^{-5} T - 7.70319 \times 10^{-3} \quad (63a)$$

Because of the uncertainty values quoted in Table 63c values cannot be considered to be more accurate than four significant figures.

Direct density measurements of Stankus and Khairulin 1987 (293-1340 K), as reviewed by Stankus and Khairulin 1991, showed an anomaly at 702 K. However, electrical resistivity measurements on very high purity europium by Güntherodt et al. 1976 and Ten Cate et al. 1980 showed no evidence of any anomalies between room temperature and the melting point which clearly indicated that any such anomalies were impurity induced, possibly by non-metallic elements which were not determined in the samples used by Stankus and Khairulin 1987. The possible presence of such elements may explain the much larger thermal expansion obtained by the direct density measurements. On a length change basis as 100$\Delta\varepsilon$ the extrapolated difference reaches 0.83 high at the melting point, equivalent to a density difference of 2.4%.

Table 63a. Lattice parameter of beta europium at 293.15 K

References	Original Temperature K	*a* nm	Note
Spedding et al. 1958	298	0.45817	
Beaudry and Palmer 1974	297	0.45822	a
	Selected	0.45822 (4)	

Note for Table 63a

a. Temperature of measurement given by Gschneidner 1990

In agreement with Gschneidner 1990 the value determined by Beaudry and Palmer 1974 for electropolished wires was selected.

At 293.15 K: Density 5246 (1) kg m^{-3} Molar volume 28.970 (8) cm^3 mol^{-1}.

Table 63b. Crystallographic properties of alpha europium

T K	100 ε_T avr	*a* nm	*c* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	- 0.672	0.45514	0.45514	0.39416	28.389	5353
10	- 0.669	0.45516	0.45516	0.39418	28.392	5352
20	- 0.662	0.45519	0.45519	0.39420	28.398	5351
30	- 0.654	0.45522	0.45522	0.39423	28.405	5350
35	- 0.650	0.45524	0.45524	0.39425	28.408	5349
40	- 0.644	0.45526	0.45528	0.39427	28.414	5348
45	- 0.635	0.45529	0.45536	0.39431	28.421	5347
50	- 0.624	0.45531	0.45545	0.39435	28.430	5345
55	- 0.611	0.45534	0.45557	0.39441	28.442	5343
60	- 0.594	0.45538	0.45573	0.39447	28.456	5340
65	- 0.573	0.45542	0.45593	0.39456	28.474	5337
70	- 0.546	0.45548	0.45620	0.39467	28.498	5332
75	- 0.528	0.45554	0.45631	0.39473	28.513	5330
80	- 0.514	0.45562	0.45634	0.39479	28.525	5327
85	- 0.499	0.45572	0.45636	0.39485	28.538	5325
90	- 0.478	0.45584	0.45641	0.39493	28.556	5322
90.4	- 0.476	0.45585	0.45642	0.39494	28.558	5321

$$d = (a^{2}/2 + c^{2}/4)^{\frac{1}{2}}$$

65c. Crystallographic properties of beta europium

T K	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
90.4	- 0.508	0.45589	0.39481	28.530	5326
100	- 0.485	0.45600	0.39491	28.550	5323
110	- 0.461	0.45611	0.39500	28.571	5319
120	- 0.436	0.45622	0.39510	28.592	5315
130	- 0.412	0.45633	0.39520	28.613	5311
140	- 0.388	0.45644	0.39529	28.634	5307
150	- 0.363	0.45656	0.39539	29.655	5303
160	- 0.339	0.45667	0.39549	28.676	5299
170	- 0.314	0.45678	0.39558	28.698	5295
180	- 0.289	0.45689	0.39568	28.719	5291
190	- 0.264	0.45701	0.39578	28.741	5287
200	- 0.239	0.45712	0.39588	28.762	5283
210	- 0.214	0.45724	0.39598	28.784	5279
220	- 0.189	0.45735	0.39608	28.806	5275
230	- 0.163	0.45747	0.39618	28.828	5271
240	- 0.138	0.45759	0.39628	28.850	5267
250	- 0.112	0.45771	0.39638	28.872	5263
260	- 0.086	0.45782	0.39649	28.895	5259
270	- 0.060	0.45794	0.39659	28.917	5255
280	- 0.034	0.45806	0.39669	28.940	5251
290	- 0.008	0.45818	0.39680	28.962	5247
293.15	0	0.45822	0.39683	28.970	5246
300	0.018	0.45830	0.39690	28.985	5243
400	0.281	0.45951	0.39794	29.214	5202
500	0.444	0.46071	0.39899	29.445	5161
600	0.806	0.46191	0.40003	29.676	5121
700	1.069	0.46312	0.40107	29.909	5081
800	1.332	0.46432	0.40212	30.143	5041
900	1.595	0.46553	0.40316	30.378	5002
1000	1.857	0.46673	0.40420	30.614	4964
1095	2.107	0.46788	0.40519	30.840	4928

$$d = \sqrt{3}a/2$$

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64 GADOLINIUM Gd

Atomic Weight: 157.25 (3) (Meija 2017)

Allotropy: Alpha phase: Hexagonal close-packed (hP2)
Beta phase: Body-centered cubic (cI2)

Gschneidner 1990 selects 1508 K for the alpha-beta transformation temperature and 1586 K for the melting point. It is noted that the transformation temperature, which was determined on the purest samples available at the Iowa State University, is notably lower than a consensus value of 1534 (5) K obtained on materials of more commercial purity (Konings and Beneš 2010). Dan'kov et al. 1998 determined that the second order Curie transition temperature was within the range 294 (1) K.

64.1 Alpha Phase: Hexagonal close-packed (hP2): 0 K to 1508 K

Low temperature region

In the room temperature region selected values are based on the thermal expansion coefficient power equations of Dolejsi and Swenson 1981 (271-319 K) which are given in detail in Part 64.5. Different values for the Curie temperature of 293.358 K and 293.425 K were obtained for the *a* and *c* axes respectively but these values were not averaged because this would lead to a distortion of the thermal expansion coefficients away from the experimental values. Above the Curie temperature the *a* axis showed a minimum thermal expansion coefficient at 308 K while values for the *c* axis were extrapolated to zero thermal expansion at 323.2 K. These power equations are considered as superseding earlier values by Robinson and Lanchester 1978 and Lanchester et al. 1980. Dilatometric measurements of Cadieu and Douglass 1968 (279-306 K) along the c axis were only shown graphically with actual data points given by Touloukian et al. 1975. On the basis $100\Delta\varepsilon$ these trend from initially 0.022 high to an average of 0.005 low at 291 K and above.

In the low temperature region all lattice parameter values apart from those of Banister et al. 1954 were shown only graphically with actual data points as length change values given by Touloukian et al. 1975. In the case of the *a* axis below 271 K only the measurements of Vorobev et al. 1971 (80-319 K) were compatible with the room temperature values and these were fitted to the following equation to cover the range from 80 to 271 K:

$$\varepsilon_T\, a = 1.23388 \times 10^{-7}\, T + 4.74399 \times 10^{-8}\, T^{\,2} - 9.11240 \times 10^{-11}\, T^{\,3} - 1.85638 \times 10^{-3} \qquad (64a)$$

Measurements of Ergin 1965 (79-316 K) and Vorob'ev et al. 1965 (80-319 K) along the *a* axis show poor agreement with the selected values and on the basis $100\Delta\varepsilon$ trend from 0.089 high and 0.060 high respectively. The measurements of Darnell 1963 (101-366 K) trend from an average of 0.007 low below 140 K to a maximum of 0.027 low at 214 K then trend to 0.041 high at 366 K while those of Banister et al. 1954 (106-349 K) scatter

from 0.091 low to 0.094 high. Along the *c* axis below 280 K an average of the measurements of Ergin 1965 (83-315 K) and Vorobev et al. 1971 (79-319 K) show satisfactory agreement with the room temperature values and were fitted to the following equations to cover the range from 80 to 280 K:

$$80 - 160\ K: \quad \varepsilon_T c = 2.30000 \times 10^{-6} T - 7.80303 \times 10^{-9} T^2 - 7.57876 \times 10^{-12} T^3 + 2.31180 \times 10^{-3} \qquad (64b)$$

$$160 - 230\ K: \quad \varepsilon_T c = 1.48778 \times 10^{-5} T - 2.47460 \times 10^{-8} T^2 - 9.66952 \times 10^{-11} T^3 + 1.10065 \times 10^{-3} \qquad (64c)$$

$$230 - 280\ K: \quad \varepsilon_T c = -3.51979 \times 10^{-4} T + 1.61936 \times 10^{-6} T^2 - 2.55059 \times 10^{-9} T^3 + 2.83609 \times 10^{-2} \qquad (64d)$$

Measurements of Darnell 1963 (131-371 K) scatter 0.025 low to 0.013 high below the Curie temperature but then trend to 0.088 low at 371 K while measurements of Vorob'ev et al. 1965 (124-366 K) trend from 0.055 high to 0.028 low below the Curie temperature then scatter 0.041 low to 0.030 high. The measurements of Banister et al. 1954 (106-349 K) scatter from 0.18 low to 0.10 high.

High temperature region

Extrapolation to 293.15 K of the *c* axis lattice parameter values of Spedding et al. 1961 (295-917 K) as deduced from the length change values given by Touloukian et al. 1975 leads to 5.781 Å whereas Touloukian et al. 1975 appear to have chosen an arbitrary value of 5.784 Å which does not appear to be related to the experimental values. With the present selected value then derived length change values over the range 316 to 917 K less 670 K were fitted to equation 64g with an overall accuracy of ± 100 ε_T as ± 0.002 However, at 323.2 K equation 64g leads to a value of 100 ε_T as 0.031 whereas the value derived from the power equations leads to – 0.034. Therefore, equation 64g was modified over the range 323.2 to 400 K in order to reconcile these differences:

$$323.2 - 345\ K: \quad \varepsilon_T c = -4.42695 \times 10^{-4} T + 6.84862 \times 10^{-7} T^2 + 7.12015 \times 10^{-2} \qquad (64e)$$

$$345 - 400\ K: \quad \varepsilon_T c = 1.49237 \times 10^{-4} T - 1.73008 \times 10^{-7} T^2 - 3.08943 \times 10^{-2} \qquad (64f)$$

$$400 - 800\ K: \quad \varepsilon_T c = 8.15061 \times 10^{-6} T + 3.34981 \times 10^{-9} T^2 - 2.67722 \times 10^{-3} \qquad (64g)$$

Using the higher reference lattice parameter at 293 K, then the equation selected by Touloukian et al. 1975 leads to notably lower length change values than indicated by equation 64g. This allowed Touloukian et al. 1975 to ignore the *a* axis length change values of Spedding et al. 1961 and instead calculated *a* axis values by subtracting from dilatometric length change values obtained from a combination of the measurements of Barson et al. 1957 (129-1208 K) and Birss 1960 (76-746 K) with both sets of measurements being given by Toulokian et al. 1975. However, with the higher c axis values given by equation 64g then the subtraction leads to values for the *a* axis which were far too low to be consistent with the selected minimum thermal expansion value of

6.47 x 10^{-6} K^{-1} at 308 K. Therefore, the length change values derived by Touloukian et al. 1975 from the lattice parameter values of Spedding et al. 1961 were reconsidered and selected values over the range 522 to 917 K were combined with the selected values at 308 K to give the following equation to cover the range from 308 to 800 K with an overall accuracy of ± 100 ε_T as ± 0.027:

$$\varepsilon_T a = 5.69022 \times 10^{-6} T + 1.25971 \times 10^{-9} T^2 - 1.77309 \times 10^{-3} \quad (64h)$$

Table 64a. Lattice parameters of alpha gadolinium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Notes
Spedding et al. 1956	RT	0.36362	0.57829	
Darnell 1963a	296/291	0.36310	0.57817	a
Vorob'ev et al. 1965	297/293	0.36331	0.57776	a
Harris et al. 1966	298	0.36339	0.57826	
Norman et al. 1967	295	0.36339	0.57821	
Gupta and Anantharaman 1971	RT	0.36317	0.57773	
Vorobev et al. 1971	293	0.36318	0.57776	a
Spedding and Beaudry 1971	297	0.36337	0.57821	b
	Selected	0.36337 (4)	0.57821(5)	

Notes for Table 64a

a. Values given by Touloukian et al. 1975

b. Temperature of measurement given by Gschneidner 1990

In agreement with Gschneidner 1990 the values determined by Spedding and Beaudry 1971 for electropolished wires are selected.

At 293.15 K: Density 7899 (2) kg m^{-3} Molar volume 19.908 (5) cm^3 mol^{-1}.

64.2 Bulk properties of alpha gadolinium

On the basis 100Δε dilatometric measurements of Barson et al. 1957 (129-1208) and Birss 1960 (76-476 K) when considered above 293.15 K trend to 0.070 low at 900 K. Direct density measurements of Stankus et al. 1981 (293-1850 K), as corrected by Stankus and Khairlulin 1991, when corrected to length change values show satisfactory agreement with the selected values up to 800 K and are therefore considered as being representative of the bulk properties above this temperature and up to the transition temperature at 1508 K. The direct density mesurements were fitted to the length change equation:

$$\varepsilon_T = 3.46182 \times 10^{-6} T + 4.73029 \times 10^{-9} T^2 - 1.42040 \times 10^{-3} \quad (64i)$$

64.3 Beta Phase: Body-centered cubic (cI2): 1508 K to 1586 K

Direct density measurements of Stankus et al. 1981 (1536-1586 in the gamma region), as corrected by Stankus and Khairlulin 1991, were refitted to lattice parameter and length change values as derived as below:

a (nm) = 1.91680 x 10^{-5} T + 0.380546 (64j)

ε_T = 4.74028 x 10^{-5} T – 5.89006 x 10^{-2} (64k)

The derived thermal expansion coefficient is 46.8 x 10^{-6} K^{-1}. The molar volume difference at the alpha-beta transition temperature derived from the density measurements is a contraction of 0.12 (6) cm^3 mol^{-1} (0.58%). Jayaraman 1965 determined an initial slope of the pressure curve to be – 0.015 K Mpa^{-1}, which together with an entropy of transition of 2.312 J mol^{-1} K^{-1} selected by Arblaster 2013, leads to a contraction of 0.035 cm^3 mol^{-1}, in reasonable agreement considering possible experimental difficulties and sample purities.

64.4 Thermal expansion power equations for alpha gadolinium

Thermal expansion coefficients determined by Dolejsi and Swenson 1981 were fitted to the power equation $\alpha = A \left| t^* \right|^{-a} + B + E\ t$ where $t^* = (T - T_c) / T_c$ and T_c is the Curie temperature:

a axis

T_c = 293.358 K B = 10.50 x 10^{-6} K^{-1} E = 5.2 x 10^{-6} K^{-1}

Range t*	Range K	10^6 A	a
-7.6 x 10^{-2} to – 8 x 10^{-4}	271.063 293.123	- 8.91	- 0.279
- 8 x 10^{-4} to – 3 x 10^{-5}	293.123 – 293.349	- 198.2	- 0.713
5 x 10^{-5} to 2.5 x 10^{-4}	293.373 – 293.431	-43.4 x 10^6	- 1.98
2.5 x 10^{-4} to 8.6 x 10^{-2}	293.431 – 317.707	- 5.14	- 0.060

c axis

T_c = 293.425 K B = - 87.40 x 10^{-6} K^{-1} E = 2.0 x 10^{-5} K^{-1}

Range t*	Range K	10^6 A	a
-5 x 10^{-2} to – 6 x 10^{-3}	278.754 – 291.664	212.0	- 0.515
- 6 x 10^{-3} to – 1.2 x 10^{-5}	291.664 – 293.421	490	- 0.676
3 x 10^{-5} to 1.3 x 10^{-3}	293.434 – 293.806	- 4.37 x 10^6	- 1.71
1.3 x 10^{-3} to 6.6 x 10^{-2}	293.806 – 312.791	112.6	- 0.121

Table 64b. Low temperature crystallographic properties of alpha gadolinium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 ε_T *a*	100 ε_T *c*	100 ε_T avr
80	6.0	0.9	4.3	- 0.159	0.244	- 0.025
90	6.5	0.7	4.5	- 0.153	0.245	- 0.020
100	6.9	0.5	4.8	- 0.146	0.246	- 0.016
110	7.3	0.3	4.9	- 0.139	0.246	- 0.011
120	7.6	0.1	5.1	- 0.132	0.246	- 0.006
130	7.8	- 0.1	5.2	- 0.124	0.246	- 0.005
140	8.1	- 0.3	5.3	- 0.116	0.246	0.005
150	8.2	- 0.6	5.3	- 0.108	0.246	0.010
160	8.3	- 0.8	5.3	- 0.100	0.245	0.015
170	8.4	- 1.9	4.9	- 0.091	0.244	0.021
180	8.4	- 3.4	4.4	- 0.083	0.241	0.025
190	8.3	- 5.0	3.8	- 0.075	0.237	0.029
200	8.2	- 6.6	3.2	- 0.066	0.231	0.033
210	8.0	- 8.3	2.6	- 0.058	0.224	0.036
220	7.8	- 10.0	1.8	- 0.050	0.215	0.038
230	7.5	- 11.8	1.1	- 0.043	0.204	0.039
240	7.2	- 15.4	- 0.4	- 0.035	0.190	0.040
250	6.8	- 20.5	- 2.3	- 0.028	0.172	0.039
260	6.3	- 27.1	- 4.8	- 0.022	0.149	0.035
270	5.8	-35.3	- 7.9	- 0.016	0.117	0.029
280	6.50	- 45.0	- 10.7	- 0.0097	0.077	0.019
285	7.05	- 53.9	- 13.3	- 0.0064	0.053	0.013
290	7.88	- 66.2	- 16.8	- 0.0026	0.023	0.0059
291	8.14	- 69.6	- 17.8	- 0.0018	0.016	0.0042
292	8.49	- 74.1	- 19.0	- 0.0010	0.0090	0.0023
292.5	8.74	- 77.5	- 20.0	- 0.0006	0.0052	0.0013
293	9.12	- 81.5	- 21.1	- 0.0001	0.0012	0.0003
293.15	9.37	- 83.0	- 21.4	0	0	0

Table 64c. High temperature crystallographic properties of alpha gadolinium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 ε_T *a*	100 ε_T *c*	100 ε_T avr
293.15	9.37	- 83.0	- 21.4	0	0	0
293.2	9.57	- 83.6	- 21.5	0.0001	- 0.0004	< 0.0001
293.3	10.05	- 84.8	- 21.6	0.0001	- 0.0017	- 0.0005
293.358	10.50	- 85.7	- 21.6	0.0002	- 0.0018	- 0.0005
239.4	9.44	- 86.5	- 22.5	0.0002	- 0.0021	- 0.0006
293.425	7.82	- 87.4	- 23.9	0.0003	- 0.0023	- 0.0006
293.5	7.25	- 84.3	- 23.3	0.0003	- 0.0030	- 0.0008
293.6	7.15	- 74.0	- 19.9	0.0004	- 0.0038	- 0.0010
293.7	7.08	- 58.4	- 14.7	0.0005	- 0.0044	- 0.0011
293.8	7.03	- 38.1	- 8.01	0.0005	- 0.0049	- 0.0013
293.9	6.99	- 35.6	- 7.21	0.0006	- 0.0053	- 0.0014
294.0	6.95	- 34.4	- 6.83	0.0007	- 0.0056	- 0.0014
294.5	6.84	- 30.2	- 5.51	0.0010	- 0.0072	- 0.0017
295	6.76	- 27.5	- 4.66	0.0014	- 0.0087	- 0.0020
296	6.67	- 23.7	- 3.45	0.0020	- 0.012	- 0.002
298	6.57	- 19.0	- 1.95	0.0024	- 0.015	- 0.003
300	6.52	- 15.8	- 0.92	0.0047	- 0.019	- 0.003
305	6.47	- 10.5	- 0.81	0.0079	- 0.025	- 0.003
310	6.47	- 6.76	2.07	0.011	- 0.030	- 0.003
315	6.48	- 3.82	3.05	0.014	- 0.032	- 0.001
320	6.50	- 1.38	3.87	0.018	- 0.033	0.001
323.2	6.50	0	4.33	0.020	- 0.034	0.002
330	6.52	9.32	7.45	0.024	- 0.031	0.006
340	6.54	23.0	12.0	0.031	- 0.014	0.016
350	6.57	28.1	13.8	0.037	0.015	0.030
360	6.59	24.7	12.6	0.044	0.041	0.043
370	6.62	21.2	11.5	0.050	0.064	0.055
380	6.64	17.7	10.3	0.057	0.083	0.066
390	6.67	14.3	9.21	0.064	0.099	0.076
400	6.69	10.8	8.07	0.070	0.112	0.084
450	6.82	11.1	8.26	0.104	0.167	0.125
500	6.94	11.5	8.45	0.139	0.224	0.167
600	7.19	12.1	8.84	0.209	0.342	0.254
700	7.43	12.8	9.21	0.283	0.467	0.344
800	7.68	13.4	9.60	0.359	0.599	0.439

Table 64d. Crystallographic properties of alpha gadolinium

T K	*a* nm	*c* nm	*c*/*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
80	0.36279	0.57962	1.5977	0.35758	19.894	7905
90	0.36282	0.57963	1.5976	0.35759	19.896	7904
100	0.36284	0.57963	1.5975	0.35760	19.899	7902
110	0.36286	0.57963	1.5974	0.35761	19.902	7901
120	0.36289	0.57963	1.5973	0.35762	19.905	7900
130	0.36292	0.57963	1.5971	0.35763	19.908	7899
140	0.36295	0.57963	1.5970	0.35764	19.911	7898
150	0.36298	0.57963	1.5969	0.35765	19.914	7896
160	0.36301	0.57963	1.5967	0.35765	19.917	7895
170	0.36304	0.57962	1.5966	0.35766	19.921	7894
180	0.36307	0.57961	1.5964	0.35767	19.923	7893
190	0.36310	0.57958	1.5962	0.35767	19.926	7892
200	0.36313	0.57955	1.5960	0.35766	19.928	7891
210	0.36316	0.57950	1.5957	0.35766	19.930	7890
220	0.36319	0.57945	1.5955	0.35764	19.931	7890
230	0.36321	0.57939	1.5952	0.35763	19.932	7889
240	0.36324	0.57931	1.5948	0.35761	19.932	7889
250	0.36327	0.57921	1.5944	0.35757	19.931	7890
260	0.36329	0.57907	1.5940	0.35752	19.929	7890
270	0.36331	0.57889	1.5934	0.35746	19.925	7892
280	0.36333	0.57866	1.5926	0.35737	19.920	7894
285	0.36335	0.57852	1.5922	0.35732	19.916	7896
290	0.36336	0.57834	1.5917	0.35725	19.912	7897
291	0.36336	0.57830	1.5915	0.35724	19.911	7898
292	0.36337	0.57826	1.5914	0.35722	19.910	7898
292.5	0.36337	0.57824	1.5913	0.35721	19.909	7898
293	0.36337	0.57822	1.5913	0.35721	19.909	7899
293.15	0.36337	0.57821	1.5912	0.35720	19.908	7899
293.4	0.36337	0.57820	1.5912	0.35720	19.908	7899
295	0.36337	0.57816	1.5911	0.35716	19.907	7899
300	0.36339	0.57810	1.5909	0.35710	19.906	7899
310	0.36341	0.57804	1.5906	0.35715	19.907	7899
320	0.36343	0.57802	1.5904	0.35715	19.909	7899
330	0.36346	0.57803	1.5904	0.35716	19.911	7897
340	0.36348	0.57815	1.5905	0.35721	19.918	7895
350	0.36351	0.57829	1.5909	0.35728	19.926	7892
360	0.36353	0.57845	1.5912	0.35735	19.934	7889
370	0.36355	0.57858	1.5915	0.35742	19.941	7886
380	0.36358	0.57869	1.5917	0.35747	19.948	7883
390	0.36360	0.57878	1.5918	0.35751	19.954	7881
400	0.36363	0.57886	1.5919	0.35755	19.959	7879
450	0.36375	0.57918	1.5922	0.35772	19.983	7869
500	0.36387	0.57950	1.5926	0.35790	20.008	7859
600	0.36413	0.58019	1.5933	0.35826	20.060	7839
700	0.36440	0.58091	1.5942	0.35864	20.115	7818
800	0.36467	0.58167	1.5951	0.35905	20.171	7796

$$d1 = (a^2/3 + c^2/4)^{½} \quad d2 = a$$

Table 64e. Bulk properties of alpha gadolinium

T K	100 ε_T	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
800	0.439	20.171	7796
900	0.553	20.240	7769
1000	0.677	20.316	7740
1100	0.811	20.397	7710
1200	0.955	20.484	7677
1300	1.107	20.577	7642
1400	1.270	20.676	7605
1500	1.442	20.782	7567
1508	1.456	20.790	7564

This Table is considered to be identical toTables 64c and 64d at 800 K and below

Table 64f. Crystallographic properties of beta gadolinium

T K	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1508	1.258	0.4095	0.3546	20.67	7608
1550	1.457	0.4103	0.3553	20.79	7563
1586	1.628	0.4109	0.3559	20.90	7525

$$d = \sqrt{3}a/2$$

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65 TERBIUM Tb

Atomic Weight: 158.925354 (8) (Meija 2017)

Allotropy: Alpha phase: Orthorhombic (oS4)
Beta phase: Hexagonal close-packed (hP2)
Gamma phase: Body-centered cubic (cI2)

The alpha phase undergoes a first order transformation to the beta phase at the Curie temperature 221.45 K which then undergoes a second order Néel transformation at a temperature of 229.95 K (Arblaster 2013). Gschneidner 1990 selected 1562 K for the beta-gamma transformation and 1629 K for the melting point.

65.1 Alpha Phase: Orthorhombic (oS4): 0 K to 221.45 K

The distortion to the orthorhombic phase from the hexagonal close-packed phase occurs when the ideal value $b_{hcp} = \sqrt{3}\ a_{hcp}$ alters to $b_{ortho} \neq \sqrt{3}\ a_{ortho}$. Length change values are derived from the lattice parameter values of Finkel' and Belovol 1973 (77-300 K) which are preferred because the metal purity of 99.8% was much higher than that available for previous measurements. Unfortunately the measurements were only shown graphically and therefore, values were estimated from the graph with the accuracy of the derived length change values estimated to be about 5%. Because values were estimated no attempt was made to extrapolate below the minimum experimental temperature or to derive thermal expansion coefficients.

Other lattice parameter measurements in this region were made with material of only about 99.5% purity and were also only shown graphically with data points as length change values given by Touloukian et al. 1975. Those of Finkel' et al. 1966 (121-295 K) suggested that the *b* axis expanded with increasing temperature whereas measurements of both Darnell 1963 (76-298 K) and the selected values of Finkel' and Belovol 1973 showed that it decreased. The deviations of other values in this region are evaluated as $100\Delta\varepsilon$ in Table 65a:

Table 65a. Deviations from the selected values for the alpha phase

References	Alpha Range K	Deviations $100\Delta\varepsilon$
Darnell 1963	76-221	*a* axis: Average deviation 0.031 high up to 150 K and then scatter 0.024 low to 0.041 high *b* axis: Average deviation 0.005 high *c* axis: Average deviation 0.052 high below 160 K trending to average 0.031 low above 200 K
Finkel' et al. 1966	121-221	*a* axis: Trends from initially 0.16 high *b* axis: Not considered because appears to show incorrect behavior *c* axis: Trends from 0.060 high to 0.097 low
Finkel and Vorob'ev 1967	117-221	*a* axis: Trends from 0.15 high to 0.062 high *c* axis: Trends from 0.058 high to 0.071 low
Alberts and du Plessis 1968	84-217	*c* axis: Trends 0.072 high to 0.008 low

65.2 Beta Phase: Hexagonal close-packed (hP2): 221.45 K to 1562 K

Up to 293.15 K length changes derived from the graphical representation of Finkel' and Belovol 1973 (77-300 K) were again selected. As a result, at the crystallographic transition at the Curie temperature the *a* axis increased 0.00012 nm, the *b* axis decreased 0.00009 nm and the *c* axis decreased 0.00013 nm. Sensitive dilatometry by Tindall and Steinitz 1983 confirmed that the Néel transformation was second order.

Above the Curie temperature the values of Finkel' and Belovol 1973 were adjusted in order to show a smooth continuity with the high temperature selected data, equations 65a and 65b, which were extrapolated to 260 K along the *a* axis and 275 K along the *c* axis but with the thermal expansion coefficients along the *c* axis at 275 K and 280 K adjusted to give a smooth curve. Other values in this region are considered in Table 65b:

Table 65b. Deviations from the selected values for the beta phase

References	Beta Range K	Deviations $100\Delta\varepsilon$
Darnell 1963	223-298	*a* axis: Scatters from 0.025 low to 0.006 high *c* axis: Trends from initially 0.065 low to maximum of 0.033 high at 268 K
Finkel' et al. 1966	222-295	*a* axis: Trends from 0.037 high *c* axis: Trends from 0.083 low
Finkel' and Vorob'ev 1967	223-300	*a* axis: Trends from 0.023 high to 0.006 low *c* axis: Trends from 0.061 low to 0.011 high
Alberts and du Plessis 1968	223-315	*c* axis: Average 0.011 high

In the high temperature region the equations selected by Touloukian et al. 1975, which were based on the lattice parameter values of Spedding et al. 1961 (297-1125 K), showed maximum values in the derived thermal expansion coefficients at 1045 K for the *a* axis and 987 K for the *c* axis which is considered to be abnormal behavior. A fit to quadratic equations eliminates this problem and therefore the measurements of Spedding et al. 1961 were fitted to the following equations to cover the range from 293.15 K to 1200 K:

$$\varepsilon_T a = 7.58802 \times 10^{-6} T + 1.50653 \times 10^{-9} T^2 - 2.35390 \times 10^{-3} \quad (65a)$$

$$\varepsilon_T c = 1.05775 \times 10^{-5} T + 5.77910 \times 10^{-9} T^2 - 3.59743 \times 10^{-3} \quad (65b)$$

Table 65c. Lattice parameters of beta terbium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Notes
Spedding et al. 1956	RT	0.36012	0.56939	
Darnell 1963	293	0.36077	0.57004	a
Finkel' et al. 1966	293	0.36092	0.56973	a
Finkel' and Vorob'ev 1967	293	0.36098	0.56976	a
Speight et al. 1968	295	0.36060	0.56975	
Gupta and Anantharaman 1971	RT	0.35992	0.56963	
Spedding and Beaudry 1971	297	0.36056	0.56966	b
	Selected	0.36056 (4)	0.56966 (6)	

Notes for Table 65c

a. Values given by Touloukian et al. 1975

b. Temperature of measurement given by Gschneidner 1990

In agreement with Gschneidner 1990 the values determined by Spedding and Beaudry 1971 for electropolished wires are selected.

At 293.15 K for β-Tb: Density 8229 (2) kg m^{-3} Molar volume 19.312 (5) cm^3 mol^{-1}

65.3 Bulk properties of beta terbium

Direct density measurements of Stankus and Basin 1983 (293-1900 K), as reviewed by Stankus and Khairulin 1991, show anomalies at 570 K and 1323 K but no evidence of the beta-gamma transformation. Length change values derived from the density measurements initially show poor agreement with the selected crystallographic values for the beta phase, on the basis $100\Delta\varepsilon$ the difference reaching 0.21 low at 1200 K. Because the crystallographic properties were obtained over the wide temperature range 293 to 1200 K then equations 65a and 65b have been extrapolated to the transition temperature but because of the extrapolation the values obtained are considered to be highly tentative. The apparent bulk thermal expansion increases rapidly above 1323 K and the difference decreases to only 0.02 low at the transition temperature.

65.4 Gamma Phase: Body-centered cubic (cI2): 1562 K to 1629 K

Stankus and Basin 1983a did not detect the beta gamma transition. Jayaraman 1965 determined an initial slope of the pressure curve to be 0.004 K Mpa^{-1}, which together with an entropy of transition of 2.852 J mol^{-1} K^{-1} selected by Arblaster 2013, leads to a molar volume expansion of 0.011 cm^3 mol^{-1} and fixes the molar volume of the gamma phase as 20.372 cm^3 mol^{-1} at 1562 K. Selecting a thermal expansion coefficient of 25.5 x 10^{-6} K^{-1} obtained from the direct density measurements of Stankus and Basin 1983a then the variation with temperature of the lattice parameter and the length change values can be calculated although all values are again considered to be highly tentative:

$$a \text{ (nm)} = 1.03907 \times 10^{-5} T + 0.391248 \quad (65c)$$

$$\varepsilon_T = 2.59584 \times 10^{-5} T - 2.25716 \times 10^{-2} \quad (65d)$$

Table 65d. Crystallographic properties of alpha terbium

T K	100 ε_T *a*	100 ε_T *b*	100 ε_T *c*	100 ε_T avr
80	- 0.592	0.218	0.182	- 0.065
90	- 0.563	0.201	0.191	- 0.057
100	- 0.534	0.183	0.199	- 0.051
110	- 0.505	0.164	0.209	- 0.045
120	- 0.477	0.145	0.216	- 0.039
130	- 0.448	0.127	0.224	- 0.033
140	- 0.419	0.111	0.230	- 0.026
150	- 0.390	0.091	0.237	- 0.021
160	- 0.361	0.075	0.240	- 0.016
170	- 0.333	0.055	0.241	- 0.013
180	- 0.300	0.030	0.239	- 0.011
190	- 0.265	0.006	0.226	- 0.011
200	- 0.229	- 0.015	0.206	- 0.013
210	- 0.193	- 0.035	0.168	- 0.020
220	- 0.126	- 0.061	0.111	- 0.025
221.45	- 0.112	- 0.066	0.103	- 0.025

Table 65e. Crystallographic properties of alpha terbium

T K	*a* nm	*b* nm	*c* nm	*b*/*a*	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
80	0.35843	0.62587	0.57070	1.7462	19.274	8245
90	0.35853	0.62577	0.57075	1.7454	19.279	8244
100	0.35863	0.62565	0.57080	1.7445	19.282	8242
110	0.35874	0.62553	0.57085	1.7437	19.286	8241
120	0.35884	0.62541	0.57089	1.7429	19.289	8239
130	0.35895	0.62530	0.57094	1.7421	19.293	8238
140	0.35095	0.62520	0.57097	1.7413	19.297	8236
150	0.35915	0.62508	0.57101	1.7404	19.300	8235
160	0.35926	0.62498	0.57102	1.7396	19.303	8233
170	0.35936	0.62485	0.57103	1.7388	19.304	8233
180	0.35948	0.62469	0.57102	1.7378	19.305	8232
190	0.35961	0.62454	0.57095	1.7367	19.305	8232
200	0.35973	0.62441	0.57083	1.7358	19.304	8233
210	0.35986	0.62429	0.57062	1.7361	19.300	8234
220	0.36010	0.62413	0.57030	1.7332	19.297	8236
221.45	0.36015	0.62410	0.57025	1.7329	19.297	8236

b values calculated from reference value at 293.15 K: $b = \sqrt{3}\ a = 0.62451$ nm

Table 65f: Crystallographic properties of beta terbium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
221.45	18.6	- 107	- 23.2	- 0.080	0.080	- 0.027
225	17.7	-88	- 17.4	- 0.074	0.046	- 0.034
229.95	16.4	-63	- 10.1	- 0.065	0.008	- 0.041
235	15.0	-41	-3.5	- 0.057	- 0.018	- 0.044
240	13.7	-21	2.2	- 0.050	- 0.033	- 0.044
245	12.4	-10	4.8	- 0.044	- 0.035	- 0.041
250	11.0	- 4.7	5.8	- 0.038	- 0.037	- 0.037
255	9.70	0	6.5	- 0.032	- 0.038	- 0.034
260	8.37	2.9	6.6	- 0.028	- 0.037	- 0.031
270	8.40	9.8	8.9	- 0.020	- 0.031	- 0.023
280	8.43	13.5	10.1	- 0.011	- 0.011	- 0.011
290	8.46	13.9	10.3	- 0.003	- 0.004	- 0.003
293.15	8.47	14.0	10.3	0	0	0
300	8.49	14.0	10.3	0.006	0.010	0.007
400	8.79	15.2	10.4	0.092	0.156	0.113
500	9.08	16.3	11.5	0.182	0.314	0.226
600	9.37	17.4	12.1	0.274	0.483	0.344
700	9.66	18.5	12.6	0.370	0.664	0.468
800	9.95	19.9	13.2	0.468	0.856	0.597
900	10.2	20.8	13.7	0.570	1.060	0.733
1000	10.5	21.9	14.3	0.674	1.276	0.875
1100	10.8	22.9	14.9	0.782	1.503	1.022
1200	11.1	24.0	15.9	0.892	1.742	1.175

Table 65g. Crystallographic properties of beta terbium

T K	*a* nm	*c* nm	*c*/*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
221.45	0.36027	0.57011	1.5825	0.35288	19.296	8236
225	0.36029	0.56992	1.5818	0.35281	19.292	8238
229.95	0.36033	0.56971	1.5811	0.35273	19.288	8240
235	0.36035	0.56956	1.5805	0.35268	19.286	8240
240	0.36038	0.56947	1.5802	0.35265	19.286	8240
245	0.36040	0.56946	1.5801	0.35266	19.288	8240
250	0.36042	0.56945	1.5799	0.35266	19.290	8239
255	0.36044	0.56944	1.5798	0.35267	19.292	8238
260	0.36046	0.56945	1.5798	0.35267	19.294	8237
270	0.36049	0.56948	1.5797	0.35270	19.298	8235
280	0.36052	0.56960	1.5799	0.35275	19.305	8232
290	0.36055	0.56963	1.5799	0.35278	19.310	8230
293.15	0.36056	0.56966	1.5799	0.35279	19.312	8229
300	0.36058	0.56971	1.5800	0.35282	19.316	8228
400	0.36089	0.57055	1.5809	0.35326	19.378	8202
500	0.36122	0.57145	1.5820	0.35374	19.443	8174
600	0.36155	0.57241	1.5832	0.35424	19.512	8145
700	0.36189	0.57344	1.5846	0.35477	19.584	8115
800	0.36225	0.57454	1.8560	0.35534	19.660	8084
900	0.36261	0.57570	1.5876	0.35593	19.740	8051
1000	0.36299	0.57693	1.5894	0.35656	19.823	8017
1100	0.36338	0.57822	1.5912	0.35721	19.910	7982
1200	0.36378	0.57958	1.5932	0.35790	20.000	7946

$$d1 = (a^2/3 + c^2/4)^{1/2} \qquad d2 = a$$

Table 65h. Bulk properties of beta terbium

All values are tentative

T K	$100\ \varepsilon_T$	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1200	1.175	20.000	7946
1300	1.334	20.095	7909
1400	1.499	20.194	7870
1500	1.670	20.296	7830
1562	1.779	20.361	7805

This Table is considered to be identical to Tables 65f and 65g at 1200 K and below.

Table 65i. Crystallographic properties of gamma terbium

All values are tentative

T K	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1562	1.798	0.4075	0.3529	20.37	7801
1600	1.896	0.4079	0.3532	20.43	7779
1629	1.971	0.4082	0.3535	20.48	7761

$$d = \sqrt{3}a/2$$

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66 DYSPROSIUM Dy

Atomic Weight: 162.500 (1) (Mweija 2017)

Allotropy: Alpha phase: Orthorhombic (oS4)
Beta phase: Hexagonal close-packed (hP2)
Gamma phase: Body-centered cubic (cI2)

The alpha phase undergoes a first order transformation to the beta phase at the Curie temperature 90.5 K which then undergoes a second order Néel transformation at a temperature of 180.0 K (Arblaster 2013). Gschneidner 1990 selected 1654 K for the beta-gamma transformation and 1685 K for the melting point.

66.1 Alpha Phase: Orthorhombic (oS4): 0 K to 90.5 K

The distortion to the orthorhombic phase from the hexagonal close-packed phase occurs when the ideal value $b_{hcp} = \sqrt{3}\ a_{hcp}$ alters to $b_{ortho} \neq \sqrt{3}\ a_{ortho}$. Selected values are based on the lattice parameter measurements of Chernyshov et al. 2008 (10-130 K in the alpha range) which were only shown graphically with actual data points given by Pecharsky 2013. Although there were significant differences between measurements obtained on heating and cooling cycles the values were averaged except that above 60 K for the *c* axis the differences were too diverse and therefore values were obtained above this temperature by extrapolating to the beta phase value at 90.5 K. Because the lattice parameter measurements did not show the sudden very sharp decrease in the thermal expansion coefficient centering at 86.9 K, as found in the thermal expansion coefficients of Amitin et al. 1984 (58-92 K in the alpha range), then the latter were not considered because it was unsure if this was the behavior in the alpha-beta transition temperature region.

Lattice parameter measurements of Darnell 1963 and Finkel' and Vorob'ev 1966 and dilatometric measurements of Clark et al. 1965 were only shown graphically with actual data points given by Touloukian et al. 1975. Lattice parameter measurements of Darnell and Moore 1963 (30-293 K) were also only shown graphically. Length change values were directly derived from the lattice parameter measurements of Banister et al. 1954. The deviations from the selected values are given in Table 66a.

Table 66a. Deviations from the selected values for the alpha phase

References	Alpha Range K	Deviations 100ε
Banister et al. 1954	49, 76	*a* axis: 0.41 low and 0.33 low *c* axis: 0.031 low and 0.078 high
Darnell 1963	9-85	*a* axis: Scatter 0.030 high to 0.099 high *b* axis: Trends from 0.71 high to 0.47 high *c* axis: Average deviation 0.17 high to 76 K then trends to 0.20 low at 81 K
Clark et al. 1965	79-88	*a* axis: Trends from 0.37 low to 0.19 low
Finkel' and Vorob'ev 1966	73-89	*a* axis: Average 0.84 low to 81 K then average 0.22 low above *b* axis: Trends 0.30 high to 0.11 high *c* axis: Averages 0.14 high to 83 K then trends to 0.006 low

66.2 Beta Phase: Hexagonal close packed: 90.5 K to 1654 K

Along the c axis thermal expansion coefficients determined by Amitin et al. 1984 (93-299 K in the beta range) were selected while along the *a* axis the lattice parameter measurements of Chernyshov et al. 2008 (70-300 K in the beta range) were selected. The latter were only shown graphically with actual data points given by Pecharsky 2013. Values obtained for both heating and cooling cycles were combined. The second order Néel transition at 180.0 K has a marked effect with a large negative decrease in the thermal expansion along the *c* axis while the *a* axis shows a marked change in the thermal expansion coefficient. The heating and cooling values diverge above 180 K and therefore the results are correlated by using a linear equation between 180 K and 293.15 K. On the basis $100\varepsilon_T$ above 180 K the heating values trend to 0.035 high at 250 K and the cooling values trend to 0.018 low at the same temperature:

$$90.5 \text{ to } 180 \text{ K} \quad : \varepsilon_T a = 2.69684 \times 10^{-6} T + 4.50841 \times 10^{-8} T^2 - 2.72483 \times 10^{-3} \qquad (66a)$$

$$180 - 293.15 \text{ K}: \varepsilon_T a = 6.88181 \times 10^{-6} T - 2.01740 \times 10^{-3} \qquad (66b)$$

Between the Curie transition and the Néel transition there is the formation of an incommensurate helical antiferromagnetic state in which at certain turn angles are commensurate with the basal plane of the hexagonal structure. Nine such transitions occur for dysprosium (Arblaster 2013) but with only minor effects on the *c* axis thermal expansion, as observed by Greenough et al. 1981, and therefore these are not considered further in the evaluation.

At the transition from the orthorhombic phase to the hexagonal phase the evaluation leads to a decrease of 0.00038 nm (0.11%) in the *a* axis and an increase of 0.00072 nm (0.12%) in the *b* axis while the *c* axis value for the beta phase was used as an input value for the alpha phase. However, in consideration of the same data Chernyshov et al. 2008 suggests a decrease of 0.24% in the *a* axis, an increase of 0.33% in the *b* axis, and a decrease of 0.10% in the *c* axis. Chernyshov et al. 2008 pointed out that Darnell 1963

obtained a decrease of 0.2% in the *a* axis, and increase of 0.5% in the *b* axis and a decrease of 0.3% in the *c* axis. However, the graphical representations of Darnell 1963 clearly showed a distinction between the alpha and beta phase lattice parameters and not the convergence as shown in the values of Chernyshov et al. 2008.

As with the alpha phase, lattice parameter measurements of Darnell 1963 and Finkel' and Vorob'ev 1966 and dilatometric measurements of Clark et al. 1965 were only shown graphically with actual data points given by Touloukian et al. 1975. Length change values were directly derived from the lattice parameter values given by Banister et al. 1954 while the beta phase *c* axis values of Chernyshov et al. 2008 were shown only graphically with actual data points given by Pecharsky 2013. The deviations from the selected values are given in Table 66b. Lattice parameter measurements of Darnell and Moore 1963 (30-293 K) were also only showed graphically. The marked scatter in the different sets of measurements above 180 K justified the use of only a linear thermal expansion relationship above this temperature.

Table 66b. Deviations from the selected values for the beta phase

References	Beta Range K	Deviations $100\Delta\varepsilon$
Banister et al. 1954	92-302	*a* axis: Scatters from 0.054 low to 0.071 high *c* axis: Scatters from 0.20 low to 0.024 low
Darnell 1963	92-298	*a* axis: Scatters from 0.031 low to 0.042 high *c* axis: Initially scatters 0.035 low to 0.023 high but averages 0.009 high above 178 K
Clark et al. 1965	91-273	*a* axis: Averages 0.016 high above 160 K *c* axis: Trends from 0.068 low to 0.020 low below 180 K and averages 0.004 high above
Finkel' and Vorob'ev 1966	91-300	*a* axis: Initially 0.034 low then trends towards selected value at 172 K then averages 0.017 low above 175 K. *b* axis equivalent trends from 0.019 low to a maximum 0.028 high at 159 K then averages 0.002 high above 190 K *c* axis: Trends from initially 0.013 low to a maximum of 0.057 low at 140 K then trends to average 0.020 high above 190 K
Chernyshov et al. 2008	90-300	*c* axis: Average of heating and cooling cycles. Trends 0.072 low to maximum 0.081 low at 130 K then trends to average of 0.009 low above 180 K

In the high temperature region length change values derived by Touloukian et al. 1975 from the lattice parameter values of Spedding et al. 1961 (293-958 K) showed satisfactory agreement with the low temperature thermal expansion along the *c* axis but the *a* axis values can generally be considered to be incompatible although in the absence of other data these measurements were accepted although the derived equation 66c did show a minimum in the thermal expansion coefficient at 580 K. The following equations are used to represent the thermal expansion from 293.15 K to 950 K:

$$\varepsilon_T a = 1.39155 \times 10^{-5} T - 1.60594 \times 10^{-8} T^2 + 9.23219 \times 10^{-12} T^3 - 2.93181 \times 10^{-3} \quad (66c)$$

$\varepsilon_T\, c = 1.80604 \times 10^{-5}\, T - 6.95836 \times 10^{-9}\, T^2 + 8.41410 \times 10^{-12}\, T^3 - 4.90841 \times 10^{-3}$ (66d)

On the basis $100\Delta\varepsilon$, length change values derived from the direct density measurements of Stankus and Tyagel'skii 2000 (293-1950 K), which supercede preliminary values of Stankus and Khairulin 1991, do not agree with the selected values, the difference reaching 0.060 low at 900 K and with no convergence above this temperature. Therefore, satisfactory thermal expansion data is only available to 950 K. Although it is possible that either of the high temperature measurements could be subject to systematic errors it is noted that the volume thermal expansion coefficient at 293 K determined by Stankus and Tyagel'skii 2000 at $20.8 \times 10^{-6}\ K^{-1}$ is much lower than the value of $29.9 \times 10^{-6}\ K^{-1}$ selected from the low temperature data.

Table 66c. Lattice parameters of beta dysprosium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Notes
Spedding et al. 1956	RT	0.35905	0.56478	
Darnell 1963	293	0.35946	0.56543	a
Finkel' and Vorob'ev 1966	293	0.35915	0.56509	a
Harris and Raynor 1969	RT	0.35932	0.56540	
Gupta and Anantharaman 1971	RT	0.35925	0.56548	
Spedding and Beaudry 1971	297	0.35916	0.56501	b
	Selected	0.35916 (1)	0.56501 (4)	

Notes for Table 66c

a. Values given by Touloukian et al. 1975

b. Temperature of measurement given by Gschneidner 1990

In agreement with Gschneidner 1990 the values determined by Spedding and Beaudry 1971 for electropolished wires are selected.

At 293.15 K: Density 8550 (1) kg m^{-3} Molar volume 19.006 (2) $cm^3\ mol^{-1}$.

Table 66d. Crystallographic properties of alpha dysprosium

T K	100 ε_T *a*	100 ε_T *b*	100 ε_T *c*	100 ε_T avr
10	0.132	- 0.745	0.232	- 0.127
20	0.132	- 0.727	0.236	- 0.120
30	0.129	- 0.711	0.240	- 0.114
40	0.116	- 0.676	0.245	- 0.106
50	0.100	- 0.628	0.251	- 0.093
60	0.076	- 0.571	0.244	- 0.084
70	0.032	- 0.504	0.235	- 0.079
80	- 0.025	- 0.426	0.223	- 0.076
90	- 0.103	- 0.331	0.209	- 0.075
90.5	- 0.106	- 0.326	0.208	- 0.075

Table 66e. Crystallographic properties of alpha dysprosium

T K	*a* nm	*b* nm	*c* nm	*b*/*a*	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
10	0.35963	0.61745	0.56632	1.7169	18.933	8583
20	0.35963	0.61756	0.56634	1.7172	18.937	8581
30	0.35962	0.61766	0.56637	1.7175	18.940	8580
40	0.35958	0.61788	0.56639	1.7183	18.945	8577
50	0.35952	0.61817	0.56643	1.7194	18.953	8574
60	0.35943	0.61853	0.56639	1.7209	18.958	8572
70	0.35928	0.61895	0.56634	1.7228	18.961	8570
80	0.35907	0.61943	0.56627	1.7251	18.962	8570
90	0.35879	0.62002	0.56619	1.7281	18.963	8569
90.5	0.35878	0.62005	0.56619	1.7282	18.963	8569

b values calculated from reference value at 293.15 K: $b = \sqrt{3}\ a = 0.62208$ nm

Table 66f: Crystallographic properties of beta dysprosium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
90.5	10.9	- 11.3	3.5	- 0.211	0.208	- 0.071
95	11.3	- 12.7	3.3	- 0.206	0.203	- 0.070
100	11.7	- 14.4	3.0	- 0.200	0.196	- 0.068
110	12.6	- 18.6	2.2	- 0.188	0.179	- 0.066
120	13.5	- 23.7	1.1	- 0.175	0.158	- 0.064
130	14.4	- 29.6	- 0.2	- 0.161	0.132	- 0.064
140	15.3	- 36.5	- 1.9	- 0.146	0.099	- 0.065
150	16.2	- 44.2	- 3.9	- 0.131	0.058	- 0.068
160	17.1	- 57.2	- 7.6	- 0.114	0.008	- 0.073
170	18.0	- 70.0	- 11.3	- 0.096	- 0.055	- 0.083
175	18.5	- 78.8	- 13.9	- 0.087	- 0.093	- 0.089
176	18.6	- 81.3	- 14.7	- 0.085	- 0.101	- 0.090
177	18.7	- 84.2	- 15.6	- 0.084	- 0.109	- 0.092
178	18.8	- 87.5	- 16.7	- 0.081	- 0.117	- 0.094
179	18.9	- 91.3	- 17.9	- 0.080	- 0.126	- 0.095
180	18.9	- 95.8	- 19.3	- 0.078	- 0.136	- 0.097
181	6.9	- 8.9	1.6	- 0.077	- 0.142	- 0.099
182	6.9	- 5.9	2.6	- 0.076	- 0.142	- 0.098
183	6.9	- 3.3	3.5	- 0.076	- 0.142	- 0.098
184	6.9	- 1.1	4.2	- 0.075	- 0.142	- 0.098
185	6.9	0.7	4.8	- 0.074	- 0.142	- 0.097
190	6.9	6.0	6.8	- 0.071	- 0.140	- 0.094
195	6.9	8.0	7.3	- 0.068	- 0.137	- 0.091
200	6.9	9.3	7.7	- 0.064	- 0.133	- 0.087
210	6.9	11.4	8.4	- 0.057	- 0.122	- 0.079
220	6.9	12.8	8.9	- 0.050	- 0.110	- 0.070
230	6.9	13.7	9.2	- 0.043	- 0.097	- 0.061
240	6.9	14.5	9.4	- 0.037	- 0.083	- 0.052
250	6.9	15.1	9.6	- 0.030	- 0.068	- 0.042
260	6.9	15.5	9.8	- 0.023	- 0.052	- 0.033
270	6.9	15.7	9.8	- 0.016	- 0.037	- 0.023
280	6.9	15.9	9.9	- 0.009	- 0.021	- 0.013
290	6.9	16.1	10.0	- 0.002	- 0.005	- 0.003
293.15	6.9	16.2	10.0	0	0	0
300	6.8	16.2	9.9	0.005	0.011	0.007
400	5.5	16.5	9.2	0.066	0.174	0.102
500	4.8	17.4	9.0	0.117	0.343	0.192
600	4.6	18.7	9.3	0.163	0.524	0.283
700	5.0	20.5	10.2	0.211	0.721	0.381
800	5.9	22.9	11.6	0.265	0.939	0.490
900	7.4	25.7	13.5	0.331	1.184	0.616
950	8.4	27.3	14.7	0.371	1.318	0.687

Table 66g. Crystallographic properties of beta dysprosium

T K	*a* nm	*c* nm	*c*/*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
90.5	0.35840	0.56619	1.5798	0.35065	18.965	8568
95	0.35842	0.56616	1.5796	0.35065	18.966	8568
100	0.35844	0.56612	1.5794	0.35064	18.967	8568
110	0.35848	0.56602	1.5789	0.35062	18.968	8567
120	0.35853	0.56590	1.5784	0.35058	18.969	8567
130	0.35858	0.56575	1.5778	0.35054	18.969	8566
140	0.35863	0.56557	1.5770	0.35048	18.969	8567
150	0.35869	0.56534	1.5761	0.35041	18.967	8567
160	0.35875	0.56506	1.5751	0.35031	18.964	8569
170	0.35881	0.56470	1.5738	0.35019	18.959	8571
175	0.35885	0.56449	1.5731	0.35012	18.955	8573
176	0.35885	0.56444	1.5729	0.35011	18.954	8573
177	0.35886	0.56439	1.5727	0.35009	18.953	8574
178	0.35887	0.56435	1.5726	0.35007	18.952	8574
179	0.35887	0.56430	1.5724	0.35005	18.951	8575
180	0.35888	0.56424	1.5723	0.35003	18.950	8575
181	0.35888	0.56421	1.5721	0.35002	18.949	8575
182	0.35889	0.56421	1.5721	0.35002	18.950	8575
183	0.35889	0.56421	1.5721	0.35002	18.950	8575
184	0.35889	0.56421	1.5721	0.35002	18.950	8575
185	0.35889	0.56421	1.5721	0.35002	18.950	8575
190	0.35890	0.56422	1.5721	0.35003	18.952	8574
195	0.35892	0.56424	1.5721	0.35004	18.954	8573
200	0.35893	0.56426	1.5721	0.35006	18.956	8572
210	0.35895	0.56432	1.5721	0.35009	18.961	8570
220	0.35898	0.56439	1.5722	0.35013	18.966	8568
230	0.35900	0.56446	1.5723	0.35017	18.971	8566
240	0.35903	0.56454	1.5724	0.35021	18.976	8563
250	0.35905	0.56463	1.5725	0.35025	18.982	8561
260	0.35908	0.56471	1.5727	0.35029	18.987	8558
270	0.35910	0.56480	1.5728	0.35034	18.993	8556
280	0.35913	0.56489	1.5730	0.35038	18.998	8553
290	0.35915	0.56498	1.5731	0.35042	19.004	8551
293.15	0.35916	0.56501	1.5731	0.35044	19.006	8550
300	0.35918	0.56507	1.5732	0.35047	19.010	8548
400	0.35940	0.56599	1.5748	0.35092	19.064	8524
500	0.35958	0.56695	1.5767	0.35136	19.115	8501
600	0.35975	0.56797	1.5788	10.35183	19.168	8478
700	0.35992	0.56908	1.5812	0.35234	19.223	8453
800	0.36011	0.57032	1.5837	0.35291	19.286	8426
900	0.36035	0.57170	1.5865	0.35355	19.358	8394
950	0.36049	0.57246	1.5880	0.35390	19.399	8377

$$d1 = (a^2/3 + c^2/4)^{½} \qquad d2 = a$$

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67 HOLMIUM Ho

Atomic Weight: 164.930328 (7) (Meija 2017)

Structure: Hexagonal close-packed (hP2)

The melting point was selected by Gschneidner 1990 as 1747 K. In the low temperature region there is a first order Curie transformation at 17.8 K and a second order Néel transition at 132.26 K (Arblaster 2013).

67.1 Low temperature

Up to the Néel transition selected values are based on the sensitive dilatometric thermal expansion coefficients of White 1989 (2.5-140, 283 K). At the Curie temperature these include an increase in the *a* axis lattice parameter given by $\Delta a/a$ = 85 (5) x 10^{-6} and a decrease in the *c* axis by $\Delta c/c$ = 245 (15) x 10^{-6}. Also by dilatometry Steinitz et al. 1987 obtained 47 x 10^{-6} and 310 x 10^{-6} respectively in reasonable agreement. Between the Curie transition and the Néel transition there is the formation of an incommensurate helical antiferromagnetic state in which at certain turn angles are commensurate with the basal plane of the hexagonal structure. The commensurate structure is given by τ_m = M/N where the basal plane moment rotates by Mπ every N atomic planes. Using both elastic neutron diffraction and ultrasonic velocity measurements Bates et al. 1988 determined the following commensurate temperatures with values of τ_m given by Willis and Ali 1992:

Table 67a. Commensurate transition temperatures for holmium

τ_m	1/6	2/11	5/27	1/5	2/9
T K	17.8 (T_c)	19.8	24.5	40.5	97.4

It is uncertain as to the direct effect of the 2/11 transition being so close to the Curie temperature but White 1989 determined a second order transition at 17.3 K and the first order transition to occur at 19.5 K. To agree with the selected Curie temperature the transition at 17.3 K was ignored and values in the range 17.8 to 22 K were obtained by extrapolating a fit to values from 22 K to 30 K. From specific heat measurements Gerstein et al. 1957 determined the Curie temperature to be at 19.4 K while Lounasmaa and Sundström 1966 obtained a lower value of 17.5 K in agreement with Bates et al. 1988. The thermal expansion coefficients showed a maximum in the *a* axis direction at 100 K and a minimum in the *c* axis direction at an interpolated 94.6 K. These values agree so closely with the 97.4 K temperature that to within experimental accuracy it would appear that this may be a significant second order transition.

Between the Néel transition and 293.15 K the dilatometric measurements of Rhyne et al. 1967 (5-299 K) were combined with length change values derived from the lattice parameter values of Finkel' and Palatnik 1970 (76-300 K). In both cases the actual values were given by Touloukian et al. 1975 with a correction to the measurements of Finkel' and Palatnik 1970 in that the values tabulated by Touloukian et al. 1975 for the *a* axis appear to be for the *c* axis thermal expansion and vice versa. Because Rhyne et al. 1967

gave values along both the *a* axis and the equivalent *b* axis then the two sets of measurements were given approximately equal weight by doubling the weight given to the *a* axis values of Finkel' and Palatnik 1970. On the basis ± 100ε_T the accuracy of equation 67a is equal to ± 0.002 and for equation 67b ± 0.004:

$$\varepsilon_T a = 1.21214 \times 10^{-5} T - 2.54205 \times 10^{-8} T^2 + 2.80463 \times 10^{-11} T^3 - 2.07538 \times 10^{-3} \quad (67a)$$

$$\varepsilon_T c = -2.14684 \times 10^{-5} T + 1.35042 \times 10^{-7} T^2 - 1.52322 \times 10^{-10} T^3 - 1.47429 \times 10^{-3} \quad (67b)$$

The decrease in the *a* axis thermal expansion coefficient between the Curie temperature and room temperature confirms the trend given by White 1989. At the isolated temperature at 283 K White 1989 obtains lower values of $\alpha_a = 3.7 \times 10^{-6} K^{-1}$ and $\alpha_c = 16.8 \times 10^{-6} K^{-1}$.

On the basis 100Δε then from 20 K to the Néel transition the combined *a* and *b* axis values of Rhyne et al. 1967 trend from 0.006 high to 0.007 low while the *c* axis values scatter from initially 0.026 low to 0.002 low. The measurements of Finkel' and Palatnik 1970 scatter 0.008 to 0.045 high along the *a* axis and 0.088 to 0.003 low along the *c* axis. Length change values derived by Touloukian et al. 1975 from the lattice parameters of Darnell 1963 (8-299 K) trend from initially 0.11 high along the *a* axis and from initially 0.12 low along the *c* axis. Dilatometric measurements of Tindall et al. 1977 (4.2-150 K) were only shown in the form of small graphs.

67.2 High temperature

Length change values derived by Touloukian et al. 1975 from the lattice parameter measurements of Spedding et al. 1961 (295-981 K) were combined with the selected thermal expansion values at 293.15 K and fitted to the following equations which are assumed to represent the thermal expansion from 293.15 to 1000 K:

$$\varepsilon_T a = 3.34689 \times 10^{-6} T + 2.07168 \times 10^{-9} T^2 - 4.40296 \times 10^{-13} T^3 - 1.14808 \times 10^{-3} \quad (67c)$$

$$\varepsilon_T c = 1.75503 \times 10^{-5} T + 1.56155 \times 10^{-9} T^2 - 3.44587 \times 10^{-13} T^3 - 5.27038 \times 10^{-3} \quad (67d)$$

Table 67b. Lattice parameters of holmium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Notes
Spedding et al. 1956	RT	0.35775	0.56161	
Darnell et al. 1963	293	0.35830	0.56280	a
Harris and Raynor 1969	RT	0.35798	0.56275	
Finkel' and Palatnik 1970	293	0.35766	0.56143	b
Gupta and Anantharaman 1971	RT	0.35763	0.56177	
Spedding and Beaudry 1971	297	0.35780	0.56177	c
	Selected	0.35780 (2)	0.56177 (3)	

Notes for Table 67b

a. Values estimated by Donohue 1974 from a graphical representation

b. Values given by Touloukian et al. 1975

c. Temperature of measurement given by Gschneidner 1990

In agreement with Gschneidner 1990 the values determined by Spedding and Beaudry 1971 for electropolished wires are selected.

At 293.15 K for Ho: Density 8795 (1) kg m^{-3} Molar volume 18.753 (2) cm^3 mol^{-1}

67.3 Bulk properties of holmium

Direct density measurements of Basin and Stankus 1979 (293-1893 K) were assumed to be superseded by the later measurements of Stankus and Basin 1984 (293-1950 K) which were given in analytical form by Stankus and Khairulin 1991. However, these indicated that when converted to length change values that on the basis $100\varepsilon_T$ the differences from the selected values were not constant but increased with increasing temperature, the difference reaching 0.10 higher than the crystallographic average at 1000 K. Further, these measurements showed a distinct change in density at 1700 K which is due to impurity stabilization of a high temperature body-centered cubic phase. Stankus and Khairulin 2000 obtained a density value for the liquid at the melting point and a change in density on melting which indicated that the density of the solid at the melting point was 8327 kg m^{-3} which when compared to the selected density at 293.15 K leads to an equivalent length change at the melting point which, on the basis 100ε, is 1.84 which is much higher than the value obtained from a large extrapolation of the selected crystallographic properties. These differences suggest that currently there are no satisfactory thermal expansion values above 1000 K.

Table 67c. Crystallographic properties of holmium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 ε_T *a*	100 ε_T *c*	100 ε_T avr
0	0	0	0	- 0.422	0.436	- 0.136
5	0.48	- 0.88	0.02	- 0.422	0.436	- 0.136
10	3.94	- 7.97	- 0.02	- 0.421	0.434	- 0.136
15	10.6	- 23.5	- 0.77	- 0.417	0.426	- 0.136
17.8	15.8	- 30	- 0.53	- 0.414	0.418	- 0.136
17.8	30	- 102	- 14	- 0.405	0.394	- 0.139
18	29	- 99	- 14	- 0.405	0.392	- 0.139
20	23	- 76	- 10	- 0.400	0.375	- 0.142
25	13	- 38	- 4.0	- 0.391	0.347	- 0.145
30	11	- 26	- 1.0	- 0.386	0.333	- 0.146
35	12	- 25	- 0.3	- 0.380	0.320	- 0.147
40	13	- 26	0	- 0.374	0.308	- 0.147
50	17	- 30	1.3	- 0.359	0.280	- 0.146
60	21.5	- 37	2.0	- 0.340	0.246	- 0.145
70	27	- 47	2.3	- 0.316	0.204	- 0.143
80	35	- 60	3.3	- 0.285	0.151	- 0.140
90	41	- 75	2.3	- 0.247	0.084	- 0.137
94.6	43	- 83	1.0	- 0.228	0.047	- 0.136
100	43	- 80	2.0	- 0.205	0.003	- 0.136
110	40	- 75	1.7	- 0.163	- 0.075	- 0.134
120	35.5	- 70	0.3	- 0.125	- 0.147	- 0.133
130	31	- 66	- 1.3	- 0.092	- 0.215	- 0.133
132.26	29.5	- 65	- 2.0	- 0.085	- 0.230	- 0.133
132.26	6.87	6.25	6.67	- 0.085	- 0.230	- 0.133
140	6.65	7.38	6.90	- 0.080	- 0.224	- 0.128
150	6.39	8.75	7.18	- 0.073	- 0.216	- 0.121
160	6.14	10.0	7.44	- 0.067	- 0.207	- 0.114
170	5.91	11.2	7.68	- 0.061	- 0.196	- 0.106
180	5.70	12.3	7.91	- 0.055	- 0.185	- 0.098
190	5.50	13.3	8.11	- 0.050	- 0.172	- 0.090
200	5.32	14.2	8.30	- 0.044	- 0.158	- 0.082
210	5.16	15.1	8.46	- 0.039	- 0.143	- 0.074
220	5.01	15.8	8.61	- 0.034	- 0.128	- 0.065
230	4.88	16.4	8.73	- 0.029	- 0.112	- 0.057
240	4.77	17.0	8.84	- 0.024	- 0.095	- 0.048
250	4.67	17.4	8.93	- 0.020	- 0.078	- 0.039
260	4.59	17.8	9.00	- 0.015	- 0.060	- 0.030
270	4.53	18.1	9.05	- 0.010	- 0.042	- 0.021
280	4.48	18.3	9.08	- 0.006	- 0.024	- 0.012
290	4.45	18.4	9.09	- 0.004	- 0.006	- 0.003
293.15	4.45	18.4	9.09	0	0	0
300	4.47	18.4	9.11	0.003	0.013	0.006
400	4.79	18.6	9.39	0.049	0.198	0.099
500	5.08	18.8	9.65	0.099	0.385	0.194
600	5.35	18.9	9.88	0.151	0.575	0.292
700	5.59	19.1	10.1	0.206	0.766	0.393
800	5.80	19.2	10.3	0.263	0.959	0.495
900	5.99	19.3	10.4	0.322	1.154	0.599
1000	6.15	19.4	10.6	0.383	1.350	0.705

Table 67d. Crystallographic properties of holmium

T K	*a* nm	*c* nm	*c*/*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.35629	0.56422	1.5836	0.34914	18.676	8831
5	0.35629	0.56422	1.5836	0.34914	18.676	8831
10	0.35629	0.56421	1.5836	0.34914	18.676	8831
15	0.35630	0.56416	1.5834	0.34912	18.676	8831
17.8	0.35631	0.56412	1.5832	0.34911	18.676	8831
17.8	0.35635	0.56398	1.5827	0.34907	18.675	8832
18	0.35635	0.56397	1.5826	0.34906	18.675	8832
20	0.35637	0.56387	1.5823	0.34903	18.673	8832
25	0.35640	0.56372	1.5817	0.34898	18.672	8833
30	0.35641	0.56364	1.5814	0.34895	18.671	8834
35	0.35643	0.53657	1.5811	0.34893	18.671	8834
40	0.35646	0.56350	1.5808	0.34891	18.671	8834
50	0.35651	0.56334	1.5802	0.34866	18.671	8834
60	0.35658	0.56315	1.5793	0.34881	18.672	8833
70	0.35666	0.56292	1.5783	0.34874	18.673	8833
80	0.35677	0.56262	1.5770	0.34866	18.675	8832
90	0.35691	0.56224	1.5753	0.34855	18.676	8831
94.6	0.35698	0.56204	1.5744	0.34850	18.677	8831
100	0.35706	0.56179	1.5734	0.34842	18.677	8831
110	0.35721	0.56135	1.5715	0.34830	18.678	8830
120	0.35735	0.56094	1.5694	0.34818	18.679	8830
130	0.35747	0.56056	1.5682	0.34807	18.679	8830
132.26	0.35749	0.56048	1.5678	0.34804	18.678	8830
140	0.35751	0.56051	1.5678	0.34806	18.681	8829
150	0.35753	0.56055	1.5678	0.34809	18.685	8827
160	0.35755	0.56061	1.5679	0.34812	18.689	8825
170	0.35758	0.56067	1.5680	0.34815	18.694	8823
180	0.35760	0.56073	1.5681	0.34818	18.698	8821
190	0.35762	0.56081	1.5682	0.34822	18.703	8819
200	0.35764	0.56088	1.5683	0.34826	18.707	8816
210	0.35766	0.56096	1.5685	0.34830	18.712	8814
220	0.35767	0.56105	1.5686	0.34834	18.717	8812
230	0.35769	0.56114	1.5688	0.34838	18.721	8810
240	0.35771	0.56124	1.5690	0.34842	18.726	8807
250	0.35772	0.56133	1.5692	0.34847	18.731	8805
260	0.35774	0.56143	1.5694	0.34851	18.736	8803
270	0.35776	0.56155	1.5696	0.34856	18.742	8800
280	0.35777	0.56163	1.5698	0.34861	18.747	8798
290	0.35779	0.56174	1.5700	0.34865	18.752	8795
293.15	0.35780	0.56177	1.5701	0.34867	18.753	8795
300	0.35781	0.56184	1.5702	0.34870	18.757	8793
400	0.35797	0.56288	1.5724	0.34918	18.809	8769
500	0.35815	0.56393	1.5746	0.34966	18.863	8744
600	0.35834	0.56500	1.5767	0.35015	18.918	8718
700	0.35853	0.56607	1.5789	0.35056	18.975	8692
800	0.35874	0.56716	1.5810	0.35116	19.033	8666
900	0.35895	0.56825	1.5831	0.35168	19.092	8639
1000	0.35917	0.56935	1.8552	0.35219	19.152	8612

$$d1 = (a^2/3 + c^2/4)^{½} \qquad d2 = a$$

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68 ERBIUM Er

Atomic Weight: 167.259 (3) (Meija 2017)

Structure: Hexagonal close-packed (hP2)

The melting point was selected by Gschneidner 1990 as 1802 K. In the low temperature region there is a first order Curie transformation at 18.7 K, a weak first order Néel transition with ordering on cubic sites at 52 K, and a second order Néel transition with ordering on hexagonal sites at 87 K (Arblaster 2013).

68.1 Crystallographic properties above 90 K

Along the *a* axis lattice parameter measurements of Finkel' and Palatnik 1970 (72-293 K) were accepted. These were only shown graphically with actual data points as length change values given by Touloukian et al. 1975 and these were fitted to equation 68a. Above room temperature length change values derived by Touloukian et al. 1975 from the lattice parameter measurements of Spedding et al. 1961 (293-1190 K), but specifically in the range 332 to 949 K, were adjusted to the selected thermal expansion coefficient at 293.15 K and given as equation 68b. This was considered to be valid to 725 K but above this temperature the equation given by Touloukian et al. 1975 to cover the range 745 to 1200 K was accepted as equation 68c even though it did not appear to be based on actual experimental data:

$$90 - 293.15\ \text{K}: \quad \varepsilon_T a = 4.38967 \times 10^{-6} T - 1.10935 \times 10^{-10} T^2 + 5.12074 \times 10^{-12} T^3 - 1.40630 \times 10^{-3} \qquad (68a)$$

$$293.15 - 725\ \text{K}: \quad \varepsilon_T a = -9.67394 \times 10^{-8} T + 1.77583 \times 10^{-8} T^2 - 2.31106 \times 10^{-11} T^3 + 1.27340 \times 10^{-14} T^4 - 1.00957 \times 10^{-3} \qquad (68b)$$

$$725 - 1200\ \text{K}: \quad \varepsilon_T a = 8.13117 \times 10^{-6} T - 4.77250 \times 10^{-9} T^2 + 4.70000 \times 10^{-12} T^3 - 2.22229 \times 10^{-3} \qquad (68c)$$

For the *c* axis, in agreement with Touloukian et al. 1975 the lattice parameter values of Finkel' and Palatnik 1970 (79-300 K) are considered to be incorrect and were rejected. Therefore, length change values derived by Touloukian et al. 1975 from the c axis lattice parameter values of Spedding et al. (293-1190 K), but specifically in the range 423 to 899 K, were fitted to the quadratic equation 68f. In order to derive low temperature *c* axis values length change dilatometric values of Barson et al. 1953 (94-349 K) as given by Touloukian et al. 1975 were correlated as an average of three runs:

$$\varepsilon_T = 5.49408 \times 10^{-6} T + 1.27119 \times 10^{-8} T^2 - 1.39054 \times 10^{-11} T^3 - 2.35270 \times 10^{-3} \qquad (68d)$$

The *c* axis length change values were then obtained by subtracting the selected *a* axis values from the dilatometric values but the resulting fit of these values showed a maximum in the derived thermal expansion coefficient at 246 K. In order to overcome

this problem the high temperature equation 68f was extrapolated to 246 K and the equation representing the *c* axis values was adjusted until as equation 68e it conformed to a thermal expansion coefficient of $\alpha^* = 17.36 \times 10^{-6}$ K^{-1} at 246 K derived from equation 68f. This adjustment was allowed because equation 68d may give only an approximate value of average thermal expansion because it may be subject to anisotropic effects. The equation given by Touloukian et al. 1975 to show the *c* axis thermal expansion above 745 K showed peculiar behavior with a minimum in the derived thermal expansion equation at 771 K, while above 900 K the thermal expansion coefficient rose rapidly and was therefore inconsistent with the behavior up to that temperature. On these grounds, equation 68f was extrapolated to 1200 K:

$$90 - 246 \text{ K:} \quad \varepsilon_T c = 7.77646 \times 10^{-6} T + 3.89004 \times 10^{-8} T^2 - 5.26473 \times 10^{-11} T^3 - 4.29634 \times 10^{-3} \qquad (68e)$$

$$246 - 1200 \text{ K:} \quad \varepsilon_T c = 1.60016 \times 10^{-6} T + 2.75261 \times 10^{-9} T^2 - 4.92741 \times 10^{-3} \qquad (68f)$$

Table 68a. Lattice parameters of erbium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Notes
Spedding et al. 1956	RT	0.35590	0.55877	
Darnell 1963	293	0.35634	0.55997	a
Norman et al. 1966, 1967	295	0.35612	0.55930	
Finkel' and Palatnik 1970	293	0.35552	0.55839	a
Gupta and Anantharaman 1971	RT	0.35592	0.55923	
Spedding and Beaudry 1971	297	0.35593	0.55849	b
	Selected	0.35593 (2)	0.55849 (3)	

Notes for Table 68a

a. Values given by Touloukian et al. 1975

b. Temperature of measurement given by Gschneidner 1990

In agreement with Gschneidner 1990 the values determined by Spedding and Beaudry 1971 for electropolished wires are selected.

At 293.15 K: Density 9065 (1) kg m^{-3} Molar volume 18.450 (2) cm^3 mol^{-1}.

68.2 Crystallographic properties below 90 K

Neutron diffraction measurements of Habenschuss et al. 1974 (6-84 K) were unfortunately only shown graphically but in combination with higher temperature values then values can be discerned from this graph. These confirm that the upper Nèel transition is second order but the lower Nèel transition, although supposedly weak first order, was observed only as a sharp change in slope of the thermal expansion coefficient. The Curie temperature was confirmed as being first order. With rising temperature there was an estimated 0.0003_4 nm increase in the *a* axis lattice parameter and a decrease of

0.0022_1 nm decrease in the *c* axis value. These values are accepted but the graphical representation of Tadakuma et al. 1995 (13-22 K) suggests a decrease of 0.0019_7 nm in the c axis lattice parameter at the Curie transition.

In order to correlate the isolated values of Habenschuss et al. 1974 with the higher temperature values, then for the *a* axis it is assumed that at 18.7 K $\alpha^* = 0\ K^{-1}$ and at 90 K $\alpha^* = 4.50 \times 10^{-6}\ K^{-1}$ and $\varepsilon_a = -1.008 \times 10^{-3}$. These values were fitted to equation 68g while over the range 0 to 18.7 K it is assumed that $\alpha^* = 0\ K^{-1}$ and $\varepsilon_a = -2.123 \times 10^{-3}$.

$$18.7 - 90\ K: \varepsilon_T a = -1.18022 \times 10^{-6} T + 3.15568 \times 10^{-8} T^2 - 1.15737 \times 10^{-3} \quad (68g)$$

For the *c* axis it is assumed that at 52 K $\alpha^* = 0\ K^{-1}$ and at 90 K $\alpha^* = 13.50 \times 10^{-6}\ K^{-1}$ and $\varepsilon_c = -3.320 \times 10^{-3}$ and these values were fitted to equation 68i. For the range 18.7 to 52 K values estimated from the graph were combined with the length change value derived from equation 68i at 52 K and fitted to equation 68h. Over the range 0 to 18.7 K it is assumed that $\alpha^* = 0\ K^{-1}$ and $\varepsilon_c = +2.052 \times 10^{-3}$.

$$18.7 - 52\ K: \varepsilon_T c = -5.78697 \times 10^{-5} T + 1.63104 \times 10^{-6} T^2 - 2.67383 \times 10^{-8} T^3 - 1.21800 \times 10^{-3} \quad (68h)$$

$$52 - 90\ K: \quad \varepsilon_T c = -1.84737 \times 10^{-5} T + 1.77632 \times 10^{-7} T^2 - 3.09619 \times 10^{-3} \quad (68i)$$

The isolation of the measurements of Habenschuss et al. 1974 can be judged from the fact that the estimated values at 10 K of 0.3541 nm along the *a* axis and 0.5584 nm along the *c* axis differ significantly from the selected values of 0.3552 nm and 0.5596 nm respectively. However, the c axis lattice parameters determined by Tadakuma et al. 1995 at the Curie transition of 0.5592 nm below the transition and 0.5573 nm above are in satisfactory agreement with the selected values of 0.5596 nm and 0.5574 nm.

Between the Curie transition and the lower Nèel transition the structure is in an incommensurate helical antiferromagnetic state in which various turn angles are commensurate with the basal plane of the hexagonal structure. Eight such transitions occur for erbium (Arblaster 2013) and although the transitions are generally found to be first order and should be detectable by sensitive dilatometry no quantitative values have been reported.

68.3 Comparison with other low temperature values

Lattice parameter measurements of Banister et al. 1954 (43-301 K) were converted to length change values and on the basis $100\Delta\varepsilon$ the *a* axis values average 0.12 high at 65 K and above while the *c* axis values scatter 0.043 low to 0.087 high. Lattice parameter measurements of Darnell 1963 (7-297 K) were only shown graphically with actual values given as length change values by Touloukian et al. 1975. The *a* axis values are initially on average 0.041 low below 19 K, trending to 0.055 high at 61 K and then to an average of 0.022 high above 150 K. For the *c* axis, values are initially an average of 0.093 low below 19 K, averaging 0.059 low over the range 20 to 40 K and then trending to an

average 0.039 low over the range 90 to 240 K. The rejected *c* axis values of Finkel' and Palatnik 1970 trend from 0.069 low at 90 K. Dilatometric measurements of Petrenko et al. 1975 (2-300 K) are only given in the form of a small graph.

68.4 Bulk properties of erbium

Dilatometric measurements of Barson et al. 1957 (293-1207 K) were shown only graphically with actual data points given by Touloukian et al. 1975. These show a trend to an average of 0.066 low at 1000 K and above. Direct density measurements of Khairulin and Stankus 1988 (293-1950 K), as discussed by Stankus and Khairulin 1991, were assumed to be superseded by the later measurements of Stankus et al. 1995-1996 (293-2000 K). However, these indicated that when converted to length change values then on the basis 100ε the differences from the selected values were not constant but increased with increasing temperature, the difference reaching 0.16 lower than the crystallographic average at 1200 K. Because of these differences it can be considered that currently there are no satisfactory measurements of thermal expansion above 1200 K.

Table 68b. Crystallographic properties of erbium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 ε_T *a*	100 ε_T *c*	100 ε_T avr
0 – 18.7	0	0	0	- 0.212	0.205	- 0.073
18.7	0	- 25	- 8.3	- 0.117	- 0.190	- 0.141
20	0.08	- 25	- 8.3	- 0.117	- 0.194	- 0.142
25	0.40	- 27	- 8.6	- 0.117	- 0.206	- 0.147
30	0.71	- 32	- 10.3	- 0.116	- 0.221	- 0.151
35	1.03	- 42	- 13.3	- 0.116	- 0.239	- 0.157
40	1.35	- 56	- 17.7	- 0.115	- 0.263	- 0.165
45	1.66	- 74	- 23.5	- 0.115	- 0.296	- 0.175
50	1.98	- 96	- 30.6	- 0.114	- 0.338	- 0.188
52	2.10	- 106	- 33.8	- 0.113	- 0.358	- 0.195
52	2.10	0	1.40	- 0.113	- 0.358	- 0.195
60	2.61	2.85	2.69	- 0.111	- 0.357	- 0.193
70	3.24	6.42	4.30	- 0.109	- 0.352	- 0.190
80	3.87	9.98	5.91	- 0.105	- 0.344	- 0.185
90	4.50	13.5	7.52	- 0.101	- 0.332	- 0.178
100	4.53	14.0	7.69	- 0.096	- 0.318	- 0.170
110	4.56	14.5	7.86	- 0.092	- 0.304	- 0.163
120	4.59	14.9	8.02	- 0.087	- 0.289	- 0.155
130	4.62	15.3	8.17	- 0.083	- 0.274	- 0.147
140	4.66	15.6	8.31	- 0.078	- 0.259	- 0.138
150	4.71	15.9	8.45	- 0.073	- 0.243	- 0.130
160	4.75	16.2	8.57	- 0.069	- 0.227	- 0.121
170	4.80	16.5	8.69	- 0.064	- 0.211	- 0.113
180	4.85	16.7	8.80	- 0.059	- 0.194	- 0.104
190	4.90	16.9	8.90	- 0.054	- 0.178	- 0.095
200	4.96	17.0	8.99	- 0.049	- 0.161	- 0.086
210	5.02	17.2	9.07	- 0.044	- 0.144	- 0.077
220	5.09	17.3	9.15	- 0.039	- 0.126	- 0.068
230	5.15	17.3	9.21	- 0.034	- 0.109	- 0.059
240	5.22	17.4	9.27	- 0.029	- 0.092	- 0.050
250	5.30	17.4	9.33	- 0.024	- 0.075	- 0.041
260	5.37	17.4	9.39	- 0.018	- 0.058	- 0.032
270	5.45	17.5	9.47	- 0.013	- 0.041	- 0.022
280	5.53	17.5	9.54	- 0.007	- 0.023	- 0.013
290	5.62	17.6	9.61	- 0.002	- 0.006	- 0.003
293.15	5.64	17.6	9.63	0	0	0
300	5.69	17.7	9.68	0.004	0.012	0.007
400	6.27	18.2	10.2	0.064	0.191	0.106
500	6.62	18.7	10.6	0.128	0.376	0.211
600	7.24	19.2	11.2	0.198	0.566	0.321
700	8.24	19.7	12.1	0.275	0.762	0.437
800	9.48	20.2	13.1	0.364	0.964	0.564
900	10.9	20.7	14.2	0.466	1.170	0.701
1000	12.6	21.2	15.5	0.584	1.383	0.850
1100	14.6	21.7	17.0	0.720	1.600	1.014
1200	16.9	22.2	18.6	0.878	1.824	1.194

Table 68c. Crystallographic properties of erbium

T K	*a* nm	*c* nm	*c*/*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0 – 18.7	0.35517	0.55964	1.5757	0.34691	18.409	9086
18.7	0.35551	0.55743	1.5680	0.34614	18.372	9104
20	0.35551	0.55741	1.5679	0.34613	18.371	9104
25	0.35551	0.55734	1.5677	0.34610	18.369	9105
30	0.35552	0.55726	1.5675	0.34607	18.367	9107
35	0.35552	0.55716	1.5672	0.34603	18.363	9108
40	0.35552	0.55702	1.5668	0.34598	18.359	9110
45	0.35552	0.55684	1.5663	0.34591	18.353	9113
50	0.35553	0.55661	1.5656	0.34581	18.346	9117
52	0.35553	0.55650	1.5653	0.34577	18.343	9119
52	0.35553	0.55650	1.5653	0.34577	18.343	9119
60	0.35553	0.55650	1.5653	0.34577	18.343	9118
70	0.35554	0.55653	1.5653	0.34579	18.345	9117
80	0.35556	0.55658	1.5654	0.34581	18.348	9116
90	0.35557	0.55664	1.5655	0.34584	18.352	9114
100	0.35559	0.55672	1.5658	0.34588	18.356	9112
110	0.35560	0.55680	1.5658	0.34591	18.360	9110
120	0.35562	0.55688	1.5659	0.34595	18.365	9108
130	0.35564	0.55696	1.5661	0.34599	18.369	9105
140	0.35565	0.55705	1.5663	0.34603	18.374	9103
150	0.35567	0.55714	1.5664	0.34607	18.378	9101
160	0.35569	0.55723	1.5666	0.34612	18.383	9099
170	0.35570	0.55732	1.5668	0.34616	18.388	9096
180	0.35572	0.55741	1.5670	0.34620	18.393	9094
190	0.35574	0.55750	1.5672	0.34624	18.397	9091
200	0.35575	0.55760	1.5674	0.34629	18.402	9089
210	0.35577	0.55769	1.5676	0.34633	18.407	9087
220	0.35579	0.55779	1.5677	0.34638	18.412	9084
230	0.35581	0.55789	1.5679	0.34642	18.418	9082
240	0.35583	0.55798	1.5681	0.34647	18.423	9079
250	0.35585	0.55807	1.5683	0.34651	18.428	9077
260	0.35587	0.55817	1.5685	0.34656	18.433	9074
270	0.35588	0.55827	1.5687	0.34660	18.438	9071
280	0.35590	0.55837	1.5689	0.34665	18.443	9069
290	0.35592	0.55846	1.5691	0.34670	18.449	9066
293.15	0.35593	0.55849	1.5691	0.34671	18.450	9065
300	0.35594	0.55856	1.5692	0.34674	18.454	9064
400	0.35616	0.55956	1.5711	0.34722	18.509	9037
500	0.35639	0.56060	1.5730	0.34771	18.567	9008
600	0.35664	0.56166	1.5749	0.34823	18.628	8979
700	0.35691	0.56275	1.5767	0.34876	18.693	8948
800	0.35722	0.56388	1.5785	0.34932	18.764	8914
900	0.35759	0.56503	1.5801	0.34991	18.840	8878
1000	0.35801	0.56622	1.5816	0.35053	18.924	8838
1100	0.35849	0.56743	1.5828	0.35119	19.016	8795
1200	0.35906	0.56868	1.5838	0.35189	19.118	8749

$$d1 = (a^2/3 + c^2/4)^{½} \qquad d2 = a$$

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69 THULIUM Tm

Atomic Weight: 168.934218 (6) (Meija 2017)

Structure: Hexagonal close-packed (hP2)

The melting point was selected by Gschneidner 1990 as 1818 K. In the low temperature region there is a first order Curie transition at 32.6 K and a second order Néel transition at 56.6 K (Arblaster 2013).

69.1 Low temperature

The selected transition temperatures were determined using calorimetry by Berezovsky et al. 1991. Lattice parameter measurements of Bulatov and Dolzhenko 1988 (4.2-300 K) were shown only in the form of a graph. However, it was possible to estimate values from the graph which suggested in the room temperature region that the *a* axis value was 0.00044 nm higher than the selected value and the *c* axis value 0.00081 nm higher which suggests a significant contamination, possible with hydrogen, which is contrary to the suggestion of using high purity samples. However, derived length change values are assumed to be independent of the original lattice parameters values. At the Curie temperature the *a* axis is only effected by a change in thermal expansion but the *c* axis shows a discontinuity which is estimated as a jump of 0.00017 nm. The *a* axis length change values vary little with temperature and have been determined with sufficient precision to derive a thermal expansion coefficient of 3.6×10^{-6} K^{-1} in the room temperature region. For the *c* axis the derived thermal expansion values decrease rapidly from 25×10^{-6} K^{-1} at 200 K to 13×10^{-6} K^{-1} at 300 K which is considered to be abnormal behavior. Therefore, the *a* axis values were accepted but the *c* axis values were only accepted below 245 K because high temperature values were extrapolated to this temperature in order to match length change values and remove the abnormal thermal expansion behavior. On the basis $\pm 100\varepsilon$ the low temperature length change values are probably accurate to better than ± 0.005 while the *c* axis values are probably accurate to ± 0.02 at the lowest temperatures improving to value better than ± 0.01 above 200 K.

On the basis $100\Delta\varepsilon$, length change values derived by Touloukian et al. 1975 from the lattice parameter measurements of Singh et al. 1971 (100-300 K) initially show marked deviations from the selected values being 0.14 low along the *a* axis and 0.31 high along the *c* axis before converging towards the selected values. Dilatometric measurements of Petrenko and Popov 1973 (2-300 K) were also only shown in the form of a small graph but did confirm the first order transition behavior at the Curie temperature and the second order transition behavior at the Néel temperature.

69.2 High temperature

Length change values for the *c* axis derived by Touloukian et al. 1975 from the lattice parameter measurements of Spedding et al. 1961 (293-1126 K), but specifically in the range 671 to 1126 K, were fitted to equation 69b and were considered to be not only representative of the thermal expansion from 293.15 to 1100 K but was also extrapolated to 245 K in the low temperature region for the reasons given above. For the *a* axis, compatibility with the low temperature data was only achieved by combining the selected thermal expansion coefficient at 293.15 K with length change values at 1000, 1050 and 1100 K derived from equation 69e to derived equation 69a. This equation showed a minimum in the derived thermal expansion coefficient at 801 K which is considered to be unsatisfactory behavior. However, from 293.15 K to 1100 K equations 69a and 69b were used to represent the thermal expansion:

$$\varepsilon_T\, a = -5.66092 \times 10^{-6}\, T + 1.93778 \times 10^{-8}\, T^2 - 8.06895 \times 10^{-12}\, T^3 - 1.97509 \times 10^{-4} \quad (69a)$$

$$\varepsilon_T\, c = 2.00553 \times 10^{-5}\, T + 4.43327 \times 10^{-10}\, T^2 - 5.91731 \times 10^{-3} \quad (69b)$$

In view of the fact that values were derived either from the graphically shown measurements of Bulatov and Dolzhenko 1988 or the low accuracy lattice parameter values of Spedding et al. 1961 then apart from the room temperature values no other thermal expansion values were derived.

On the basis $100\Delta\varepsilon$ length change values derived by Touloukian et al. 1975 from the lattice parameter measurements of Spedding et al. 1961 trend along the *a* axis from a maximum deviation of 0.11 high at 414 K and then converge to the selected values while for the *c* axis there is only a maximum deviation of 0.035 high at 505 K.

Table 69a. Lattice parameters of thulium at 293.15 K

Values were corrected to 293.15 K using selected room temperature thermal expansion values of $\alpha_a = 3.6 \times 10^{-6}\ K^{-1}$ and $\alpha_c = 20.3 \times 10^{-6}\ K^{-1}$ derived from equations 69a and 69b respectively.

References	Original Temperature K	*a* nm	*c* nm	Notes
Spedding et al. 1956	RT	0.35377	0.55549	
Harris and Raynor 1969	RT	0.35428	0.55711	
Singh et al. 1971	293	0.35169	0.55735	a
Spedding and Beaudry 1971	297	0.35377	0.55539	b
	Selected	0.35377 (4)	0.55539 (2)	

Notes for Table 69a

a. Values given by Touloukian et al. 1975

b. Temperature of measurement given by Gschneidner 1990

In agreement with Gschneidner 1990 the values determined by Spedding and Beaudry 1971 for electropolished wires are selected.

At 293.15 K for Tm: Density 9320 (2) kg m^{-3} Molar volume 18.126 (4) cm^3 mol^{-1}

69.3 Bulk properties of thulium

Length change values derived from the direct density measurements of Stankus and Khairulin 1987 (293-1950 K), as summarized by Stankus and Khairulin 1991, agree very closely with the average selected length change value at 1100 K and can be considered to be a natural extension up to the melting point. The length change value derived from the bulk measurements at 1200 K was combined with an extrapolation of the *c*/*a* ratio to this temperature in order to derive the selected properties, but further extrapolation of the c/*a* ratio was not justified in view of the highly tentative nature of equations 69a and 69b. Length change values derived from the high temperature density measurements were used to represent bulk properties up to the melting point as derived in Table 69c.

69.4 Comments on the measurements of Spedding et al. 1961

Length change values were derived by Touloukian et al. 1975 from the lattice parameter measurements of Spedding et al. 1961 (293-1126 K). These values were fitted to the following equations by considering *a* axis values only above 459 K and *c* axis only above 671 K. After rejecting the a axis value at 671 K the measurements were fitted to the following equations as length change values:

$$\varepsilon_T a = 1.18991 \times 10^{-5} T - 5.09537 \times 10^{-9} T^2 + 2.15267 \times 10^{-12} T^3 - 3.10456 \times 10^{-3} \quad (69e)$$

$$\varepsilon_T c = 2.49618 \times 10^{-5} T - 7.17114 \times 10^{-9} T^2 + 3.54569 \times 10^{-12} T^3 - 6.79061 \times 10^{-3} \quad (69f)$$

Equation 69e showed a minimum in the derived thermal expansion coefficient at 789 K and equation 69f at 674 K. In order to overcome the abnormal behavior for the *c* axis the data was refitted to quadratic equation 69b which showed a normal behavior.

Table 69b. Crystallographic properties of thulium

T K	100 ε_T *a*	100 ε_T *c*	100 ε_T avr
0	- 0.048	- 0.854	- 0.317
32	- 0.048	- 0.854	- 0.317
32	- 0.048	- 0.823	- 0.307
40	- 0.052	- 0.767	- 0.291
50	- 0.055	- 0.698	- 0.270
60	- 0.058	- 0.645	- 0.254
70	- 0.060	- 0.592	- 0.238
80	- 0.062	- 0.543	- 0.222
90	- 0.063	- 0.508	- 0.211
100	- 0.063	- 0.474	- 0.200
110	- 0.062	- 0.442	- 0.189
120	- 0.061	- 0.412	- 0.178
130	- 0.059	- 0.383	- 0.167
140	- 0.056	- 0.355	- 0.156
150	- 0.052	- 0.329	- 0.145
160	- 0.048	- 0.304	- 0.134
170	- 0.045	- 0.281	- 0.123
180	- 0.041	- 0.259	- 0.114
190	- 0.037	- 0.232	- 0.102
200	- 0.034	- 0.206	- 0.091
210	- 0.030	- 0.180	- 0.080
220	- 0.026	- 0.156	- 0.070
230	- 0.023	- 0.132	- 0.059
240	- 0.019	- 0.109	- 0.049
250	- 0.016	- 0.088	- 0.040
260	- 0.012	- 0.067	- 0.030
270	- 0.008	- 0.047	- 0.021
280	- 0.005	- 0.027	- 0.012
290	- 0.001	- 0.006	- 0.007
293.15	0	0	0
300	0.003	0.014	0.006
400	0.052	0.218	0.107
500	0.120	0.422	0.221
600	0.203	0.628	0.345
700	0.296	0.834	0.475
800	0.394	1.041	0.609
900	0.492	1.249	0.744
1000	0.585	1.458	0.875
1100	0.668	1.668	1.000
1200	0.768	1.890	1.141

Table 69c. Crystallographic properties of thulium

T K	*a* nm	*c* nm	*c*/*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.35360	0.55065	1.5573	0.34276	17.954	9410
32	0.35360	0.55065	1.5573	0.34276	17.954	9410
32	0.35360	0.55082	1.5577	0.34282	17.959	9407
40	0.35359	0.55113	1.5587	0.34294	17.968	9402
50	0.35357	0.55151	1.5598	0.34309	17.979	9396
60	0.35356	0.55181	1.5607	0.34321	17.988	9392
70	0.35356	0.55210	1.5616	0.34332	17.996	9387
80	0.35355	0.55237	0.5624	0.34343	18.005	9383
90	0.35355	0.55257	0.5629	0.34351	18.011	9379
100	0.35355	0.55276	1.5635	0.34358	18.017	9376
110	0.35355	0.55293	1.5639	0.34366	18.023	9373
120	0.35356	0.55310	1.5644	0.34373	18.029	9370
130	0.35356	0.55326	1.5648	0.34379	18.035	9367
140	0.35357	0.55342	1.5652	0.34386	18.041	9364
150	0.35358	0.55356	1.5656	0.34392	18.047	9361
160	0.35360	0.55370	1.5659	0.34398	18.053	9358
170	0.35361	0.55383	1.5662	0.34404	18.059	9355
180	0.35363	0.55395	1.5665	0.34409	18.064	9352
190	0.35364	0.55410	1.5669	0.34416	18.070	9349
200	0.35365	0.55425	1.5672	0.34422	18.076	9346
210	0.35366	0.55439	1.5676	0.34428	18.082	9343
220	0.35368	0.55453	1.5679	0.34434	18.088	9340
230	0.35369	0.55466	1.5682	0.34440	18.093	9337
240	0.35370	0.55479	1.5685	0.34445	18.099	9334
250	0.35371	0.55490	1.5688	0.34451	18.104	9331
260	0.35373	0.55502	1.5691	0.34456	18.109	9329
270	0.35374	0.55513	1.5693	0.34461	18.114	9326
280	0.35375	0.55524	1.5696	0.34466	18.119	9324
290	0.35377	0.55535	1.5698	0.34470	18.124	9321
293.15	0.35377	0.55539	1.5699	0.34472	18.126	9320
300	0.35378	0.55547	1.5701	0.34475	18.129	9318
400	0.35395	0.55660	1.5725	0.34527	18.184	9290
500	0.35420	0.55773	1.5747	0.34581	18.246	9259
600	0.35449	0.55888	1.5766	0.34637	18.314	9225
700	0.35482	0.56002	1.5783	0.34695	18.385	9189
800	0.35516	0.56117	1.5800	0.34753	18.459	9152
900	0.35551	0.52623	1.5818	0.34811	18.533	9115
1000	0.35584	0.56349	1.5836	0.34869	18.605	9080
1100	0.35613	0.56465	1.5855	0.34926	18.675	9046
1200	0.35649	0.56589	1.5874	0.34988	18.753	9008

$$d1 = (a^2/3 + c^2/4)^{1/2} \quad d2 = a$$

Table 69d. Bulk properties of thulium

T K	100 ε_T	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1200	1.141	18.753	9008
1300	1.283	18.832	8970
1400	1.429	18.914	8932
1500	1.579	18.998	8892
1600	1.732	19.084	8852
1700	1.888	19.172	8812
1800	2.049	19.263	8770
1818	2.078	19.279	8763

This Table is considered to be identical to Tables 69b and 69c at 1200 K and below.

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70 YTTERBIUM Yb

Atomic Weight: 173.045 (10) (Meija 2017)

Allotropy: Alpha phase: Hexagonal close-packed (hP2)
Beta phase: Face-centered cubic (cF4)
Gamma phase: Body-cented cubic (cI2)

For pure ytterbium Kayser 1970 showed that the alpha-beta transformation was martensitic with the transformation on cooling starting at 260 K and the reverse on heating at 280 K so an "equilibrium" transformation temperature of 270 K was selected. Gschneidner 1990 selected 1068 K for the beta-gamma transformation temperature and 1092 K for the melting point.

For hydrogen contaminated samples, Spedding et al. 1961 found that there was a transformation to an hexagonal close-packed structure (hP2) between 533 and 993 K. A similar behavior was observed in the divalent metals calcium and strontium which Peterson and Fattore 1961 and Peterson and Colburn 1966 respectively again showed was due to hydrogen. While this would appear to be definate proof as to the origin of the intermediate phase, subsequent electrical resistivity and other measurements by Hurd and Alderson 1973, Vedernikov et al. 1974, 1977 and Zinov'ov et al. 1975 suggested that this phase was actually genuine and direct density measurements of Stankus and Basin 1986 also appeared to indicate the existence of the phase between 615 and 990 K. However, there was a general lack of chemical composition details whereas for the pure metal Beaudry and Gschneidner 1974 showed only the existence of the beta and gamma phases but for samples saturated with hydrogen they reproduced the transition temperatures reported by Hurd and Alderson 1973. Further, electrical resistivity measurements on pure samples by Güntherodt et al. 1976 and Ten Cate et al. 1980 established there there were no anomalies corresponding to the intermediate phase.

70.1 Alpha ytterbium: Hexagonal close-packed (hP2): 0 K to 270 K

Bucher et al. 1970 initially determined the structure while Kayser 1970, 1971 determined precision lattice parameter measurements at 296 K. In the absence of thermal expansion values correction to 293.15 K was made by assuming that the thermal expansion coefficients for both the alpha and beta phases are the same while the *c*/*a* ratio is unaltered over the very narrow temperature range from 296 K to 293.15 K. On this basis derived crystallographic properties at 293.15 K are lattice parameter values *a* 0.38798 (2) nm *c* 0.63858 (2) nm while the derived density is 6904 (2) kg m^{-3} and the molar volume 25.066 (7) cm^3 mol^{-1}.

It is noted that thermal expansion coefficients, presumably for the alpha phase, were determined in isolation by Andres 1963 (1.69-10 K).

70.2 Beta ytterbium: Face-centered cubic: 270 K to 1068 K

In agreement with Touloukian et al. 1975, the dilatometric measurements of Barson et al. 1957 (298-1047 K) were selected. These were shown only graphically with actual data points given by Touloukian et al. 1975. Selecting measurements from 540 to 994 K with increasing temperature and 735 to 910 K with decreasing temperature then on the basis $\pm 100\varepsilon_T$ the overall accuracy is ± 0.010:

$$\varepsilon_T = 1.95175 \times 10^{-5} T + 8.14287 \times 10^{-9} T^2 + 6.60779 \times 10^{-14} T^3 - 6.42299 \times 10^{-3} \quad (70a)$$

On the basis $100\Delta\varepsilon$ length change values derived by Touloukian et al. 1975 from the lattice parameter measurements of Spedding et al. 1961 (296-849 K) trend to 0.17 high. Length change values derived from the direct density measurements of Stankus and Basin 1986, as summarized by Stankus and Khairulin 1991, over the range 293 to 615 K, described as being the face-centered cubic phase, trend to 0.12 low while measurements over the range 615 to 990 K, described as being the hexagonal close-packed phase, trend from 0.30 high to 0.088 high.

Table 70a. Lattice parameter of beta ytterbium at 293.15 K

References	Original Temperature K	*a* nm	Notes
Spedding et al. 1956	RT	0.54865	
Evans and Raynor 1961	RT	0.54864	
Harris and Raynor 1969	RT	0.54850	
Kayser 1970, 1971	296	0.54846	
Beaudry and Palmer 1974	297	0.54846	a
	Selected	0.54846 (5)	

Notes for Table 70b

a. Temperature of measurement given by Gschneidner 1990

In agreement with Gschneidner 1990 the value obtained by Beaudry and Palmer 1974 for electropolished wires was selected although it is noted that the value of Kayser 1970, 1971 is identical.

At 293.15 K: Density 6967 (2) kg m^{-3} Molar volume 24.839 (7) cm^3 mol^{-1}.

At 293.15 K the molar volume of the alpha phase is 0.227 (4) cm^3 mol^{-1} or 0.91 (2) % greater than that of the beta phase.

70.3 Gamma ytterbium: Body-centered cubic: 1068 K to 1092 K

From the entropy of transformation of 1.795 J mol^{-1} K^{-1} selected by Arblaster 2013, and the initial slope of the transformation curve of – 0.16 K MPa^{-1} determined by Jayaraman 1964, then the molar volume contraction as determined by the Clausius Clapeyron equation is 0.287 cm^3 mol^{-1} (1.08 %) leading to a molar volume of the gamma phase as

26.367 cm^3 mol^{-1} at 1068 K. Direct density measurements of Stankus and Basin 1983 (990 to 1098 K in the gamma region), as summarized by Stankus and Khairulin 1991, were determined in isolation but lead to a molar volume at 1068 K which was 0.285 cm^3 mol^{-1} higher than the above value. If the derived molar volume determined by the direct density technique at 1092 K is reduced by this amount then derived lattice parameters and length change values over the range 1068 to 1092 K are determined as:

$$a \text{ (nm)} = 1.63720 \times 10^{-5} T + 0.426579 \quad (70b)$$

$$\varepsilon_T = 3.76097 \times 10^{-5} T - 2.00637 \times 10^{-2} \quad (70c)$$

The derived thermal expansion coefficient is 36.9 x 10^{-6} K^{-1}. The calculated lattice parameter value of 0.4437 nm at 1047 K is in excellent agreement with the experimental value of 0.444 nm determined by Spedding et al. 1961.

Table 70b. Crystallographic properties of alpha ytterbium

T K	*a* nm	*c* nm	*c*/*a*	*d*1 nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
293.15	0.38798	0.63858	1.6459	0.39003	25.066	6904

$$d1 = (a^2/3 + c^2/4)^{1/2} \quad d2 = a$$

Table 70c. Crystallographic properties of beta ytterbium

T K	α x 10^6 K^{-1}	100 ε_T	*a* nm	*d* nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
270	23.94	- 0.056	0.54815	0.37860	24.797	6979
280	24.10	- 0.032	0.54829	0.38770	24.815	6974
290	24.26	- 0.008	0.54842	0.38779	24.833	6969
293.15	24.31	0	0.54846	0.38782	24.839	6967
300	24.42	0.017	0.54855	0.38788	24.851	6964
400	25.99	0.269	0.54994	0.38886	25.040	6911
500	27.56	0.538	0.55141	0.38991	25.242	6856
600	29.12	0.823	0.55298	0.39101	25.457	6798
700	30.67	1.125	0.55463	0.39218	25.686	6737
800	32.21	1.444	0.55638	0.39342	25.930	6674
900	33.74	1.779	0.55822	0.39472	26.188	6608
1000	35.25	2.130	0.56014	0.39608	26.476	6540
1068	36.27	2.379	0.56151	0.39705	26.654	6492

$$d = a/\sqrt{2}$$

Table 70d. Crystallographic properties of gamma ytterbium

T K	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1068	2.010	0.4441	0.3846	26.37	6563
1092	2.101	0.4445	0.3849	26.44	6546

$$d = \sqrt{3}a/2$$

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71 LUTETIUM Lu

Atomic Weight: 174.9668 (1) (Meija 2017)

Structure: Hexagonal close-packed (hP2)

The melting point was selected by Gschneidner 1990 as 1936 K.

71.1 Low temperature

The dilatometric thermal expansion coefficients of very high purity single crystals as determined by Swenson 1996 (1-300 K) were selected. The results were given in the form of equations and the *c* axis value showed a maximum at 280 K. Earlier lattice parameter measurements by Singh et al. 1971 (90-301 K), on commercial purity material, showed a different behavior with a negative thermal expansion coefficient along the *a* axis from 90 to 209 K so that on the basis 100Δε the length change value at 90 K was 0.267 higher than the selected value. The *c* axis showed more conventional behavior but was still 0.065 higher than the selected value at 90 K. The dilatometric measurements of Tonnies et al. 1971 (4.2-301 K), also on high purity single crystals, surprisingly showed a different behavior along the *a* axis compared to the measurements of Swenson 1996 with a maximum in the derived thermal expansion coefficient of 8.1 x 10^{-6} K^{-1} at 130 K falling to 4.8 x 10^{-6} K^{-1} at 301 K which is 2.3 x 10^{-6} K^{-1} lower than the selected value. The *c* axis thermal expansion behaves more normally with the value at 301 K agreeing exactly with the selected value although there is a scatter in the measurements above 260 K. On the basis 100Δε the smooth length change values along the *a* axis trend from 0.015 low at 4.2 K to 0.008 high at 210 K while for the *c* axis values the trend is from 0.008 high at 4.2 K to 0.015 high at 127 K.

71.2 High temperature

Length change values derived by Touloukian et al. 1975 from the lattice parameter measurements of Spedding et al. 1961 (291-1229 K) as discussed in Part 71.3 lead to equations 71c and 71d. An incompatibility between the low and high temperature thermal expansion for the *a* axis data was overcome by combining the length change value at 1200 K calculated from equation 71c with the selected thermal expansion value at 293.15 K and fitting to equation 71a. In the case of the *c* axis the agreement between low and high temperature measurements was relatively satisfactory so that values from equation 71d at 800 K and above were combined with the selected thermal expansion coefficient at 293.15 K to obtain equation 71b. Equations 71a and 71b were used to represent the thermal expansion from 293.15 K to 1200 K. The decreasing thermal expansion coefficient up to about 800 K found for the *c* axis is consistent with the maximum value found for the low temperature data at 280 K.

$$\varepsilon_T a = 5.25103 \times 10^{-6} T + 3.08062 \times 10^{-9} T^2 - 1.80408 \times 10^{-3} \quad (71a)$$

$$\varepsilon_T c = 2.52140 \times 10^{-5} T - 1.07684 \times 10^{-8} T^2 + 4.65284 \times 10^{-12} T^3 - 6.58329 \times 10^{-3} \quad (71b)$$

71a. Lattice parameters of lutetium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Notes
Spedding et al. 1956	RT	0.35033	0.55512	
Harris and Raynor 1969	RT	0.35101	0.55669	
Singh et al. 1971	293	0.35359	0.55578	a
Spedding and Beaudry 1971	297	0.35053	0.55493	b
	Selected	0.35053 (4)	0.55493 (5)	

Notes for Table 71a

a. Values given by Touloukian et al. 1975

b. Temperature of measurement given by Gschneidner 1990

In agreement with Gschneidner 1990 the values determined by Spedding and Beaudry 1971 for electropolished wires are selected.

At 293.15 K: Density 9840 (2) kg m^{-3} Molar volume 17.780 (4) cm^3 mol^{-1}.

71.3 Bulk properties of lutetium

Direct density measurements of Khairulin and Stankus 1989 (293-2030 K) were summarized by Stankus and Khairulin 1991. The quality of the material used can be considered from the fact that their density value at 293 K of 9826 kg m^{-3} is notably lower than the selected value of 9840 kg m^{-3} obtained from lattice parameter measurements and the volume thermal expansion coefficient at 293 K of 26.6 x 10^{-6} K^{-1} is also much lower than the selected value of 34.2 x 10^{-6} K^{-1}. When converted to length change values then on the basis 100ε the differences from the selected values was not constant but increased with increasing temperature reaching 0.16 lower than the crystallographic average at 1200 K. On these grounds it is considered that currently there are no satisfactory thermal expansion measurements above 1200 K

71.3 Comments on the measurements of Spedding et al. 1961

Length change values derived by Touloukian et al. 1975 from the lattice parameter measurements of Spedding et al. 1961 (291-1229 K) were fitted to the following equations except that the *a* axis value at 410 K, 498 K and 1021 K were not included:

$$\varepsilon_T a = 4.77249 \times 10^{-7} T + 8.29988 \times 10^{-9} T^2 - 1.60781 \times 10^{-12} T^3 - 8.12667 \times 10^{-4} \quad (71c)$$

$$\varepsilon_T c = 2.55886 \times 10^{-5} T - 1.13117 \times 10^{-8} T^2 + 4.88784 \times 10^{-12} T^3 - 6.65233 \times 10^{-3} \quad (71d)$$

Equation 71c shows a maximum in the derived thermal expansion coefficient at 1721 K and Equation 71d a minimum at 771 K.

Table 71b. Crystallographic properties of lutetium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
0	0	0	0	- 0.149	- 0.479	- 0.259
10	< 0.01	0.77	0.25	- 0.149	- 0.479	- 0.259
20	0.27	3.60	1.38	- 0.149	- 0.477	- 0.258
30	1.22	7.20	3.21	- 0.148	- 0.472	- 0.256
40	2.35	10.25	4.98	- 0.147	- 0.463	- 0.252
50	3.27	12.50	6.34	- 0.144	- 0.452	- 0.246
60	3.97	14.13	7.36	- 0.140	- 0.438	- 0.240
70	4.50	15.37	8.12	- 0.136	- 0.423	- 0.232
80	4.89	16.29	8.69	- 0.131	- 0.408	- 0.223
90	5.17	19.94	9.09	- 0.126	- 0.391	- 0.215
100	5.38	17.46	9.41	- 0.121	- 0.374	- 0.205
110	5.53	17.90	9.66	- 0.116	- 0.356	- 0.196
120	5.65	18.27	9.85	- 0.110	- 0.338	- 0.186
130	5.74	18.57	10.02	- 0.104	- 0.320	- 0.176
140	5.81	18.83	10.15	- 0.098	- 0.301	- 0.166
150	5.88	19.03	10.27	- 0.093	- 0.282	- 0.156
160	5.96	19.20	10.37	- 0.087	- 0.263	- 0.146
170	6.03	19.35	10.47	- 0.081	- 0.244	- 0.135
180	6.11	19.47	10.57	- 0.075	- 0.225	- 0.125
190	6.20	19.57	10.66	- 0.069	- 0.205	- 0.114
200	6.29	19.66	10.75	- 0.062	- 0.186	- 0.103
210	6.38	19.75	10.84	- 0.056	- 0.166	- 0.093
220	6.47	19.82	10.92	- 0.050	- 0.146	- 0.082
230	6.56	19.89	11.00	- 0.043	- 0.126	- 0.071
240	6.65	19.95	11.08	- 0.036	- 0.107	- 0.060
250	6.73	20.01	11.15	- 0.030	- 0.087	- 0.049
260	6.80	20.06	11.22	- 0.023	- 0.067	- 0.038
270	6.87	20.09	11.28	- 0.016	- 0.047	- 0.026
280	6.95	20.11	11.33	- 0.009	- 0.026	- 0.015
290	7.03	20.11	11.39	- 0.002	- 0.006	- 0.004
293.15	7.06	20.10	11.40	0	0	0
300	7.10	20.01	11.40	0.005	0.014	0.008
400	7.71	18.79	11.41	0.079	0.208	0.122
500	8.32	17.89	11.50	0.159	0.391	0.237
600	8.93	17.22	11.69	0.246	0.567	0.353
700	9.53	16.85	11.97	0.338	0.739	0.471
800	10.14	16.77	12.35	0.437	0.908	0.594
900	10.74	16.95	12.81	0.542	1.078	0.720
1000	11.34	17.42	13.37	0.653	1.252	0.852
1100	11.93	18.15	14.01	0.770	1.432	0.990
1200	12.53	19.16	14.74	0.893	1.621	1.135

Table 71c: Crystallographic properties of lutetium

T K	*a* nm	*c* nm	*c*/*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.35001	0.55227	1.5779	0.34218	17.642	9917
10	0.35001	0.55227	1.5779	0.34218	17.642	9917
20	0.35001	0.55228	1.5779	0.34218	17.643	9917
30	0.35001	0.55231	1.5780	0.34220	17.644	9916
40	0.35002	0.55236	1.5781	0.34222	17.646	9915
50	0.35003	0.55242	1.5782	0.34225	17.649	9914
60	0.35004	0.55250	1.5784	0.34228	17.653	9912
70	0.35005	0.55258	1.5786	0.34232	17.657	9909
80	0.35007	0.55267	1.5787	0.34236	17.661	9907
90	0.35009	0.55276	1.5789	0.34240	17.666	9904
100	0.35011	0.55285	1.5791	0.34245	17.671	9901
110	0.35013	0.55295	1.5793	0.34249	17.676	9899
120	0.35014	0.55305	1.5795	0.34254	17.681	9896
130	0.35016	0.55315	1.5797	0.34259	17.687	9893
140	0.35018	0.55326	1.5799	0.34264	17.692	9890
150	0.35021	0.55336	1.5801	0.34269	17.697	9887
160	0.35023	0.55347	1.5803	0.34274	17.703	9884
170	0.35025	0.55357	1.5805	0.34279	17.708	9880
180	0.35027	0.55368	1.5807	0.34284	17.714	9877
190	0.35029	0.55379	1.5809	0.34289	17.720	9874
200	0.35031	0.55390	1.5812	0.34294	17.725	9871
210	0.35033	0.55401	1.5814	0.34299	17.731	9868
220	0.35036	0.55412	1.5816	0.34304	17.737	9865
230	0.35038	0.55423	1.5818	0.34309	17.743	9861
240	0.35040	0.55434	1.5820	0.34315	17.748	9858
250	0.35043	0.55445	1.5822	0.34320	17.754	9855
260	0.35045	0.55456	1.5824	0.34325	17.760	9852
270	0.35047	0.55467	1.5826	0.34331	17.766	9848
280	0.35050	0.55478	1.5828	0.34336	17.772	9845
290	0.35052	0.55490	1.5831	0.34341	17.778	9842
293.15	0.35053	0.55493	1.5831	0.34343	17.780	9840
300	0.35055	0.55501	1.5833	0.34347	17.784	9838
400	0.35081	0.55608	1.5852	0.34399	17.845	9805
500	0.35109	0.55710	1.5868	0.34450	17.907	9771
600	0.35139	0.55808	1.5882	0.34499	17.969	9737
700	0.35172	0.55903	1.5894	0.34549	18.033	9703
800	0.35206	0.55997	1.5905	0.34599	18.099	9667
900	0.35243	0.56091	1.5916	0.34649	18.167	9631
1000	0.35282	0.53187	1.5925	0.34702	18.239	9593
1100	0.35323	0.56287	1.5935	0.34756	18.314	9554
1200	0.35366	0.56392	1.5945	0.34813	18.393	9513

$$d1 = (a^2/3 + c^2/4)^{½} \quad d2 = a$$

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72 HAFNIUM Hf

Atomic Weight: 178.49 (2) (Meija 2017)

Allotropy: Alpha phase: Hexagonal close-packed (hP2)
Beta phase: Body-centered cubic (cI2)

Values of 2016 (20) K for the alpha-beta transformation temperature and 2502 (20) K for the melting point were selected by Arblaster 2014.

72.1 Alpha Phase: Hexagonal close-packed: 0 K to 2016 K

Length changes derived from the lattice parameter measurements of Romans et al. 1965 (298-1773 K) and Krug and Davis 1970 (296-1873 K) disagree significantly with the bulk dilatometric measurements of Petukhov 2002 (1235-2221 K). While it is possible that the lattice parameter measurements could have been susceptible to lattice expansion due to oxidation effects the measurements were carried out in a very high vacuum so this would appear to be unlikely. However, the dilatometric measurements were subject to oxidation because the alpha-beta transformation temperature was not observed even 205 K above the selected value. In view of the limitations of bulk dilatometric mesurements in being able to represent crystallographic data, then the lattice parameter measurements were accepted, especially those of Krug and Davis 1970 which were fitted to the following equations which were extrapolated to the alpha-beta transformation temperature:

$$\varepsilon_T a = 5.94631 \times 10^{-6} T + 2.52099 \times 10^{-10} T^2 - 1.76482 \times 10^{-3} \quad (72a)$$

$$\varepsilon_T c = 6.14847 \times 10^{-6} T + 2.76660 \times 10^{-9} T^2 - 2.04018 \times 10^{-3} \quad (72b)$$

Deviations of experimental values from the selected values are given in Table 72b. Lattice parameter measurements of Ross and Hume-Rothery 1963 (1693-2388 K) were given only in the form of a small graph. A review of the data for the alpha phase by Onufriev et al. 2008 gave various weights to the different experimental data but the selected dilatometric curve agrees closely with the values of Petukhov 2002.

Table 72a. Lattice parameters of alpha hafnium at 293.15 K – Original values

References	Original Temperature K	Original values corrected to 293.15 K	
		a nm	*c* nm
Litton 1951	RT	0.31949	0.50527
Duwez 1951	RT	0.31954	0.50572
Fast 1952	RT	0.3193_6	0.5051_5
Russell 1953	297	0.31947	0.50511
Swanson et al. 1954	299	0.31968	0.50579
Taylor et al. 1961	296	0.31970	0.50585
Rudy and Stecher 1963	RT	0.3194_2	0.5052_3
Silver et al. 1963	RT	0.31979	0.50609
Domagala and Ruh 1965	RT	0.31980	0.50553
Krug and Davis 1970	296	0.31957	0.50548
Azhazha et al. 2008	298	0.31951	0.50543

Table 72b. Lattice parameters of alpha hafnium at 293.15 K - Corrected values

References	at % Zr	Vegards Law correction for Zr content		Notes
		a nm	*c* nm	
Litton 1951	?	-	-	
Duwez 1951	?	-	-	
Fast 1952	0	0.3193_6	0.5051_5	a, b
Russell 1953	0	0.31947	0.50511	a, b
Swanson et al. 1954	1.9	0.31961	0.50562	c
Taylor et al. 1961	4.4	0.31954	0.50544	
Rudy and Stecher 1963	0	0.3194_2	0.50523	a
Silver et al. 1963	4.4	0.31963	0.50569	
Domagala and Ruh 1965	3.3	0.31968	0.50521	
Krug and Davis 1970	4.0	0.31942	0.50509	a, b
Azhazha et al. 2008	0.6	0.31949	0.50537	
	Selected	0.31942 (6)	0.50512 (2)	

Notes for Table 72b

a. *a*-axis value included in the fit

b. *c*-axis value included in the fit

c. Actual range 0.1 to 3.8 at% Zr

At 293.15 K: Density 13281 (5) kg m^{-3} Molar volume 13.439 (5) cm^3 mol^{-1}.

Table 72c. Deviations of high temperature experimental values from the selected value for the alpha phase

References	Temperature Range K	Deviations 100Δε
Andenstadt 1949	293-1255	Trends to 0.19 lower
Baldwin 1954	293-1973	Trends to 0.22 lower
Fieldhouse and Lang 1961	294-1833	Trends to 0.25 higher above 1600 K
Siemans et al. 1964	298-1773	*a* axis trends to 0.36 high and *c* axis to 0.53 higher
Goluvtin and Maslennikov 1970	293-1302	Average bias 0.020 higher above 700 K
Petukhov 2002	1235-2221	Initially 0.11 lower then trends to 0.15 lower above 1500 K

72.2 Beta Phase: Body-centered cubic (cI2): 2016 K to 2502 K

Low accuracy lattice parameter measurements by Ross and Hume-Rothery 1963, Siemans et al. 1964, and Romans et al. 1965, established that the structure to be body-centered cubic. Higher accuracy values were obtained indirectly from direct density measurements of Paradis et al. 2003 (1950-2500 K) and volume ratio measurements of Cagran et al. 2008 (1500-2471 K). Both sets of determinations were carried out on metal containing 3 wt% (5.7 at%) zirconium. Based on the selected lattice parameters for the pure metals then a Vegards Law interpolation would lead to lattice parameters of *a* 0.31964 nm and *c* 0.50567 nm at 293.15 K for 5.7 at% Zr. The derived molar volume is 13.472_3 cm^3 mol^{-1} compared to 13.439_1 cm^3 mol^{-1} for pure hafnium. After recalculation of the measurements of Paradis et al. 2003 and Cagan et al. 2008 to conform to molar volumes, then molar volumes for pure beta hafnium were calculated from the experimental values as: $V_{pure} = (13.439_1/13.472_3)\ V_{experimental}$. The values for the pure element were then converted to length change values and lattice parameters and fitted to the following equations:

$$a\ (\text{nm}) = 2.98339 \times 10^{-6}\,T + 2.73048 \times 10^{-10}\,T^{2} + 0.353580 \qquad (72c)$$

$$\varepsilon_T = 8.41061 \times 10^{-6}\,T + 7.69761 \times 10^{-10}\,T^{2} - 3.20741 \times 10^{-3} \qquad (72d)$$

Extrapolation of equation 72c into the room temperature region leads to 0.3545 nm in exact agreement with the value obtained by Aurelio and Fernández-Guillermet 2000 by extrapolating the lattice parameters of hafnium alloys to the pure metal. Because of this agreement the values for the beta phase are considered to be self consistent.

The selected alpha–beta molar volume change at the transition temperature is an expansion of 0.65% while the values selected for the alpha phase by Onufriev et al. 2008 would lead to an even larger value of 1.1%. In contrast, the direct determination of lattice parameters in the region of the transformation by Ross and Hume-Rothery 1963 would lead to a contraction of 1.1%. Unfortunately the measurements of Ross and Hume-Rothery 1963 must be treated with caution because the samples used were highly oxidized as indicated by the fact that the derived alpha–beta transformation temperature was 250 K higher then the selected value. Comparison with zirconium would suggest that

there should be a contraction but the transition temperature to melting point ratios are so different for zirconium and hafnium then it is unsure if this is the correct behavior. Therefore, whether the transformation involves an expansion or a contraction cannot be properly determined until further high precision thermal expansion data becomes available.

Table 72d. Crystallographic properties of alpha hafnium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 ε_T *a*	100 ε_T *c*	100 ε_T avr
293.15	6.09	7.77	6.65	0	0	0
300	6.10	7.81	6.67	0.0042	0.0053	0.0046
400	6.14	8.35	6.88	0.065	0.086	0.072
500	6.19	8.90	7.09	0.127	0.173	0.142
600	6.24	9.44	7.31	0.189	0.264	0.214
700	6.28	9.99	7.52	0.252	0.362	0.289
800	6.33	10.53	7.73	0.315	0.465	0.365
900	6.38	11.06	7.94	0.379	0.573	0.444
1000	6.42	11.60	8.15	0.443	0.687	0.525
1100	6.47	12.14	8.36	0.508	0.807	0.608
1200	6.51	12.67	8.57	0.573	0.932	0.693
1300	6.56	13.20	8.77	0.639	1.063	0.780
1400	6.61	13.73	8.98	0.705	1.199	0.870
1500	6.65	14.26	9.19	0.772	1.341	0.962
1600	6.70	14.78	9.39	0.839	1.488	1.056
1700	6.74	15.30	9.60	0.907	1.641	1.152
1800	6.79	15.82	9.80	0.976	1.799	1.250
1900	6.83	16.34	10.00	1.044	1.963	1.351
2000	6.88	16.86	10.20	1.114	2.132	1.453
2016	6.89	16.94	10.24	1.125	2.160	1.470

Table 72e. Crystallographic properties of alpha hafnium

T K	*a* nm	*c* nm	*c*/*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
293.15	0.31942	0.50512	1.5814	0.31272	13.439	13281
300	0.31943	0.50515	1.5814	0.31274	13.441	13280
400	0.31963	0.50556	1.5817	0.31297	13.468	13253
500	0.31983	0.50599	1.5821	0.31321	13.497	13225
600	0.32002	0.50646	1.5826	0.31347	13.526	13196
700	0.32023	0.50695	1.5831	0.31374	13.556	13167
800	0.32043	0.50747	1.5837	0.31402	13.587	13137
900	0.32063	0.50802	1.5844	0.31431	13.619	13106
1000	0.32084	0.50859	1.5852	0.31461	13.652	13075
1100	0.32104	0.50920	1.5861	0.31492	13.686	13042
1200	0.32125	0.50983	1.5870	0.31525	13.720	13009
1300	0.32146	0.51049	1.5880	0.31559	13.756	12975
1400	0.32167	0.51118	1.5891	0.31594	13.793	12941
1500	0.32189	0.51189	1.5903	0.31630	13.830	12906
1600	0.32210	0.51264	1.5916	0.31667	13.869	12870
1700	0.32232	0.51341	1.5929	0.31706	13.909	12833
1800	0.32254	0.51421	1.5943	0.31746	13.949	12791
1900	0.32276	0.51504	1.5957	0.31787	13.991	12758
2000	0.32298	0.51589	1.5973	0.31829	14.033	12719
2016	0.32301	0.51603	1.5976	0.31836	14.040	12713

$$d1 = (a^2/3 + c^2/4)^{1/2} \quad d2 = a$$

Table 72f. Crystallographic properties of beta hafnium

T K	$\alpha \times 10^6\ K^{-1}$	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
2016	11.32	1.688	0.36070	0.31238	14.131	12631
2050	11.37	1.727	0.36084	0.31250	14.147	12616
2100	11.44	1.785	0.36105	0.31268	14.172	12595
2150	11.51	1.843	0.36126	0.31286	14.196	12573
2200	11.58	1.902	0.36147	0.31304	14.221	12551
2250	11.65	1.961	0.36168	0.31322	14.245	12530
2300	11.71	2.021	0.36189	0.31340	14.270	12508
2350	11.78	2.081	0.36210	0.31359	14.296	12486
2400	11.85	2.141	0.36231	0.31377	14.321	12464
2450	11.92	2.202	0.36253	0.31396	14.347	12441
2500	11.99	2.263	0.36275	0.31415	14.372	12419
2502	11.99	2.265	0.36275	0.31415	14.373	12418

$$d = \sqrt{3}a/2$$

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73 TANTALUM Ta

Atomic weight: 180.94788 (2) (Meija 2017)

Structure: Body-centered cubic (cI2)

Inaba 1980 determined the superconducting transition temperature to be 4.4924 K while a melting point of 3293 ± 15 K is selected as an average after correction to ITS-90 of values of 3292 K determined by Rudy and Harmon 1965, and 3294 K determined by Pemsler 1961 where in both cases the material used was of particularly high purity.

73.1 Allotropy

Similar for vanadium and niobium, dilatometric measurements of Bollinger et al. 2011 on pure tantalum indicated a structural distortion below 300 K leading to the formation of a structure which was not cubic. However, although given in smooth form, neither specific heat measurements of Sterrett and Wallace 1958 (12-543 K) or electrical resistivity measurements by Williams et al. 1982 (80-400 K) showed any evidence of an anomaly that would be involved in a phase transition while lattice parameter measurements of Smirnov and Finkel' 1965 (127-396 K) established that the structure remained body-centered cubic down to at least 127 K. Therefore, until the observations of Bollinger et al. 2011 are independently verified and the supposed new low temperature structure is fully characterized then it is assumed that the body-centered cubic structure exists over the whole temperature range.

73.2 Low Temperatures

Above the superconducting temperature, thermal expansion coefficients of White 1962 (5-85 K) were accepted. Above this temperature length change values of Nix and MacNair 1942 (92-301 K) were adjusted from a 273.15 K base to a 293.15 K base and fitted to the equation:

$$\varepsilon_T = 9.40257 \times 10^{-7} T + 3.24640 \times 10^{-8} T^2 - 9.04753 \times 10^{-11} T^3 + 9.87359 \times 10^{-14} T^4 - 1.51538 \times 10^{-3} \quad (73a)$$

This equation was then differentiated in order to obtain thermal expansion coefficients which were combined with the values of White 1962 and the selected thermal expansion coefficient at 293.15 K as derived in Table 73a and correlated using Equation A, and the corrected specific heat values of Sterrett and Wallace 1958 (12-543 K) as given in Part 73.6:

0 to 75 K: $\alpha\ (K^{-1}) = C_p\ (2.45312 \times 10^{-7} + 1.73800 \times 10^{-10} T - 4.38000 \times 10^{-7} / T)$ (73b)

75 to 180 K: $\alpha\ (K^{-1}) = C_p\ (2.76981 \times 10^{-7} - 5.13469 \times 10^{-11} T - 1.54036 \times 10^{-6} / T)$ (73c)

180 to 293.15 K: $\alpha\ (K^{-1}) = C_p\ (2.69273 \times 10^{-7} - 1.53501 \times 10^{-11} T - 1.35446 \times 10^{-6} / T)$ (73d)

Table 73a. Thermal expansion coefficient of tantalum at 293.15 K

References	Method	$\alpha \times 10^6$ K^{-1}
Hidnert 1929	Fit to dilatometric equation 293 – 773 K	6.58
Nix and MacNair 1942	Fit to length change values 279 to 294 K	6.55
Lisovskii 1972	Reported value at 300 K	6.58
	Selected	6.57

The thermal expansion coefficient values of Lisovskii 1972 (55-300 K) were only shown graphically with data points being given by Touloukian et al. 1975. However, these suggested that the actual value at 293 K was 6.07 x 10^{-6} K^{-1} compared to the above reported value. When converted to length change values then on the basis $100\Delta\varepsilon$ these measurements are initially 0.009 high and then trend towards the selected values. Lattice parameter values of Smirnov and Finkel' 1965 (127-396 K) were also only shown graphically with actual data points as length change values given by Touloukian et al. 1975. In the low temperature region these are initially 0.058 high and then trend towards the selected values. Dilatometric measurements of Hidnert 1929 (83-773 K) in the low temperature region are initially 0.016 low but above 100 K tend to agree to within 0.001.

73.3 High Temperatures

Length change values of Petukov et al. 1977 (1244-2267 K) and Miiller and Cezairliyan 1982, 1991 (1500-3200 K) were accepted and were joined with the selected value of the thermal expansion coefficient at 293.15 K and considered as covering the range from this temperature up to the melting point. On the basis $\pm 100\varepsilon_T$ the fit to the equation is equal to ± 0.002:

$$\varepsilon_T = 6.20553 \times 10^{-6} T + 7.16013 \times 10^{-10} T^2 - 2.42131 \times 10^{-13} T^3 + 7.04518 \times 10^{-17} T^4 - 1.87510 \times 10^{-3} \quad (73e)$$

Because the selected high temperature values are dilatometric measurements they cannot truly be considered as representing the crystallographic properties because of the onset of thermal vacancy effects. The enthalpy of vacancy formation (H_V) has been determined using Doppler broadening and positron annihilation mean lifetimes.

Table 73b. Thermal vacancy parameters for tantalum

References	Method	H_V eV
Maier et al. 1977	Doppler broadening	2.2 (2)
Maier et al. 1979	Doppler broadening	2.8 (6)
Schaffer et al. 1987	Mean lifetimes	2.9 (4)
	Weighted average	2.4 (4)

Estimating the vacancy concentration parameter (C_V) at 1.0 x 10^{-3} for refractory metals would lead to an entropy of vacancy formation of $S_V/k = 1.5$. However, because of the speculation over the value of C_V no thermal vacancy corrections were applied.

Dilatometric measurements of Hidnert 1929 (83-773 K) in the high temperature region agree closely and deviate only up to 0.009 low at 773 K while length change values derived from the lattice parameter values of Smirnov and Finkel' 1965 (127-396 K) in the high temperature region deviate up to 0.035 low. The deviations of other experimental lattice parameter and dilatometric measurements are given in part 73.3.

73c. Lattice parameter values for tantalum at 293.15 K

References	Original Temperature K	*a* nm	Notes
Schramm et al. 1950	RT	0.33079	a
Geach and Summers Smith 1951-1952	293	0.33042	a
Swanson and Tatge 1953	298	0.33059	a
Smirnova and Ormont 1956	298	0.33036	a
Vasyutinskii et al. 1962	293	0.33088	a, b
Amonenko et al. 1963	293	0.33097	a, b
Smirnov and Finkel' 1965	294	0.33020	a, c
Waseda et al. 1975	298	0.33013	a
Neuburger 1936	293	0.33027	
Edwards et al. 1951	291	0.33031	
McMasters and Larsen 1961	RT	0.33032	
Bolef 1961	300	0.33029	d
Fisher et al. 1975	298	0.33030	e
Katahara et al. 1976	298	0.33031	f
Mueller 1977	296	0.33027	
	Selected	0.33029 (2)	

Notes for Table 73c

a. Not included in the average

b. Calculated from equation

c. Value given by Touloukian et al. 1975

d. From direct density measurement 16678 kg m^{-3} at 300 K

e. From direct density measurement 16677 kg m^{-3} at 298 K

f. From direct density measurement 16675 kg m^{-3} at 298 K

At 293.15 K: Density 16678 (3) kg m^{-3} Molar Volume 10.849 (2) m^3 mol^{-1}.

73.4 Deviations of high temperature experimental values from the selected values

Table 73d. Lattice parameter values

References	Temperature Range K	Deviation 100Δε
Vasyutinskii et al. 1962	293-2973	Trend 0.054 low to 0.86 high
Amonenko et al. 1963	293-2873	Trend to 0.22 high
Edwards et al. 1951	291-2495	Scatter 0.041 low to 0.059 high
Waseda et al. 1975	298-2620	Trend to 0.15 high

Table 73e. Dilatometric values

References	Temperature Range K	Deviation 100Δε
Disch 1921	273-673	Average bias only 0.001 high
Worthing 1926	300-2700	Trend to 0.018 high at 2000 K falling to 0.020 low at 2700 K
Makin et al. 1953	293-1171	Trend to 0.038 low
Fieldhouse et al. 1956	343-1871	Trend to 0.37 high
Rasor and McClelland 1957, 1960	302-3125	Run 1 to 3125 K: Trends to 0.29 high; Run 2 to 2992 K: Trends to 0.34 high; Run 3 to 3065 K: Trends to 0.45 high; Run 4 to 1918 K: Trends to 0.38 high
Saldinger and Glasier 1959	1873-3273	Trends to 0.82 high
Amonenko et al. 1964	293-2273	Trends up to 0.10 high
V'yugov and Gumenyuk 1965	293-3273	Maximum deviation 0.10 high at 2673 K
Conway et al. 1965	293-2673	Run 1 to 2577 K: Trends to 0.59 high; Run 2 to 2588 K: Trends to 0.48 high; Run 3 to 2673 K: Trends to 0.12 high
Conway and Losenkamp 1966	298-2653	Run 1 to 2959 K: Trends to 0.13 high; Run 2 to 2653 K: Trend to 0.060 hig; Run 3 to 2615 K: Trends to 0.079 high
Conway and Flagella 1967	383-2643	Run 1 to 2588 K:Trends to 0.12 high; Run 2 to 2493 K: Trensd to 0.078 high; Run 3 to 2643 K: Trends to 0.092 high
Gilchrist and Preston 1979	293-873	Trends to only 0.008 high

73.5 Comparison with previous evaluations in the high temperature region

Of the most recent reviews that of Wang and Reeber 1998 is based on similar measurements to those selected in the present review and on the basis 100Δε lead to a bias of only 0.006 high. Volume thermal expansion coefficients selected by Bodryakov 2016 in the low temperature region trend from 12.5% high at 20 K to 1.5% low at 170 K to 1.0% low at 300 K while in the high temperature region the trend is to 3.2% high at 1200 K to 1.0% low at 2800 K to 2.3% high at 3250 K.

73.6 Corrected specific heat values of Sterrett and Wallace 1958

Corrected from cal mol^{-1} K^{-1} to J mol^{-1} K^{-1} and for atomic weight 180.94788/180.88

T K	20	22	24	25	26	28	30	35	40
C_p	1.415	1.854	2.361	2.641	3.587	4.211	5.906	7.634	9.325
T K	45	50	55	60	65	70	75	80	85
C_p	9.325	10.849	12.289	13.582	14.733	15.717	16.625	17.454	18.199
T K	90	95	100	105	110	115	120	125	130
C_p	18.831	19.350	19.827	20.262	20.681	21.037	21.372	21.669	21.941
T K	135	140	145	150	155	160	165	170	175
C_p	22.192	22.435	22.619	22.807	22.987	23.159	23.309	23.452	23.577
T K	180	185	190	195	200	205	210	215	220
C_p	23.695	23.812	23.921	24.021	24.113	24.205	24.293	24.368	24.440
T K	225	230	235	240	245	250	255	260	265
C_p	24.507	24.578	24.645	24.707	24.766	24.825	24.875	24.925	24.975
T K	270	275	280	285	290	293.15	295	298.15	300
C_p	25.030	25.080	25.134	25.185	25.235	25.262	25.277	25.302	25.319

Table 73f. Low temperature crystallographic properties of tantalum

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	- 0.143	0.32982	0.28563	10.803	16750
10	0.05	- 0.143	0.32982	0.28563	10.803	16750
20	0.32	- 0.143	0.32982	0.28563	10.803	16750
30	0.99	- 0.142	0.32982	0.28563	10.803	16749
40	1.84	- 0.141	0.32982	0.28564	10.804	16749
50	2.66	- 0.139	0.32983	0.28564	10.804	16748
60	3.37	- 0.136	0.32984	0.28565	10.805	16746
70	3.95	- 0.132	0.32985	0.28566	10.807	16744
80	4.43	- 0.128	0.32987	0.28567	10.808	16742
90	4.81	- 0.123	0.32988	0.28569	10.809	16740
100	5.08	- 0.118	0.32990	0.28570	10.811	16737
110	5.32	- 0.113	0.32992	0.28572	10.813	16735
120	5.51	- 0.108	0.32993	0.28573	10.814	16732
130	5.67	- 0.102	0.32995	0.28575	10.816	16729
140	5.81	- 0.096	0.32997	0.28576	10.818	16726
150	5.91	- 0.090	0.32999	0.28578	10.820	16723
160	6.00	- 0.084	0.33001	0.28580	10.822	16720
170	6.08	- 0.078	0.33003	0.28582	10.824	16717
180	6.14	- 0.072	0.33005	0.28583	10.826	16714
190	6.20	- 0.066	0.33007	0.28585	10.828	16711
200	6.26	- 0.060	0.33009	0.28587	10.830	16708
210	6.31	- 0.054	0.33011	0.28589	10.832	16705
220	6.35	- 0.047	0.33013	0.28590	10.834	16702
230	6.39	- 0.041	0.33015	0.28592	10.836	16699
240	6.42	- 0.035	0.33018	0.28594	10.838	16695
250	6.45	- 0.028	0.33020	0.28596	10.840	16692
260	6.48	- 0.022	0.33022	0.28598	10.842	16689
270	6.51	- 0.015	0.33024	0.28600	10.845	16686
280	6.54	- 0.009	0.33026	0.28601	10.847	16682
290	6.56	- 0.002	0.33028	0.28603	10.849	16679
293.15	6.57	0	0.33029	0.28604	10.849	16678

$$d = \sqrt{3}a/2$$

Table 73g. High temperature crystallographic properties of tantalum

T K	$\alpha \times 10^6$ K^{-1}	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
293.15	6.57	0	0.33029	0.28604	10.849	16678
300	6.58	0.005	0.33030	0.28605	10.851	16676
400	6.68	0.071	0.33052	0.28624	10.872	16643
500	6.77	0.138	0.33075	0.28643	10.894	16609
600	6.85	0.206	0.33097	0.28663	10.917	16575
700	6.93	0.275	0.33120	0.28683	10.939	16541
800	7.01	0.345	0.33143	0.28703	10.962	16507
900	7.08	0.416	0.33166	0.28723	10.985	16472
1000	7.16	0.487	0.33190	0.28743	11.009	16437
1100	7.24	0.560	0.33214	0.28764	11.033	16401
1200	7.32	0.633	0.33228	0.28785	11.057	16365
1300	7.41	0.707	0.33263	0.28806	11.081	16329
1400	7.50	0.782	0.33287	0.28828	11.106	16293
1500	7.61	0.858	0.33313	0.28849	11.131	16256
1600	7.72	0.936	0.33338	0.28872	11.157	16219
1700	7.85	1.014	0.33364	0.28894	11.183	16181
1800	7.99	1.094	0.33390	0.28917	11.209	16142
1900	8.14	1.176	0.33417	0.28940	11.237	16103
2000	8.31	1.259	0.33445	0.28964	11.264	16064
2100	8.50	1.344	0.33473	0.28985	11.293	16023
2200	8.72	1.431	0.33502	0.29013	11.322	15986
2300	8.95	1.521	0.33531	0.29039	11.352	15940
2400	9.21	1.613	0.33562	0.29065	11.383	15896
2500	9.49	1.708	0.33593	0.29093	11.415	15852
2600	9.79	1.806	0.33626	0.29121	11.448	15806
2700	10.13	1.908	0.33659	0.29150	11.482	15759
2800	10.50	2.013	0.33694	0.29180	11.517	15710
2900	10.89	2.122	0.33730	0.29211	11.555	15660
3000	11.22	2.235	0.73767	0.29243	11.593	15608
3100	11.78	2.354	0.33806	0.29277	11.634	15554
3200	12.28	2.477	0.33847	0.29312	11.676	15498
3293	12.78	2.596	0.33887	0.29347	11.717	15444

$$d = \sqrt{3}a/2$$

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74 TUNGSTEN W

Atomic weight: 183.84 (1) (Meija 2017)

Structure: Body-centered cubic (cI2)

The melting point is a secondary fixed point on ITS-90 at 3687 (7) K (Bedford et al. 1996).

74.1 Low temperature

Thermal expansion coefficients of White et al. 1978 (4-85, 283 K) and Kirby and Hahn 1976 (80-1800 K) were combined to represent the thermal expansion up to 293.15 K. Derived thermal expansion values were also fitted to equation A and given in Appendix A. On the basis $100\Delta\varepsilon$ length change values of Nix and MacNair 1942 (102-301 K), Rodrigues et al. 1984 (20-300 K) and the measurements of Hidnert and Sweeney 1925 (173-1273 K) below room temperature agree with the selected values to within 0.001. Thermal expansion coefficient values of Lisovskii 1972 (55-300 K), which were given only graphically with actual data points given by Touloukian et al. 1975, when converted to length change values, are initially 0.003 high and then converge to the selected values. Length change values derived from the lattice parameter values of King and Preece 1967 (18-298 K) show an average bias of 0.004 high.

74.2 High temperature

Dilatometric measurements of Kirby 1972 (293-1800 K), Petukhov and Chekhovskoi 1972 (2213-3608 K), Kirby and Hahn 1976 (80-1800 K) and Miiller and Cezairliyan 1990, 1991 (1500-3600 K) were combined with an overall accuracy on the basis $\pm 100\varepsilon_T$ as only ± 0.004:

$$\varepsilon_T = 3.94396 \times 10^{-6} T + 9.78341 \times 10^{-10} T^2 - 4.23510 \times 10^{-13} T^3 + 1.17016 \times 10^{-16} T^4 - 4.48177 \times 10^{-21} T^5 - 1.23043 \times 10^{-3} \quad (74a)$$

Because the selected high temperature values are dilatometric measurements they cannot truly be considered as an overall representation of the crystallographic properties because of the onset of thermal vacancy effects. The enthalpy of vacancy formation (H_V) has been determined using the following techniques:

Table 74a. Thermal vacancy parameters for tungsten

References	Method	H_V eV
Maier et al. 1979	Doppler broadening	4.0 (3)
Smedskjaer et al. 1985	Doppler broadening	3.76 (39)
Ziegler and Schaeffer 1987	Positron lifetime spectroscopy	4.6 (8)
Schaeffer 1987	Mean lifetimes	4.1 (2)
	Weighted average	4.1 (1)

Estimating the vacancy concentration parameter (C_V) at 1.0 x 10^{-3} for refractory metals would lead to an entropy of vacancy formation of S_V/k = 6.0. However, because of the speculation over the value of C_V no thermal vacancy corrections were applied

Dilatometric measurements of Roberts 1975 (323-1223 K) and Nasekovskii 1969 (77-1200 K) were only shown graphically.

Table 74b. Lattice parameter values for tungsten at 293.15 K

References	Original Temperature K	*a* nm	Note
Van Arkel 1928	RT	0.31649	
Owen and Iball 1932	289.7	0.31658	
Neuburger 1933	RT	0.31649	
Neuburger 1934	293	0.31655	
Jette and Foote 1935	298	0.31649	
Straumanis and Ievinš 1936	293	0.31652	
Cohen 1936	RT	0.31649	
Moeller 1937	RT	0.31654	
Lu and Chang 1941	294	0.31650	
Jaffee and Nielsen 1948	RT	0.31649	
Schramm et al. 1950	RT	0.31653	
Swanson and Tatge 1953	298	0.31649	
Pines and Kaluzhinova 1959	RT	0.31655	
Vogel and Kempter 1959, 1961	298	0.31652	
Umanskii et al. 1960a	298	0.31652	
Umanskii et al. 1960c	298	0.31653	
Perdok 1960	298	0.31654	a
Balchin 1960	298	0.31653	a
Straumanis and James 1960	298	0.31652	a
Beu 1960	298	0.31651	a
Umanskii et al. 1960b	298	0.31654	a
Kempter 1960	298	0.31653	a
Mitchell 1960	298	0.31654	a
Tournarie 1960	298	0.31654	a
Wilkens 1960	298	0.31653	a
Taylor et al. 1961	RT	0.31651	
Deshpande and Pawar 1962	298	0.31649	
Dutta and Dayal 1963b	298	0.31650	
Delf 1963	298	0.31653	
Beu 1964, 1965	298	0.31653	
Taylor et al. 1964	298	0.31654	
Taylor and Doyle 1965	RT	0.31654	
King and Russell 1965	298	0.31653	
Swanson et al. 1966	298	0.31651	
King and Preece 1967	298	0.31653	
Gerdes et al. 1970	RT	0.31652	
Swanson et al. 1970	298	0.31652	
Hart et al. 1990	294	0.31652	
	Selected	0.31652 (2)	

Note for Table 74b

a. I.U.Cr. Precision Lattice Parameter Project (Parrish 1960)

At 293.15 K for W: Density 19254 (4) kg m^{-3} Molar Volume 9.548 (2) m^3 mol^{-1}

74.3 Deviations of high temperature experimental values from the selected values

Table 74c: Dilatometric values

References	Temperature Range K	Deviations 100Δε
Worthing 1917	300-2673	Trends to 0.029 high
Goucher 1924	283-1042	Average bias 0.005 low
Benedicks et al. 1924	288-1993	Trends to 0.10 high
Hidnert and Sweeney 1925	173-1773	Average bias 0.002 low
Burger 1934	298-823	Average bias 0.002 high
Demarquay 1945	293-2423	Trends 0.022 low to 0.034 low
Apblett and Pellini 1952	294-2900	Trends 0.021 low at 811 K to 0.28 high at 2900 K
Anthony and Pearl 1960	300-1616	Trends 0.013 high to 0.010 low
Fulkerson 1960	293-1573	Trends 0.014 high to 0.005 low
Levingstein 1961	297-1422	Trends to 0.050 high
Neel et al. 1962	293-3025	Run 1: 293-2283 K: Trends to 0.48 low; Run 2: 294, 2283 K: Trends to 0.43 low; Run 3: 293-3025 K: Trends to 1.27 low
Denman 1962	297-1366	Overall trend to 0.028 low
Totskii 1964	273-1373	Trends to 0.014 low
Amonenko et al. 1964	293-2273	Trends to maximum of 0.043 low at 1600 K then increases to 0.013 high
V'Yugov and Gumenyuk 1965	1937-3322	Trends 0.089 low to 0.21 high
Yagee and Styles 1965	298-1273	Average bias 0.003 low
Takamori and Tomozawa 1965	293-848	Average bias 0.002 low
Kraftmakher and Cheremisina 1965	1300-2300	Average bias 0.003 high when fixed at selected value at 1300 K
Conway and Losenkamp 1966	298-2747	Trends to 0.053 high. Second sample of 99.0% purity not considered
Conway and Flagella 1967	533-2748	Sample 1: 533-2748 K: Trends to maximum 0.078 low at 1500 K then increase to 0.024 high; Sample 2: 548-2623 K: Trends 0.056 low to 0.036 high
Brizes 1968	782-2321	Trends to 0.12 low when fixed at selected value at 782 K
Knibbs 1969	1942-2558	Trends to 0.029 high when fixed at selected value At 1942 K
Valentich 1969	293-2489	Run 1: Trends to 0.033 low at 1260 K then increases to 0.010 low; Run 2: Trends 0.055 low to 0.016 high
Fitzer 1971	373-1273	Average of 7 participants trends to 0.024 high
Fitzer 1972	373-1573	Average of 4 participants trends to 0.041 high
Fitzer and Weisenburger 1972	373-2573	Participant No.5: 373-1573 K: Scatters 0.007 low to 0.007 high; Participant No.10: 373-2573 K: Trends to 0.053 high; Participant No. 11: 873-1773 K: Trends 0.036 to 0.10 high
Kraftmakher 1972	2050-2897	Average bias 0.004 high when fixed at selected value at 2050 K
Kollie et al. 1974	300-1000	Trends to 0.014 high
Shevchenko et al. 1986	373-673	Average bias 0.005 low
Suh et al. 1988	293-1700	Trends to 0.033 low
Reiter and Kaschnitz 2002	1000-3500	Trends to average of 0.045 high above 2700 K

Table 74d: Lattice parameter values

References	Temperature Range K	Deviations 100Δε
Shinoda 1934	288-1328	Trends to 0.23 high
Mauer and Bolz 1955	273-1613	Average bias 0.005 low except 0.014 high at 1613 K
Brand and Goldschmidt 1956	273-1573	Trends to 0.025 low
Baun 1959	291-1246	Trends to 0.003 low
Deshpande and Pawar 1962	293-773	Trends to 0.009 low
Dutta and Dayal 1963b	298-1151	Trends to 0.048 high
Houska 1964	298-2050	Average bias 0.003 low
Clark and Knight 1965	300-1499	Trends 0.034 high to 0.006 low
Frantsevich et al. 1967	293, 1473	0.004 low at 1473 K
Fitzer and Weisenburger 1972	293-1173	Average bias 0.004 low (Participant No. 2)
Waseda et al. 1975	298-2621	Trends to 0.075 max at 1600 K then trends to 0.024 max
Dubrovinsky and Saxena 1997	298-3548	Scatter 0.065 low to 0.093 high but average 0.046 high above 2600 K

74.4 Comparison with previous evaluations in the high temperature region

Touloukian et al. 1975 included the high temperature length change values of Kirby 1972 and Petukhov and Chekhovskoi 1972 but of course not the later measurements of Kirby and Hahn 1976 and Miiller and Cezairliyan 1990, 1991 so that on the basis 100Δε their selected values were 0.020 low at 3600 K. The thermal expansion table of White and Minges 1997 contained an error in that the length change values given did not agree with the selected equation but were those obtained in a previous review by White and Roberts 1983. This error was again repeated in 1998 (White 1998). Integration of the actual selected equation leads to a difference of only 0.010 high at 3400 K. The selected values of Wang and Reeber 1998 included the measurements of Deshpande and Pawar 1962 and Totskii 1964, neither of which were considered of sufficient accuracy in the present review, and the measurements of Roberts 1975 which were not considered because the values were determined on low density sintered material and were also only shown graphically. As a result the values of Wang and Reeber 1998 show maximum deviations of 0.012 low at 1500 K increasing to 0.001 high in the region of 2400 to 2700 K. Overall the bias is only 0.004 low. Bodryakov 2015 did not mention any of the high temperature length change values selected in the present review. After correction from volume thermal expansion to linear thermal expansion the selected values of Bodryalov 2015 trend from 2.1% low at 300 K to 3.3% high at 2200 K to 0.1% high at 3200 K to 2.4% high at the melting point.

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Table 74e. Low temperature crystallographic properties of tungsten

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	- 0.0876	0.31624	0.27387	9.523	19304
10	0.006	- 0.0876	0.31624	0.27387	9.523	19304
20	0.048	- 0.0876	0.31624	0.27387	9.523	19304
30	0.20	- 0.0875	0.31624	0.27387	9.523	19304
40	0.53	- 0.0871	0.31624	0.27388	9.523	19304
50	0.96	- 0.0864	0.31625	0.27388	9.524	19304
60	1.43	- 0.0852	0.31625	0.27388	9.524	19303
70	1.88	- 0.0835	0.31626	0.27389	9.524	19302
80	2.26	- 0.0814	0.31626	0.27389	9.525	19301
90	2.61	- 0.0790	0.31627	0.27390	9.526	19299
100	2.88	- 0.0762	0.31628	0.27391	9.526	19298
110	3.11	- 0.0732	0.31629	0.27391	9.527	19296
120	3.30	- 0.0700	0.31630	0.27392	9.528	19294
130	3.46	- 0.0666	0.31631	0.27393	9.529	19292
140	3.59	- 0.0631	0.31632	0.27394	9.530	19290
150	3.71	- 0.0595	0.31633	0.27395	9.531	19288
160	3.81	- 0.0557	0.31634	0.27396	9.532	19286
170	3.89	- 0.0518	0.31636	0.27397	9.533	19284
180	3.97	- 0.0479	0.31637	0.27398	9.535	19281
190	4.04	- 0.0439	0.31638	0.27399	9.536	19279
200	4.10	- 0.0398	0.31639	0.27401	9.537	19277
210	4.15	- 0.0357	0.31641	0.27402	9.538	19274
220	4.20	- 0.0315	0.31642	0.27403	9.539	19272
230	4.24	- 0.0273	0.31643	0.27404	9.540	19270
240	4.27	- 0.0231	0.31645	0.27405	9.542	19267
250	4.30	- 0.0188	0.31646	0.27406	9.543	19265
260	4.34	- 0.0145	0.31647	0.27407	9.544	19262
270	4.36	- 0.0102	0.31649	0.27409	9.545	19260
280	4.39	- 0.0058	0.31650	0.27410	9.547	19257
290	4.41	- 0.0014	0.31652	0.27411	9.548	19255
293.15	4.42	0	0.31652	0.27411	9.548	19254

$$d = \sqrt{3}a/2$$

Table 74f. High temperature crystallographic properties of tungsten

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
293.15	4.42	0	0.31652	0.27411	9.548	19254
300	4.43	0.003	0.31653	0.27412	9.549	19252
400	4.55	0.048	0.31667	0.27425	9.562	19226
500	4.66	0.094	0.31682	0.27437	9.575	19200
600	4.75	0.141	0.31697	0.27450	9.589	19172
700	4.84	0.189	0.31712	0.27462	9.603	19145
800	4.91	0.238	0.31727	0.27477	9.617	19117
900	4.99	0.288	0.31743	0.27490	9.631	19089
1000	5.06	0.338	0.31759	0.27504	9.645	19060
1100	5.13	0.389	0.31775	0.27518	9.660	19031
1200	5.20	0.441	0.31792	0.27532	9.675	19001
1300	5.28	0.494	0.31808	0.27547	9.690	18971
1400	5.36	0.547	0.31825	0.27561	9.706	18941
1500	5.45	0.602	0.31842	0.27576	9.722	18910
1600	5.56	0.657	0.31860	0.27592	9.738	18879
1700	5.67	0.713	0.31878	0.27607	9.754	18847
1800	5.80	0.771	0.31896	0.27623	9.771	18815
1900	5.94	0.830	0.31915	0.27639	9.788	18782
2000	6.11	0.891	0.31934	0.27656	9.806	18748
2100	6.29	0.954	0.31954	0.27673	9.824	18712
2200	6.49	1.018	0.31974	0.27691	9.843	18677
2300	6.72	1.085	0.31995	0.27709	9.862	18640
2400	6.97	1.154	0.32017	0.27728	9.883	18602
2500	7.24	1.226	0.32040	0.27748	9.904	18563
2600	7.55	1.301	0.32064	0.27768	9.926	18521
2700	7.88	1.379	0.32088	0.27789	9.949	18479
2800	8.24	1.461	0.32114	0.27812	9.972	18434
2900	8.63	1.546	0.32141	0.27835	9.998	18388
3000	9.05	1.636	0.32170	0.27860	10.025	18339
3100	9.51	1.730	0.32200	0.27886	10.053	18288
3200	10.00	1.830	0.32231	0.27913	10.082	18234
3300	10.52	1.934	0.32264	0.27942	10.113	18178
3400	11.08	2.044	0.32299	0.27972	10.146	18120
3500	11.68	2.161	0.32336	0.28004	10.181	18058
3600	12.31	2.283	0.32375	0.28037	10.217	17993
3687	12.90	2.395	0.32410	0.28068	10.251	17934

$$d = \sqrt{3}a/2$$

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75 RHENIUM Re

Atomic Weight: 186.207 (1) (Meija 2017)

Structure: Close-packed hexagonal (hP2)

Arblaster 1996 selected 3458 (20) K for the melting point corrected to ITS-90.

75.1 Low temperature

Thermal expansion coefficients of Petrenko and Popov 1979 (3-300 K) were accepted where above 100 K and up to 293.15 K these can be represented by the equations:

$$\alpha_a\,(K^{-1}) = 8.56667 \times 10^{-8}\,T - 4.96667 \times 10^{-10}\,T^{2} + 1.33333 \times 10^{-12}\,T^{3} - 1.33333 \times 10^{-15}\,T^{4} - 1.00000 \times 10^{-7} \quad (75a)$$

$$\alpha_c\,(K^{-1}) = 5.90000 \times 10^{-8}\,T - 3.96667 \times 10^{-10}\,T^{2} + 1.20000 \times 10^{-12}\,T^{3} - 1.33333 \times 10^{-15}\,T^{4} - 1.10000 \times 10^{-6} \quad (75b)$$

Thermal expansion coefficients of Yelenskiy et al. 1984 (4.5-300 K) were only shown in the form of small graphs but appear to confirm the values obtained by Petrenko and Popov 1979. Lattice parameter measurements of Finkel' et al. 1971 (80-300 K) were only shown graphically with actual data points as length change values being given by Touloukian et al. 1975. On the basis $100\Delta\varepsilon$ the *a* axis values are initially 0.029 low and then trend to agree with the selected values while the *c* axis values average 0.013 high below 200 K then again trend to agree with the selected values. Below the room temperature region length change values derived from the lattice parameter measurements of Sovetnikova et al. 1977 (113-1700 K) bias only 0.003 high along the *a* axis and 0.001 low along the *c* axis.

75.2 High temperature

Only length change values derived from the lattice parameter measurements of Wasilewski 1961 (298-1561 K) show satisfactory agreement with the low temperature selected thermal expansion coefficients and from 293.15 K to 1600 K are selected to represent the thermal expansion:

$$\varepsilon_T\,a = 5.72913 \times 10^{-6}\,T + 5.81392 \times 10^{-10}\,T^{2} - 1.72946 \times 10^{-3} \quad (75c)$$

$$\varepsilon_T\,c = 4.30373 \times 10^{-6}\,T + 6.58821 \times 10^{-10}\,T^{2} - 1.31826 \times 10^{-3} \quad (75d)$$

Average length change values derived from the above equations at 1400 K, 1500 K and 1600 K show exact agreement with length change values derived from the volume ratios of Hixson and Winkler 1992 (2427-3453 K) at 2684 K, 2879 K and 3321 K, and all six values were fitted to the following equation to represent the average length change from 1600 K to the melting point:

$$\varepsilon_T \text{ avr} = 6.04023 \times 10^{-6}\, T - 6.19723 \times 10^{-11}\, T^2 + 1.79646 \times 10^{-13}\, T^3 - 1.87362 \times 10^{-3} \qquad (75e)$$

On the basis $100\Delta\varepsilon$ length change values derived from the lattice parameter measurements of Medoff and Cadoff 1959 (293-1273 K) average 0.013 high below 900 K and then trend to 0.055 low along the *a* axis while for the *c* axis the average is 0.008 high up to 900 K and then trending to 0.031 low. Measurements of Pawar and Deshpande 1967 (298-627 K) scatter from 0.015 to 0.052 high along the *a* axis while the *c* axis values trend from 0.014 high to 0.005 low. Those of Lui et al. 1970 (286-701 K) scatter from 0.009 to 0.039 high along the *a* axis but bias only 0.002 high along the *c* axis. In the high temperature region the values of Sovetnikova et al. 1977 (113-1700 K) trend up to 0.19 low along the *a* axis and 0.12 low along the *c* axis. Dilatometric measurements of Petukhov et al. 1979 (1200-2300 K) were only given in the form of small graphs.

Volume ratio measurements of Hüpf et al. 2008 (1500-3458 K) supersede earlier measurements of Pottlacher et al. 1986 (2600-3453 K) but when reduced to length change values trend from 0.093 to 0.82 low while volume ratios of Thévenin et al. 1993 (2500-3453 K) corrected to length change values which trend from 1.51 to 1.69 high.

75a. Lattice parameters of rhenium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Notes
Stenzel and Weerts 1932	293	0.27610	0.44585	
Trzebiatowski 1937	RT	0.27605	0.44579	
Wasilewski 1961	298	0.27610	0.44577	
Rudy et al. 1962	RT	0.27614	0.44615	a
Taylor et al. 1963	296	0.27612	0.44589	
Pawar and Deshpande 1967	298	0.27607	0.44579	
Finkel' et al. 1971	293	0.27616	0.44569	b
Sovetnikova et al. 1977	293	0.27613	0.44596	c
	Selected	0.27610 (3)	0.44584 (7)	

Notes for Table 75a

a. *c* axis value not included in the average

b. Values given by Touloukian et al. 1975. Not included in the average

c. Calculated from equations

At 293.15 K: Density 21010 (5) kg m^{-3} Molar Volume 8.863 (2) m^3 mol^{-1}.

Table 75b. Crystallographic properties of rhenium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 ε_T *a*	100 ε_T *c*	100 ε_T avr
0	0	0	0	- 0.127	- 0.104	- 0.120
5	0.01	- 0.44	- 0.14	- 0.127	- 0.104	- 0.120
10	0.07	- 0.01	0.04	- 0.127	- 0.104	- 0.120
15	0.05	0.05	0.05	- 0.127	- 0.104	- 0.120
20	0.07	0.07	0.07	- 0.127	- 0.104	- 0.120
25	0.15	0.17	0.16	- 0.127	- 0.104	- 0.120
30	0.30	0.32	0.31	- 0.127	- 0.104	- 0.119
40	1.05	1.05	1.05	- 0.126	- 0.103	- 0.119
50	1.83	1.80	1.82	- 0.125	- 0.102	- 0.117
60	2.52	2.42	2.49	- 0.123	- 0.100	- 0.115
70	3.16	2.96	3.09	- 0.120	- 0.097	- 0.112
80	3.74	3.42	3.63	- 0.117	- 0.094	- 0.109
90	4.25	3.80	4.10	- 0.113	- 0.090	- 0.105
100	4.70	4.10	4.50	- 0.108	- 0.086	- 0.101
110	4.89	4.19	4.66	- 0.103	- 0.082	- 0.096
120	5.05	4.27	4.79	- 0.098	- 0.078	- 0.092
130	5.19	4.32	4.90	- 0.093	- 0.074	- 0.087
140	5.31	4.37	5.00	- 0.088	- 0.069	- 0.082
150	5.40	4.40	5.07	- 0.083	- 0.065	- 0.077
160	5.48	4.43	5.13	- 0.077	- 0.061	- 0.072
170	5.55	4.45	5.18	- 0.072	- 0.056	- 0.067
180	5.60	4.47	5.22	- 0.066	- 0.052	- 0.061
190	5.65	4.48	5.26	- 0.060	- 0.047	- 0.056
200	5.70	4.50	5.30	- 0.055	- 0.043	- 0.051
210	5.74	4.52	5.33	- 0.049	- 0.038	- 0.046
220	5.78	4.54	5.37	- 0.043	- 0.034	- 0.040
230	5.82	4.56	5.40	- 0.038	- 0.029	- 0.035
240	5.86	4.58	5.43	- 0.032	- 0.025	- 0.029
250	5.90	4.60	5.47	- 0.026	- 0.020	- 0.024
260	5.94	4.62	5.50	- 0.020	- 0.015	- 0.018
270	5.98	4.65	5.54	- 0.014	- 0.011	- 0.013
280	6.02	4.66	5.57	- 0.008	- 0.006	- 0.007
290	6.06	4.69	5.60	- 0.002	- 0.001	- 0.002
293.15	6.07	4.69	5.61	0	0	0
300	6.08	4.70	5.62	0.004	0.003	0.004
400	6.19	4.83	5.74	0.066	0.051	0.061
500	6.30	4.96	5.85	0.128	0.100	0.119
600	6.41	5.09	5.97	0.192	0.150	0.178
700	6.53	5.22	6.09	0.257	0.202	0.238
800	6.64	5.34	6.21	0.323	0.255	0.300
900	6.75	5.47	6.32	0.390	0.309	0.363
1000	6.86	5.60	6.44	0.458	0.364	0.427
1100	6.97	5.73	6.56	0.528	0.421	0.492
1200	7.08	5.86	6.67	0.598	0.479	0.559
1300	7.19	5.98	6.79	0.670	0.539	0.626
1400	7.30	6.11	6.91	0.743	0.600	0.695
1500	7.41	6.23	7.02	0.817	0.662	0.765
1600	7.52	6.37	7.14	0.893	0.725	0.837

Table 75c. Crystallographic properties of rhenium

T K	*a* nm	*c* nm	*c*/*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.27575	0.44538	1.6152	0.27374	8.831	21086
5	0.27575	0.44538	1.6152	0.27374	8.831	21086
10	0.27575	0.44537	1.6151	0.27374	8.831	21086
15	0.27575	0.44537	1.6151	0.27374	8.831	21086
20	0.27575	0.44537	1.6151	0.27374	8.831	21086
25	0.27575	0.44537	1.6151	0.27374	8.831	21086
30	0.27575	0.44538	1.6151	0.27374	8.831	21086
40	0.27575	0.44538	1.6151	0.27375	8.831	21085
50	0.27575	0.44538	1.6151	0.27375	8.831	21085
60	0.27576	0.44539	1.6151	0.27376	8.832	21083
70	0.27577	0.44541	1.6151	0.27376	8.833	21081
80	0.27578	0.44542	1.6151	0.27377	8.834	21079
90	0.27579	0.44544	1.6151	0.27378	8.835	21077
100	0.27580	0.44545	1.6151	0.27379	8.836	21074
110	0.27581	0.44547	1.6151	0.27381	8.837	21071
120	0.27583	0.44549	1.6151	0.27382	8.838	21068
130	0.27584	0.44551	1.6151	0.27383	8.840	21065
140	0.27586	0.44553	1.6151	0.27384	8.841	21062
150	0.27587	0.44555	1.6151	0.27386	8.842	21059
160	0.27589	0.44557	1.6150	0.27387	8.844	21056
170	0.27590	0.44559	1.6150	0.27388	8.845	21052
180	0.27592	0.44561	1.6150	0.27390	8.846	21049
190	0.27593	0.44563	1.6150	0.27391	8.848	21046
200	0.27595	0.44565	1.6150	0.27392	8.849	21042
210	0.27596	0.44567	1.6150	0.27394	8.851	21039
220	0.27598	0.44569	1.6149	0.27395	8.852	21036
230	0.27600	0.44571	1.6149	0.27396	8.853	21032
240	0.27601	0.44573	1.6149	0.27398	8.855	21029
250	0.27603	0.44575	1.6149	0.27399	8.856	21025
260	0.27605	0.44577	1.6148	0.27400	8.858	21022
270	0.27606	0.44579	1.6148	0.27402	8.859	21018
280	0.27608	0.44581	1.6148	0.27403	8.861	21015
290	0.27609	0.44583	1.6148	0.27405	8.862	21011
293.15	0.27610	0.44584	1.6148	0.27405	8.863	21010
300	0.27611	0.44585	1.6148	0.27406	8.864	21008
400	0.27628	0.44607	1.6145	0.27420	8.879	20972
500	0.27645	0.44629	1.6143	0.27435	8.894	20936
600	0.27663	0.44651	1.6141	0.27450	8.910	20899
700	0.27681	0.44674	1.6139	0.27465	8.926	20861
800	0.27699	0.44698	1.6137	0.27481	8.943	20822
900	0.27718	0.44722	1.6135	0.27497	8.959	20783
1000	0.27736	0.44747	1.6133	0.27514	8.977	20744
1100	0.27756	0.44772	1.6131	0.27530	8.994	20793
1200	0.27775	0.44978	1.6129	0.27547	9.012	20662
1300	0.27795	0.44834	1.6127	0.27565	9.030	20620
1400	0.27815	0.44851	1.6125	0.27583	9.049	20578
1500	0.27836	0.44879	1.6123	0.27601	9.068	20535
1600	0.27856	0.44907	1.6121	0.27619	9.087	20492

$$d1 = (a^2/3 + c^2/4)^{1/2} \quad d2 = a$$

Table 75d. Bulk properties of rhenium above 1600 K

T K	$\alpha \times 10^6$ K^{-1}	100 ε_T	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1600	7.14	0.837	9.087	20492
1700	7.32	0.910	9.107	20447
1800	7.49	0.985	9.127	20402
1900	7.67	1.061	9.148	20358
2000	7.86	1.140	9.169	20308
2100	8.06	1.220	9.191	20260
2200	8.27	1.303	9.214	20210
2300	8.49	1.388	9.237	20159
2400	8.72	1.475	9.261	20107
2500	8.96	1.565	9.285	20054
2600	9.21	1.657	9.311	20000
2700	9.47	1.752	9.337	19944
2800	9.74	1.850	9.364	19886
2900	10.02	1.950	9.391	19827
3000	10.31	2.054	9.420	19767
3100	10.61	2.161	9.450	19705
3200	10.91	2.271	9.480	91642
3300	11.23	2.384	9.512	19577
3400	11.56	2.501	9.544	19510
3458	11.75	2.570	9.564	19470

This Table is considered to be identical to Tables 75b and 75c at 1600 K and below.

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76 OSMIUM Os

This review is based on the assessment of Arblaster 2013.

Atomic Weight: 190.23 (3) (Meija 2017)

Structure: Close-packed hexagonal (hP2)

The melting point estimated as 3400 ± 50 K for the pure metal by Arblaster 2005 is considered to be more acceptable than values actually obtained for impure metal determined as 3318 ± 30 K by Knapton et al. 1960 for metal of only about 99.7% purity and 3283 ± 10 K by Douglass and Adkins 1961 for metal of 99.5% purity.

76.1 Crystallographic properties

The thermal expansion is only represented by three sets of lattice parameter measurements, those of Owen and Roberts 1936, 1937 (293-873 K), Schröder et al. 1972 (289-1287 K) and Finkel' et al. 1971 (79-300 K) where the latter measurements were shown only graphically and by incorrect equations with actual data points being given as length change values by Touloukian 1975. The two high temperature sets of measurements agree closely and were fitted to the following equations with accuracies expressed on the basis ± 100 ε of ± 0.004 and ± 0.002 respectively to represent the thermal expansion from 293.15 K to 1300 K:

$$\varepsilon_T a = 4.46595 \times 10^{-6} T + 1.69909 \times 10^{-10} T^2 - 1.32379 \times 10^{-3} \quad (76a)$$

$$\varepsilon_T c = 4.64427 \times 10^{-6} T + 2.04826 \times 10^{-9} T^2 - 1.53749 \times 10^{-3} \quad (76b)$$

The low temperature measurements of Finkel' et al. 1971 were fitted to smooth equations 76e and 76f as given in Part 76.2. The incompatibility of these measurements with the high temperature data can be shown by calculating thermal expansion coefficients of $\alpha_a = 5.8 \times 10^{-6}$ K^{-1} and $\alpha_c = 8.8 \times 10^{-6}$ K^{-1} at 293.15 K which are notably higher than values calculated from equations 76a and 76b as given in Tables 76b and 76c. In view of the very different value of 0.43174 nm obtained for the *c*-axis lattice parameter compared to all other values given in Table 76a then the measurements of Finkel' et al. 1971 must be treated with some suspicion and because it does not appear to be possible to reconcile the high and low temperature data then these low temperature measurements were rejected.

Therefore, in order to extrapolate below room temperature the procedure given in Part 76.3 was adopted leading to the following equations to represent the thermal expansion data below 293.15 K, where the values of C_p in J mol^{-1} K^{-1} were those selected in Part 76.4:

$$\alpha_a\,(K^{-1}) = C_p\,(1.58546 \times 10^{-7} + 1.09521 \times 10^{-11} T + 6.88982 \times 10^{-6}/T) \quad (76c)$$

$$\alpha_c\,(K^{-1}) = C_p\,(1.71988 \times 10^{-7} + 1.41412 \times 10^{-10} T + 6.95413 \times 10^{-6}/T) \quad (76d)$$

On the basis 100Δε values derived from three-point integration of these equations when compared to values obtained from the measurements of Finkel' et al. 1971 indicate for the latter that the *a*-axis values are 0.005 to 0.006 lower over the range 80 to 240 K and the c-axis values initially 0.029 lower at 80 K and then trending to agree with the selected values above this temperature.

Table 76a. Lattice parameters of osmium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Notes
Owen et al. 1935	291	0.27361	0.43189	a
Owen and Roberts 1936	291	0.27357	0.43191	a
Owen and Roberts 1937	293	0.27355	0.43194	a
Finkel' et al. 1971	292,293	0.27346	0.43174	a, b
Rudman 1965	RT	0.27341	0.43188	c
Swanson et al. 1955	299	0.27342	0.43198	
Mueller and Heaton 1961	RT	0.27345	0.43200	
Taylor et al. 1961b and Taylor et al. 1962	296	0.27342	0.43201	
Schröder et al. 1972	289	0.27340	0.43198	
	Selected	0.27342 (2)	0.43199 (2)	

Notes for Table 76a

a. Not included in the average

b. Lattice parameter values were given by Touloukian et al. 1975

c. The *c*-axis value was not included in the fit

At 293.15 K: Density 22589 (5) kg m^{-3} Molar volume 8.421 (1) cm^3 mol^{-1}.

76.2 Length change equations of Finkel' et al. 1971

Lattice parameter measurements of Finkel' et al. 1971 as given as length change values by Touloukian et al. 1975 were fitted to the following equations covering the ranges 79 to 289 K for the a-axis and 80 to 288 K for the c-axis:

$$\varepsilon_T a = 3.13600 \times 10^{-6} T + 1.37670 \times 10^{-9} T^2 + 7.27143 \times 10^{-12} T^3 - 1.22081 \times 10^{-3} \quad (78e)$$

$$\varepsilon_T c = 3.88446 \times 10^{-6} T + 3.26721 \times 10^{-9} T^2 + 1.16202 \times 10^{-11} T^3 - 1.71224 \times 10^{-3} \quad (78f)$$

76.3 Derivation of selected low temperature equations

Equations 76a and 76b were differentiated in order to obtain thermal expansion coefficients α* from which thermodynamic thermal expansion coefficients α were calculated using $\alpha = \alpha^*/(1 + \varepsilon)$. The derived values over the range 293.15 to 700 K were then combined with the specific heat values calculated from the high temperature equation 76g as given in Part 76.4 to give equations 76c and 76d. The standard deviations of the fits were 4.2 x 10^{-9} K^{-1} and 6.1 x 10^{-9} K^{-1} for the *a* and *c*-axes respectively. The limit

of 700 K was deliberately chosen because if 1000 K had been used the standard deviations would have deteriorated to 9.2 x 10^{-9} K^{-1} and 1.7 x 10^{-8} K^{-1} respectively. However, the extrapolation to absolute zero using values of low temperature specific heat given in Part 76.4 and three-point integration of equations 76c and 76d appears to be fairly insensitive to the choice of temperature range because choosing 1000 K would only increase the value of $100\Delta\varepsilon$ by 0.002 for the *a*-axis and 0.005 for the *c*-axis.

76.4: Low temperature specific heat of osmium

This is an extension of the Tables given by Arblaster 1995. C_p values in J mol^{-1} K^{-1}:

Table 76d. Low temperature specific heat values for osmium

T K	10	15	20	25	30	35	40	45	50
C_p	0.0417	0.116	0.290	0.636	1.252	2.104	3.139	4.322	5.604
T K	60	70	80	90	100	110	120	130	140
C_p	8.205	10.563	12.661	14.448	15.939	17.182	18.231	19.132	19.912
T K	150	160	170	180	190	200	210	220	230
C_p	20.577	21.085	21.533	21.975	22.377	22.695	22.928	23.163	23.441
T K	240	250	260	270	280	290	293.15	298.15	300
C_p	23.715	23.929	24.119	24.290	24.444	24.584	24.625	24.688	24.711

High temperature specific heat equation 293.15 to 3400 K:

$$C_p\,(\text{J mol}^{-1}\,\text{K}^{-1}) = 2.64636 \times 10^{-4}\,T + 1.15788 \times 10^{-6}\,T^{2} + 1.599912 \times 10^{-10}\,T^{3} - 150378/\,T^{2} + 26.1938 \qquad (76g)$$

Table 76b. Crystallographic properties of osmium

Values below 293.15 K are estimated.

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 ε_T *a*	100 ε_T *c*	100 ε_T avr
0	0	0	0	- 0.100	- 0.119	- 0.106
10	0.035	0.035	0.035	- 0.100	- 0.119	- 0.106
20	0.15	0.15	0.15	- 0.100	- 0.119	- 0.106
30	0.49	0.51	0.49	- 0.100	- 0.118	- 0.106
40	1.04	1.10	1.06	- 0.099	- 0.118	- 0.105
50	1.62	1.78	1.70	- 0.098	- 0.116	- 0.104
60	2.25	2.43	2.31	- 0.096	- 0.114	- 0.102
70	2.72	2.97	2.81	- 0.094	- 0.111	- 0.099
80	3.11	3.42	3.21	- 0.090	- 0.108	- 0.096
90	3.41	3.79	3.54	- 0.087	- 0.104	- 0.093
100	3.64	4.08	3.79	- 0.084	- 0.101	- 0.089
110	3.82	4.31	3.98	- 0.080	- 0.096	- 0.085
120	3.96	4.50	4.14	- 0.076	- 0.092	- 0.081
130	4.07	4.67	4.27	- 0.072	- 0.087	- 0.077
140	4.16	4.81	4.38	- 0.068	- 0.083	- 0.073
150	4.24	4.93	4.47	- 0.064	- 0.078	- 0.068
160	4.29	5.02	4.53	- 0.059	- 0.073	- 0.064
170	4.33	5.10	4.59	- 0.055	- 0.068	- 0.059
180	4.37	5.19	4.64	- 0.051	- 0.063	- 0.055
190	4.41	5.26	4.69	- 0.046	- 0.057	- 0.050
200	4.43	5.33	4.73	- 0.042	- 0.052	- 0.045
210	4.45	5.40	4.76	- 0.038	- 0.047	- 0.041
220	4.47	5.45	4.80	- 0.033	- 0.041	- 0.036
230	4.49	5.51	4.83	- 0.029	- 0.036	- 0.031
240	4.50	5.57	4.86	- 0.024	- 0.030	- 0.026
250	4.52	5.63	4.89	- 0.020	- 0.025	- 0.021
260	4.53	5.68	4.91	- 0.015	- 0.019	- 0.016
270	4.54	5.73	4.94	- 0.011	- 0.013	- 0.011
280	4.55	5.78	4.96	- 0.006	- 0.008	- 0.007
290	4.56	5.83	4.98	- 0.001	- 0.002	- 0.002
293.15	4.57	5.85	4.99	0	0	0
300	4.57	5.87	5.00	0.003	0.004	0.003
400	4.60	6.28	5.16	0.049	0.065	0.054
500	4.63	6.68	5.32	0.095	0.130	0.107
600	4.66	7.09	5.47	0.142	0.199	0.161
700	4.69	7.49	5.63	0.189	0.272	0.216
800	4.73	7.89	5.78	0.236	0.349	0.273
900	4.76	8.30	5.94	0.283	0.430	0.332
1000	4.79	8.70	6.09	0.331	0.516	0.393
1100	4.82	9.10	6.25	0.379	0.605	0.455
1200	4.85	9.49	6.40	0.428	0.699	0.518
1300	4.88	9.89	6.55	0.477	0.796	0.583

Table 76c. Crystallographic properties of osmium

Values below 293.15 K are estimated.

T K	*a* nm	*c* nm	*c*/*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.27315	0.43148	1.5797	0.26723	8.395	22661
10	0.27315	0.43148	1.5797	0.26723	8.395	22661
20	0.23715	0.43148	1.5797	0.26723	8.395	22661
30	0.27315	0.43148	1.5797	0.26723	8.395	22661
40	0.27315	0.43148	1.5797	0.26723	8.395	22660
50	0.27315	0.43149	1.5797	0.26724	8.395	22659
60	0.27316	0.43150	1.5797	0.26724	8.396	22658
70	0.27316	0.43151	1.5797	0.26725	8.396	22656
80	0.27317	0.43152	1.5797	0.26726	8.397	22654
90	0.27318	0.43154	1.5797	0.26727	8.398	22652
100	0.27319	0.43156	1.5797	0.26728	8.399	22649
110	0.23720	0.43157	1.5797	0.26729	8.400	22647
120	0.27321	0.43159	1.5797	0.26731	8.401	22644
130	0.27322	0.43161	1.5797	0.26731	8.402	22641
140	0.27323	0.43163	1.5797	0.26732	8.403	22638
150	0.27325	0.43165	1.5797	0.26734	8.404	22635
160	0.27326	0.43168	1.5797	0.26735	8.405	22632
170	0.27327	0.43170	1.5797	0.26736	8.406	22629
180	0.27328	0.43172	1.5798	0.26738	8.408	22626
190	0.27329	0.43175	1.5798	0.26739	8.409	22623
200	0.27331	0.43176	1.5798	0.36740	8.410	22620
210	0.27332	0.43179	1.5798	0.26742	8.411	22616
220	0.27333	0.43181	1.5798	0.26743	8.412	22613
230	0.27334	0.43183	1.5798	0.26744	8.414	22610
240	0.27335	0.43186	1.5799	0.26746	8.415	22607
250	0.27337	0.43188	1.5799	0.26747	8.416	22603
260	0.27338	0.43191	1.5799	0.26748	8.417	22600
270	0.27339	0.43193	1.5799	0.26750	8.419	22596
280	0.27340	0.43196	1.5799	0.26751	8.420	22593
290	0.27342	0.43198	1.5799	0.26753	8.421	22590
293.15	0.27342	0.43199	1.5800	0.26753	8.421	22589
300	0.27343	0.43201	1.5800	0.26754	8.422	22586
400	0.27355	0.43227	1.5802	0.26769	8.435	22552
500	0.27368	0.43255	1.5805	0.26785	8.448	22517
600	0.27381	0.43285	1.5808	0.26801	8.462	22480
700	0.27394	0.43316	1.5813	0.26818	8.476	22443
800	0.27406	0.43350	1.5817	0.26836	8.491	22404
900	0.27419	0.43385	1.5823	0.26855	8.506	22365
1000	0.27433	0.43422	1.5829	0.26874	8.521	22325
1100	0.27446	0.43460	1.5835	0.26894	8.537	22284
1200	0.27459	0.43501	1.5842	0.26915	8.553	22241
1300	0.27472	0.43543	1.5850	0.26936	8.570	22198

$$d1 = (a^2/3 + c^2/4)^{1/2} \quad d2 = a$$

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77 IRIDIUM Ir

This review is based on the assessment of Arblaster 2010

Atomic Weight: 192.217 (2) (Meija 2017)

Structure: Face-centered cubic (cF4)

The freezing point is a secondary fixed point on ITS-90 at 2719 (6) K (Bedford et al. 1996).

77.1 Low temperature region

Thermal expansion coefficients of White and Pawlowicz 1970 (3-85, 283 K) were combined with the revised value of (6.45 ± 0.05) x 10^{-6} K^{-1} at 283 K obtained by White 1988. Measurements above 21 K were fitted to Equation A using specific heat (C_p) values given in Part 77.4:

$$0 - 21\ K: \quad \alpha\ (K^{-1}) = 8.65118 \times 10^{-10}\ T + 5.00520 \times 10^{-12}\ T^{3} + 4.80639 \times 10^{-15}\ T^{5} + 1.37616 \times 10^{-17}\ T^{7} \qquad (77a)$$

$$21 - 293.15\ K: \quad \alpha\ (K^{-1}) = C_p\,(2.68909 \times 10^{-7} - 2.49303 \times 10^{-11} T - 9.14579 \times 10^{-7}/T) \qquad (77b)$$

On the basis 100Δε length changes derived from a smooth fit to the lattice parameter measurements of Schaake 1968 (4.2-298 K) overall show a bias of only 0.001 high while those of Schröder et al. 1972 (92-1918 K) are initially 0.027 low at 92 K and then converge to the room temperature values. Thermal expansion coefficients of Valentiner and Wallot 1915 (98-283 K) scatter 5% low to 4% high.

77.2 High temperature region

In addition to the lattice parameter measurements determined by Schröder et al. 1972, values were also determined by Singh 1968 (303-1138 K) while dilatometric measurements were determined by Holborn and Valentiner 1907 (1335-2004 K), Krikorian 1960 (298-2273 K) and Halvorson and Wimber 1972 (1164-2494 K). Although subsequently it was shown that the samples used by Halvorson and Wimber 1972 may have contained up to 0.5% tungsten, these measurements were revised by Wimber 1976 who gave the results in the form of an equation which incorporated the measurements of Singh 1968. Unfortunately this equation showed a maximum in the derived thermal expansion coefficient at 2399 K which could be traced to the derivative of the thermal expansion coefficient, dα/dT showing a maximum at 1351 K. In order to overcome this unnatural behavior the procedure given in Part 77.3 was adopted which still is in agreement with the measurements of Wimber 1976 up to 2000 K but above this temperature values begin to diverge. Because the adopted procedure assumes that dα/dT is constant above 1351 K then this is considered as representing the "crystallographic" properties of iridium at high temperature because the onset of thermal vacancy effects

should cause an increase in dα/dT. It was found that a best fit to the data was achieved by deriving two equations covering the ranges 293.15 – 800 K and 800 – 2719 K:

$$293.15 - 800\ K: \varepsilon_T = 5.13336 \times 10^{-6} T + 4.709895 \times 10^{-9} T^2 - 8.04620 \times 10^{-12} T^3 + 7.338225 \times 10^{-15} T^4 - 2.35176 \times 10^{-18} T^5 - 1.75600 \times 10^{-3} \quad (77c)$$

$$800 - 2719\ K: \varepsilon_T = 6.59094 \times 10^{-6} T - 1.075625 \times 10^{-9} T^2 + 1.78108 \times 10^{-12} T^3 - 4.665925 \times 10^{-16} T^4 + 4.84024 \times 10^{-20} T^5 - 1.84421 \times 10^{-3} \quad (77d)$$

Because of the procedure adopted all values given in Table 77c above 2000 K are considered to be tentative.

On the basis 100Δε the abnormal behavior of the equation given by Wimber 1976 becomes evident above about 1900 K with the deviation reaching 0.070 low at 2500 K. Length changes derived from the lattice parameters of Schröder et al. 1972 deviate in a sinusoidal manner from 0.046 high at 1400 falling to 0.056 low at 1900 K while a similar behavior is observed in the dilatometric measurements of Holborn and Valentiner 1907 which deviate up to 0.027 high at 1400 K before falling to 0.050 low at 2000 K and also in the values of Krikorian 1964 which deviate up to 0.032 at 1273 K before trending to 0.095 low at 2273 K. Volume ratios of Hüpf and Pottlacher 2011 (2000-2719 K) converted to length change values trends from 0.19 low to 0.14 low.

Table 77a. Lattice parameter of iridium at 293.15 K

References	Original Temperature K	*a* nm
Owen and Yates 1933	291	0.38392
Swanson et al. 1955	299	0.38395
Schaake 1968	298	0.38397
Singh 1968	303	0.38390
Schröder et al. 1972	297	0.38386
	Selected	0.38392(6)

At 293.15 K: Density 22562 (11) kg m^{-3} Molar volume 8.519 (4) cm^3 mol^{-1}.

77.3 Estimate of the high temperature properties of iridium

The equation given by Wimber 1976 reaches a maximum in the derivative dα/dT at 1351 K. In practice the derivative will either increase or remain constant above this temperature but because the actual increase cannot be predicted then it is assumed to remain constant at a value of 4.36 x 10^{-9} K^{-2}. Utilizing the equation given by Wimber 1976 up to 1351 K then the thermodynamic thermal expansion coefficient (α) above this temperature is given by equation 77e:

$$\alpha\ (K^{-1}) = 3.68327 \times 10^{-6} + 4.36 \times 10^{-9} T \quad (77e)$$

Relative length changes can then be calculated from equation 77f:

$$\ln(L_T) = 3.68327 \times 10^{-6} T + 2.18 \times 10^{-9} T^2 - 8.35310 \times 10^{-4} \quad (77f)$$

where $L_T = 1 + \varepsilon$. Equations 77e and 77f were combined to derive the thermal expansion coefficient relative to 293.15 K as $\alpha^* = \alpha \times L_T$. Values of α^* were then calculated at 50 K intervals from 1400 to 2700 K and combined with values at 50 K intervals from 500 to 1350 K derived from the equation given by Wimber 1976 which were then adjusted to conform to the selected value of the thermal expansion coefficient at 293.15 K. It was found that two equations covering the intervals 293.15 to 800 K and 800 to 2700 K were required to give the best fit and these equations were then integrated to derive equations 77c and 77d.

77.4 Low temperature specific heat values of iridium

Furukawa et al. 1974 gave specific heat only to the nearest 0.01 J mol^{-1} K^{-1} above 55 K in their Table 8 but also gave values to the nearest 0.001 cal mol^{-1} K^{-1} in their Appendix D. These values have been combined to give all values to three decimal places in J mol^{-1} K^{-1}.

Table 77b. Low temperature specific heat values for iridium

T K	10	15	20	25	30	35	40	45	50
C_p	0.0587	0.159	0.398	0.916	1.804	2.972	4.333	5.813	7.314
T K	60	70	80	90	100	110	120	130	140
C_p	10.109	12.460	14.393	16.000	17.359	18.510	19.472	20.267	20.933
T K	150	160	170	180	190	200	210	220	230
C_p	21.493	21.979	22.405	22.786	23.129	23.435	23.707	23.949	24.163
T K	240	250	260	270	280	290	293.15	298.15	300
C_p	24.351	24.514	24.665	24.794	24.908	25.011	25.042	25.090	25.104

Table 77c. Low temperature crystallographic properties of iridium

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	- 0.133	0.38341	0.27111	8.486	22652
10	0.014	- 0.133	0.38341	0.27111	8.486	22652
20	0.090	- 0.133	0.38341	0.27111	8.486	22652
30	0.43	- 0.132	0.38341	0.27111	8.486	22652
40	1.06	- 0.132	0.38341	0.27112	8.486	22651
50	1.82	- 0.130	0.38342	0.27112	8.486	22650
60	2.55	- 0.128	0.38343	0.27112	8.487	22649
70	3.17	- 0.125	0.38344	0.27113	8.488	22647
80	3.68	- 0.122	0.38345	0.27114	8.488	22645
90	4.10	- 0.118	0.38347	0.27115	8.489	22642
100	4.47	- 0.114	0.38348	0.27116	8.490	22639
110	4.77	- 0.109	0.38350	0.27118	8.492	22636
120	5.03	- 0.104	0.38352	0.27119	8.493	22633
130	5.24	- 0.099	0.38354	0.27120	8.494	22629
140	5.42	- 0.094	0.38356	0.27122	8.496	22626
150	5.57	- 0.088	0.38358	0.27123	8.497	22622
160	5.70	- 0.082	0.38360	0.27125	8.498	22618
170	5.81	- 0.077	0.38363	0.27126	8.500	22614
180	5.91	- 0.071	0.38365	0.27128	8.501	22610
190	6.00	- 0.065	0.38367	0.27130	8.503	22606
200	6.08	- 0.059	0.38369	0.27131	8.504	22602
210	6.15	- 0.053	0.38372	0.27133	8.506	22598
220	6.21	- 0.047	0.38374	0.27135	8.508	22594
230	6.26	- 0.040	0.38377	0.27136	8.509	22589
240	6.31	- 0.034	0.38379	0.27138	8.511	22585
250	6.35	- 0.028	0.38381	0.27140	8.512	22581
260	6.39	- 0.021	0.38384	0.27141	8.514	22577
270	6.42	- 0.015	0.38386	0.27143	8.516	22572
280	6.44	- 0.009	0.38389	0.27145	8.517	22568
290	6.47	- 0.002	0.38391	0.27147	8.519	22563
293.15	6.47	0	0.38392	0.27147	8.519	22562

$$d = a/\sqrt{2}$$

Table 77d. High temperature crystallographic properties of iridium

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
293.15	6.47	0	0.38392	0.27147	8.519	22562
300	6.48	0.044	0.38394	0.27148	8.521	22559
400	6.61	0.070	0.38419	0.27166	8.537	22515
500	6.73	0.137	0.38445	0.27184	8.554	22470
600	6.90	0.205	0.38471	0.27203	8.572	22424
700	7.12	0.275	0.38498	0.27222	8.590	22377
800	7.41	0.348	0.38526	0.27242	8.609	22328
900	7.75	0.424	0.38555	0.27262	8.628	22278
1000	8.12	0.503	0.38585	0.27284	8.649	22225
1100	8.51	0.587	0.38617	0.27307	8.670	22169
1200	8.92	0.675	0.38651	0.27330	8.693	22112
1300	9.34	0.767	0.38686	0.27355	8.717	22051
1400	9.78	0.863	0.38723	0.27382	8.742	21988
1500	10.21	0.964	0.38762	0.27409	8.768	21922
1600	10.65	1.069	0.38802	0.27438	8.796	21854
1700	11.10	1.179	0.38845	0.27467	8.824	21782
1800	11.54	1.294	0.38889	0.27498	8.854	21709
1900	11.98	1.413	0.38934	0.27531	8.886	21632
2000	12.41	1.537	0.38982	0.27564	8.918	21553
2100	12.85	1.665	0.39031	0.27599	8.952	21472
2200	13.28	1.798	0.39082	0.27635	8.987	21388
2300	13.71	1.935	0.39135	0.27673	9.024	21301
2400	14.14	2.077	0.39190	0.27711	9.062	21212
2500	14.58	2.224	0.39265	0.27751	9.101	21121
2600	15.02	2.375	0.39304	0.27792	9.141	21028
2700	15.47	2.531	0.39364	0.27834	9.183	20932
2719	15.56	2.562	0.39375	0.27843	9.191	20913

$$d = a/\sqrt{2}$$

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78 PLATINUM Pt

This review is based on the assessments of Arblaster 1997, 2006.

Atomic Weight: 195.084 (9) (Meija 2017)

Structure: Face-centered cubic (cF4)

The freezing point is a secondary fixed point on ITS-90 at 2041.3 (4) K (Bedford et al. 1996).

78.1 Low temperature region

Thermal expansion coefficients of White 1972 (3-85, 283 K) were combined with thermal expansion coefficients derived form the length change measurements of Edsinger et al. 1986 (246-841 K). Above 26 K the data were correlated using equation A and the specific heat values given in Part 78.4:

$$0 - 26\ \text{K}: \quad \alpha\ (\text{K}^{-1}) = 1.83531 \times 10^{-9}\, T + 4.86241 \times 10^{-11}\, T^{3} + 5.06150 \times 10^{-14}\, T^{5} - 6.06097 \times 10^{-17}\, T^{7} \qquad (78a)$$

$$26 - 71\ \text{K}: \quad \alpha\ (\text{K}^{-1}) = C_p\,(3.84248 \times 10^{-7} - 3.38481 \times 10^{-10} T - 1.12981 \times 10^{-6}/T) \qquad (78b)$$

$$71 - 272\ \text{K}: \quad \alpha\ (\text{K}^{-1}) = C_p\,(3.51722 \times 10^{-7} - 2.73616 \times 10^{-12} T - 5.20350 \times 10^{-7}/T) \qquad (78c)$$

Although using a completely different approach to interpolate within the region 85 to 245 K, thermal expansion coefficients selected by Kirby 1991 agree with those determined from the above equations to within $7 \times 10^{-8}\ \text{K}^{-1}$.

78.2 High temperature region

Above 272 K dilatometric measurements of Edsinger et al. 1986 (246-841 K), Holborn and Day 1901 (273-1023 K) and Austin 1932 (273-873 K) were converted to thermal expansion coefficients relative to 293.15 K (α^*) and combined with the thermal expansion values of Hahn and Kirby 1972 (293-1900 K) to give an equation accurate to the value $2 \times 10^{-8}\ \text{K}^{-1}$. The selected values of Kirby 1991 agree with equation 78d to within $5 \times 10^{-8}\ \text{K}^{-1}$.

$$\alpha^*\ (\text{K}^{-1}) = 7.08788 \times 10^{-6} + 1.04970 \times 10^{-8}\, T - 2.00846 \times 10^{-11}\, T^{2} + 2.28200 \times 10^{-14}\, T^{3} - 1.18453 \times 10^{-17}\, T^{4} + 2.37348 \times 10^{-21}\, T^{5} \qquad (78d)$$

$$\varepsilon_T = 7.08788 \times 10^{-6}\, T + 5.24850 \times 10^{-9}\, T^{2} - 6.69487 \times 10^{-12}\, T^{3} + 5.70500 \times 10^{-15}\, T^{4} - 2.36906 \times 10^{-18}\, T^{5} + 3.95580 \times 10^{-22}\, T^{6} - 2.39745 \times 10^{-3} \qquad (78e)$$

However, at high temperature equation 78d leads to bulk not lattice thermal expansion. An average thermal vacancy concentration parameter (c_V) of $(7 \pm 2) \times 10^{-4}$ at the melting point is established from measurements on copper (Hehenkamp et al. 1992), silver

(Mosig et al. 1992), aluminum (Simmons and Balluffi 1960a) and gold (Simmons and Balluffi 1962). For platinum the enthalpy of monovacancy formation is also well established as $H_V = 1.51$ eV from the measurements of Jackson 1965, Heigl and Sizmann 1972 and Senoo et al. 1973 which together with the above average value of c_V leads to an entropy of monovacancy formation of $S_V/k = 1.32$. This value is in excellent agreement with a value of 1.3 calculated by Schumacher et al. 1968 from a re-analysis of the self-diffusion experiments of Kidson and Ross 1958 and Cattaneo et al. 1962 and 1.45 estimated by Heigl and Sizmann 1972 from results using a millisecond heat pulsing technique. The resulting thermal vacancy corrections are then given by:

$$\varepsilon_T L - \varepsilon_T a = (1/3)\, e^{(1.32 - 17523/T)} \qquad \alpha_L - \alpha_a = (5841/T^2)\, e^{(1.32 - 17523/T)}$$

Equations 78d and 78e were then combined with the thermal vacancy corrections in order to give equations representing "crystallographic" values over the temperature range from 272 K to the freezing point:

$$\alpha^* (K^{-1}) = 7.03139 \times 10^{-6} + 1.08937 \times 10^{-8} T - 2.10071 \times 10^{-11} T^2 + 2.36623 \times 10^{-14} T^3 - 1.20728 \times 10^{-17} T^4 + 2.34219 \times 10^{-21} T^5 \quad (78f)$$

$$\varepsilon_T = 7.03139 \times 10^{-6} T + 5.44686 \times 10^{-9} T^2 - 7.00236 \times 10^{-12} T^3 + 5.91557 \times 10^{-15} T^4 - 2.41456 \times 10^{-18} T^5 + 3.90366 \times 10^{-22} T^6 - 2.39164 \times 10^{-3} \quad (78g)$$

Because of poor agreement and scatter in the experimental data, equations 78f and 78g are considered to give a more satisfactory representation of crystallographic data than could be obtained from actual lattice parameter measurements. On the basis $100\Delta\varepsilon$ dilatometric measurements of Dorsey 1907 (93-293 K), Scheel 1907 (83-373 K), Scheel and Heuse 1907 (90-289 K), Henning 1907 (82-289 K), Nix and MacNair 1942 (85-368 K), Branchereau et al. 1962 (573 K), Amatuni et al. 1976 (373-1273 K) and participant No.7 (373-1073 K) noted by Fitzer and Weisenburger 1972 all agree with the selected values to within 0.002.

Table 78a. Lattice parameter of platinum at 293.15 K

References	Original Temperature K	*a* nm	Note
Van Arkel 1928	RT	0.39223	
Stenzel and Weerts 1931	293	0.39232	
Owen and Yates 1933a, 1933b	291	0.39240	
Owen and Yates 1934	288	0.39244	
Moeller 1937	293	0.39226	
Esch and Schneider 1944	RT	0.39239	
Goldschmidt and Land 1947	RT	0.39242	
Grube et al. 1951	RT	0.39238	
Swanson and Tatge 1953	298	0.39232	
Kidron 1965	298	0.39237	
Evans and Fischer 1971	293	0.39236	
Schröder et al. 1972	297	0.39234	
Waseda et al. 1975	298	0.39241	
Stankus and Khairulin 1992	293	0.39240	a
	Selected	0.39236 (6)	

Note for Table 78a

a. From direct density measurement 21445 kg m^{-3}

At 293.15 K for Pt: Density 21452 (10) kg m^{-3} Molar volume 9.094 (4) cm^3 mol^{-1}

78.3 Deviations of high temperature experimental values from the selected values

Table 78b. Lattice parameter values

References	Temperature Range K	Deviations 100Δε
Owen and Yates 1934	288-873	Trends to maximum deviation of 0.030 high at 481 K
Shinoda 1934	288-1373	Trends to maximum deviation of 0.087 low at 1231 K
Esser et al. 1938	293-1373	Trends to 0.085 high
Eisenstein 1946	1148	Bias 0.093 low
Edwards et al. 1951	291-2005	Trends to maximum deviation of 0.057 low at 1705 K
Mauer and Bolz 1955	273-1663	Trends to 0.15 high
Brand and Goldschmidt 1956	273-1607	Trends to maximum deviation of 0.036 low at 1073 K
Lui et al. 1970	286-701	Trends to 0.018 low
Evans and Fischer 1971	293-1783	Trends to 0.019 high
Schröder et al. 1972	85-1933	Trends to a maximum deviation of 0.12 high at 1400 K
Waseda et al. 1975	298-2029	Over measurement range 1059-2029 K trends 0.12 low to 0.062 high

Table 78c. Dilatometric values on the basis 100Δε

References	Temperature Range K	Deviations 100Δε	Notes
Esser and Eusterbrock 1941	273-1273	Trends to 0.007 low	
Masumoto and Kobayashi 1965	313	Bias 0.006 low	
Vertogradskii 1969	356-1589	Trends to 0.36 high	
Cowder et al. 1970	293-1773	Trends to 0.045 high	a
Weisenburger 1970	573-1173	Averages bias 0.004 high	b
Fitzer 1971	573-1273	Averages bias 0.009 high	c
Fitzer and Weisenburger 1972	373-1873	Averages bias 0.007 high up to 1300 K	
Stankus and Khairulin 1992	293-2042	Trends to 0.17 low	d
Hüpf and Pottlacher 2011	1200-2042	Trends to 0.29 low	e

Notes for Table 78c

a. AGARD (Advisory Panel for Aerospace Research and Development) five participants.

b. AGARD – ten participants.

c. AGARD – four participants (fifth participant No. 7 treated separately)

d. Length changes derived from direct density measurements

e. Based on length change values derived from volume ratios $V/V_{293.15\ K}$

Thermal expansion coefficients of Valentiner and Wallot 1915 deviate to a maximum of 3% low at 217 K while values estimated from a graphical representation by Kraftmakher 1967 (1000-1900 K) trend to 25% high.

78.4 Low temperature specific heat of Platinum

This is an extension of the Tables given by Arblaster 1994. C_p values in J mol^{-1} K^{-1}**:**

Table 78d. Low temperature specific heat values for platinum

T K	10	15	20	25	30	35	40	45	50
C_p	0.230	0.690	1.550	2.793	4.323	5.994	7.632	9.210	10.699
T K	60	70	80	90	100	110	120	130	140
C_p	13.326	15.437	17.078	18.425	19.559	20.489	21.245	21.863	22.376
T K	150	160	170	180	190	200	210	220	230
C_p	22.810	23.185	23.513	23.803	24.057	24.278	24.463	24.623	24.773
T K	240	250	260	270	280	290	293.15	298.15	300
C_p	24.920	25.066	25.210	25.346	25.469	25.576	25.605	25.648	25.663

Table 78e. Bulk properties of platinum

T K	$\alpha \times 10^6$ K^{-1}	100 ε_T	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
1300	11.79	1.039	9.380	20797
1400	12.16	1.160	9.414	20723
1500	12.56	1.285	9.449	20646
1600	13.01	1.414	9.485	20567
1700	13.56	1.549	9.523	20485
1800	14.26	1.690	9.563	20400
1900	15.17	1.839	9.605	20310
2000	16.40	2.000	9.650	20214
2041.3	17.03	2.070	9.670	20173

This Table is considered to be identical to Table 78f below 1300 K

Table 78f. Crystallographic properties of platinum

T K	$\alpha \times 10^6$ K^{-1}	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	- 0.193	0.39160	0.27690	9.041	21577
10	0.071	- 0.193	0.39160	0.27690	9.041	21577
20	0.51	- 0.193	0.39160	0.27690	9.041	21576
30	1.45	- 0.192	0.39161	0.27691	9.041	21576
40	2.61	- 0.190	0.39161	0.27691	9.042	21575
50	3.69	- 0.187	0.39163	0.27692	9.043	21573
60	4.60	- 0.183	0.39164	0.27693	9.044	21570
70	5.32	- 0.178	0.39166	0.27695	9.045	21567
80	5.89	- 0.172	0.39168	0.27696	9.047	21563
90	6.37	- 0.166	0.39171	0.29698	9.049	21559
100	6.77	- 0.160	0.39173	0.27700	9.050	21555
110	7.10	- 0.153	0.39176	0.27702	9.052	21550
120	7.37	- 0.145	0.39179	0.27704	9.054	21546
130	7.59	- 0.138	0.39182	0.27706	9.056	21541
140	7.78	- 0.130	0.39185	0.27708	9.058	21536
150	7.93	- 0.122	0.39188	0.27710	9.060	21531
160	8.07	- 0.114	0.39191	0.27712	9.063	21526
170	8.19	- 0.106	0.39194	0.27715	9.065	21521
180	8.29	- 0.098	0.39198	0.27717	9.067	21515
190	8.38	- 0.090	0.39201	0.27719	9.069	21510
200	8.46	- 0.081	0.39204	0.27722	9.072	21504
210	8.53	- 0.073	0.39207	0.27724	9.074	21499
220	8.59	- 0.064	0.39211	0.27726	9.076	21493
230	8.64	- 0.056	0.39214	0.27729	9.079	21488
240	8.70	- 0.047	0.39218	0.27731	9.081	21482
250	8.75	- 0.038	0.39221	0.27733	9.083	21477
260	8.80	- 0.029	0.39224	0.27736	9.086	21471
270	8.85	- 0.021	0.39228	0.27738	9.088	21466
280	8.89	- 0.012	0.39231	0.27741	9.091	21459
290	8.92	- 0.003	0.39235	0.27743	9.093	21454
293.15	8.93	0	0.39236	0.27744	9.094	21452
300	8.95	0.006	0.39238	0.27746	9.095	21448
400	9.26	0.097	0.39274	0.27771	9.120	21389
500	9.48	0.191	0.39311	0.27797	9.146	21329
600	9.71	0.287	0.39349	0.27824	9.172	21268
700	9.94	0.386	0.39387	0.27851	9.199	21205
800	10.19	0.487	0.39427	0.27879	9.227	21142
900	10.47	0.591	0.39468	0.27908	9.256	21076
1000	10.77	0.698	0.39510	0.27938	9.285	21009
1100	11.10	0.808	0.39553	0.27968	9.316	20940
1200	11.43	0.921	0.39597	0.28000	9.347	20870
1300	11.77	1.038	0.39643	0.28032	9.380	20797
1400	12.11	1.159	0.39691	0.28066	9.414	20723
1500	12.48	1.284	0.39740	0.28100	9.448	20647
1600	12.86	1.412	0.39790	0.28136	9.484	20568
1700	13.31	1.545	0.39842	0.28173	9.522	20488
1800	13.86	1.683	0.39896	0.28211	9.561	20404
1900	14.58	1.827	0.39953	0.28251	9.601	20318
2000	15.57	1.981	0.40013	0.28294	9.645	20226
2041.3	16.07	2.047	0.40039	0.28312	9.664	20187

Interatomic distance calculations for Table 78f: $d = a/\sqrt{2}$

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79 GOLD Au

Atomic weight: 196.966570 (4) (Meija 2017)

Structure: Face-centered cubic (cF4)

The freezing point is a primary fixed point on ITS-90 at 1337.33 K (Preston-Thomas 1990).

79.1 Low temperature

Thermal expansion coefficients of White and Collins 1972 (2-85, 283 K) and McLean et al. 1972 (1-26 K) were combined with the values above 20 K fitted to Equation A using specific heat (C_p) values calculated from the equation of Martin 1987. The thermal expansion equation had an overall accuracy of 1.1 x 10^{-8} K^{-1} and was extrapolated to 293.15 K:

$$\alpha\ (K^{-1}) = C_p\ (5.43508 \times 10^{-7} + 5.73104 \times 10^{-11}\ T - 5.59154 \times 10^{-8}\ /T\ ) \qquad (79a)$$

The derived thermal expansion coefficient of 14.13 x 10^{-6} K^{-1} at 293.15 K agrees exactly with the value derived from the equation of Austin 1932 (273-1173 K) and in satisfactory agreement with the value of 14.21 x 10^{-6} K^{-1} derived from the equation of Esser and Eusterbrock 1941 (273-1223 K). However, the value of 13.4 x 10^{-6} K^{-1} determined by Straumanis 1971 (288-338 K) from lattice parameter measurements is notably lower. Thermal expansion coefficients of Kos and Lamarche 1969 (5-15 K) agree with the selected values to within 2 x 10^{-8} K^{-1}.

In order for inclusion in Table 79c thermal expansion measurements of Dorsey 1907, Dorsey 1908 and Leksina and Novikova 1963 were converted to length change values.

79.2 High temperature

Selected length change values derived from the lattice parameter values of Merryman and Kempter 1965 (293-1275 K) and the lattice parameter and dilatometric measurements of Simmons and Balluffi 1962 (293-1323 K) were combined except that the dilatometric measurements were not considered above 923 K in order to avoid values being affected by thermal vacancy effects:

$$\varepsilon_T = 1.15417 \times 10^{-5}\ T + 5.76138 \times 10^{-9}\ T^{\,2} - 3.68063 \times 10^{-12}\ T^{\,3} + 1.60423 \times 10^{-15}\ T^{\,4} - 3.79769 \times 10^{-3} \qquad (79b)$$

Lattice parameter measurements of Esser et al. 1938 (293-1323 K) were only shown graphically. Deviations of other lattice and dilatometric values are given in Part 79.4

Table 79a. Lattice parameter of gold at 293.15 K

References	Original Temperature K	*a* nm	Note
Sachs and Weerts 1930	283	0.40793	a
Stenzel and Weerts 1931	298	0.40785	
Owen and Yates 1933a	291	0.40785	
Owen and Yates 1933b	291	0.40786	
Vegard and Kloster 1934	RT	0.40786	
Jette and Foote 1935	298	0.40786	
Straumanis and Ievinš 1936	292	0.40786	
Kubaschewski and Weibke 1938	RT	0.40786	
Owen and Rowlands 1940	291	0.40785	
Fricke 1941	RT	0.40789	
Owen and Roberts 1945	291	0.40785	
Ellwood and Bagley 1951-1952	298	0.40785	
Swanson and Tatge 1953	298	0.40786	
Geach and Summers-Smith 1953-1954	293	0.40785	
Güntert and Faessler 1956	292	0.40785	
Weyerer 1956, 1957	298	0.40785	
Day 1961	RT	0.40787	
Mueller and Heaton 1961	298	0.40781	a
Calvert and Henry 1962	294	0.40787	
Dutta and Dayal 1963	298	0.40779	a
Maeland and Flanagan 1964	293	0.40784	
Merryman and Kempter 1965	298	0.40787	
Batchelder and Simmons 1965	298	0.40788	
Rolfe 1966	290	0.40786	
Nagender-Naidu and Houska 1971	298	0.40778	a
Straumanis 1971	298	0.40789	
	Selected	0.40786 (3)	

Note for Table 79a

a. Not included in the average

The accuracy assigned to the selected value takes into account the spread in the accepted values.

At 293.15 K: Density 19283 (4) kg m^{-3} Molar volume 10.215 (2) cm^3 mol^{-1}.

79.3 Bulk properties of gold

Lattice parameter and dilatometric length change values of Simmons and Balluffi 1962 extrapolated to freezing point lead to C_V = 7.2 x 10^{-4}, H_V = 0.94 eV and S_V/k = 1.0. However, self consistency requires S_V/k = 0.92 which is selected. Schaefer et al. 1987 obtain H_V = 0.89 (4) eV from positron annihilation lifetime spectrosocopy which agrees satisfactorily.

79.4 Deviations of experimental values from the selected values

Table 79b. Dilatometric values on the basis 100Δε

References	Temperature Range K	Deviations 100Δε
Dorsey 1907	93-295	Average bias 0.002 low
Dorsey 1908	103-288	Average bias 0.005 low
Kurnakow and Ageew 1931	293-873	Trends to 0.095 low
Austin 1932	293-1173	Trends to 0.017 low
Esser and Eusterbrock 1941	273-1223	Trends to 0.039 low
Nix and MacNair 1941	86-1003	Below room temperature are initially 0.002 high and then trend to agree exactly with the selected values above 160 K. Above room temperature trends to 0.025 low
Leksina and Novikova 1963	90-1323	Below room temperature are initially 0.005 high then trend towards the selected values. Above room temperature trends to 0.12 low
Fraser and Hollis Hallett 1965	8-99	Average bias 0.004 low
Vest 1971	293-1072	Trends to 0.11 low
Fitzer 1971	293-1273	Range 573 to 1173 K only - average of 10 laboratories trends to 0.006 low
Fitzer and Weisenburger 1972	293-1173	Average of 16 laboratories trends to 0.005 low
Suh et al. 1988	293-1100	Trends to 0.056 low

Table 79c. Lattice parameter values on the basis 100Δε

References	Temperature Range K	Deviations 100Δε
Shinoda 1934	288-732	Trends to 0.10 low
Warlimont 1959	388-993	Trends to maximum 0.037 high at 626 K then falls to average 0.010 low above 850 K
Dutta and Dayal 1963	298-1151	Trends to 0.086 low
Rolfe 1966	290-698	Average bias 0.010 low
Nagender-Naidu and Houska 1971	80-298	Average bias 0.009 high
Suh et al. 1988	293-1325	Scatters 0.054 low to 0.002 low
Vesnin and Shubin 1988	293-1273	Trends to 0.10 high

Table 79d. Low temperature crystallographic properties of gold

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	- 0.324	0.40654	0.28747	10.116	19471
10	0.23	- 0.324	0.40654	0.28747	10.116	19471
20	1.71	- 0.323	0.40654	0.28747	10.116	19471
30	3.97	- 0.320	0.40655	0.28748	10.117	19469
40	6.08	- 0.315	0.40657	0.28749	10.118	19466
50	7.77	- 0.308	0.40660	0.28751	10.120	19462
60	9.05	- 0.300	0.40664	0.28754	10.123	19457
70	10.01	- 0.290	0.40668	0.28756	10.126	19452
80	10.74	- 0.280	0.40672	0.28759	10.129	19446
90	11.30	- 0.269	0.40676	0.28762	10.132	19439
100	11.74	- 0.257	0.40681	0.28766	10.136	19432
110	12.09	- 0.246	0.40686	0.28769	10.140	19425
120	12.37	- 0.233	0.40691	0.28773	10.143	19418
130	12.61	- 0.221	0.40696	0.28776	10.147	19411
140	12.80	- 0.208	0.40701	0.28780	10.151	19404
150	12.97	- 0.195	0.40706	0.28784	10.155	19396
160	13.12	- 0.182	0.40712	0.28787	10.159	19389
170	13.24	- 0.169	0.40717	0.28791	10.163	19381
180	13.35	- 0.156	0.40722	0.28795	10.167	19373
190	13.45	- 0.143	0.40728	0.28799	10.171	19365
200	13.54	- 0.129	0.40733	0.28803	10.175	19358
210	13.63	- 0.115	0.40739	0.28807	10.179	19350
220	13.70	- 0.102	0.40744	0.28811	10.184	19342
230	13.77	- 0.088	0.40750	0.28815	10.188	19334
240	13.83	- 0.074	0.40756	0.28819	10.192	19326
250	13.90	- 0.060	0.40761	0.28823	10.196	19318
260	13.96	- 0.047	0.40767	0.28827	10.200	19310
270	14.01	- 0.033	0.40773	0.28831	10.205	19302
280	14.06	- 0.019	0.40778	0.28835	10.209	19293
290	14.12	- 0.004	0.40784	0.28839	10.213	19285
293.15	14.13	0	0.40786	0.28840	10.215	19283

$$d = a/\sqrt{2}$$

Table 79e. High temperature crystallographic properties of gold

T K	α x 10^6 K^{-1}	100 ε_T	*a* nm	*d* nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
293.15	14.13	0	0.40786	0.28840	10.215	19283
300	14.18	0.010	0.40790	0.28843	10.218	19277
350	14.49	0.081	0.40819	0.28864	10.240	19236
400	14.77	0.155	0.40849	0.28885	10.262	19194
450	15.04	0.229	0.40880	0.28906	10.285	19151
500	15.30	0.305	0.40911	0.28928	10.309	19107
550	15.55	0.383	0.40942	0.28950	10.332	19063
600	15.79	0.461	0.40974	0.28973	10.357	19018
650	16.04	0.541	0.41007	0.28996	10.381	18973
700	16.30	0.623	0.41040	0.29020	10.407	18927
750	16.56	0.705	0.41074	0.29043	10.432	18880
800	16.85	0.790	0.41108	0.29068	10.459	18833
850	17.15	0.875	0.41143	0.29092	10.485	18785
900	17.48	0.963	0.41179	0.29118	10.512	18736
950	17.84	1.052	0.41215	0.29143	10.540	18687
1000	18.23	1.143	0.41252	0.29170	10.569	18636
1050	18.66	1.236	0.41290	0.29197	10.598	18585
1100	19.14	1.332	0.41329	0.29224	10.628	18532
1150	19.66	1.430	0.41369	0.29253	10.659	18478
1200	20.25	1.532	0.41411	0.29282	10.691	18423
1250	20.88	1.636	0.41453	0.29312	10.724	18366
1300	21.58	1.744	0.41497	0.29343	10.758	18308
1337.33	22.15	1.827	0.41531	0.29367	10.785	18263

$$d = a/\sqrt{2}$$

Table 79f. Bulk properties of gold

$3\,(\varepsilon_T L - \varepsilon_T a) = \exp(0.92 - 10908/T)$; $\alpha_L - \alpha_a = (3636/T^2)\exp(0.92 - 10908/T)$

T K	α x 10^6 K^{-1}	100 ε	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
900	17.48	0.963	10.512	18736
950	17.94	1.053	10.541	18686
1000	18.40	1.144	10.569	18636
1050	18.91	1.239	10.599	18584
1100	19.51	1.336	10.630	18530
1150	20.18	1.438	10.661	18475
1200	20.96	1.541	10.694	18418
1250	21.83	1.649	10.729	18359
1300	22.81	1.763	10.764	18298
1337.33	23.61	1.851	10.792	18250

This Table is considered to be identical to Table 79e below 900 K.

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80 MERCURY Hg

Atomic weight: 200.592 (3) (Meija 2017)

Allotropy: Beta phase: Tetragonal (tI2)
Alpha phase: Rhombohedral (hR1)

Although unusual, the low temperature phase is denoted as the beta phase. The transition between the two phases cannot be obtained at ambient pressure but is estimated that it would occur at 79 K by extrapolation of the high pressure phase boundary (Swenson 1958, Schirber and Swenson 1962). The triple point is a primary fixed point on ITS-90 at 234.3156 K (Preston-Thomas 1990) and the freezing point is a secondary fixed point at 234.3210 (5) K (Bedford et al. 1996).

80.1 Alpha Phase: Rhombohedral (hR1): 79 K to 234.3210 K

Because of the nature of the transition the alpha phase is easily retained to the lowest temperatures and undergoes a superconducting transition at 4.15 (1) K (Schirber and Swenson 1962). Apart from the normal rhombohedral structure designated Rhomb I, the structure can also be considered in terms of a second rhombohedral structure, Rhomb II, as well as a hexagonal structure. It is the latter that is used to evaluate the variation of the lattice parameters with temperature. The relationship between the three different structure types is given below.

Most determinations of the lattice parameters assumed for the Rhomb I structure that the angle was ideal at $\alpha = 70.53°$, i.e. $\cos \alpha = ⅓$. Barrett 1957 did not assume this and obtained $\alpha = 70.74°$ at both 5 K and 78 K but Barrett 1958 admitted that the measurements at 78 K were probably in error. A summary of the various determinations of the lattice parameters as given in Table 80a clearly show a high degree of discrepancy and therefore a different approach was used in estimating the lattice parameters and their variation with temperature. Grosse 1965 selected 13690.98 kg m^{-3} for the density of the liquid at the freezing point, equal to a molar volume of 14.6514 cm^3 mol^{-1}. Houck 1977 determined the melting curve over the range 234.316 K to 273.173 K from which an initial slope is given by 19.331 (55) MPa K^{-1} was obtained and this value is selected. Molinar 1991 also determined the melting curve over the range 246.051 K to 294.974 K and extrapolation to the freezing point leads to a similar value of 19.328 (59) MPa K^{-1}. The selected pressure slope together with an enthalpy of fusion of 2301 (1) J mol^{-1} as determined by Callahan et al. 1990 leads to a volume change on fusion of 0.5080 (15) cm^3 mol^{-1} using the Clausius-Clapeyron equation in excellent agreement with a value of 0.5083 cm^3 mol^{-1} determined by Bridgeman 1911 from pressure-temperature-volume data. The molar volume of the solid at the freezing point is therefore calculated as 14.1434 (15) cm^3 mol^{-1} and the density as 14182.7 (1.5) kg m^{-3}. In the absence of other criteria possible thermal vacancy effects are ignored and it is assumed that $\cos \alpha = ⅓$ at the freezing point and all of the other lattice parameter data is calculated on this basis. This procedure is validated by the fact that there is a close agreement with the lattice parameters determined by Amand and Giessen 1978 at 83 K, the direct density

determination obtained by Dönitz 1934 at 82 K, the molar volume determined by Swenson 1958 at 100 K and below and the very close agreement to within 1 x 10^{-6} K^{-1} with the mean thermal expansion coefficients determined by Grüneisen and Sckell 1934 between 85 K and 194 K. Molar volume thermal expansion determinations by Carpenter and Oakley 1931 (183.3-233.7 K) and anisotropic thermal expansion coefficients of Hill 1935 (113-158 K) were combined by Grosse 1965 to derive thermal expansion coefficients over the range 10 K to 234.3 K. These values were used to derive the equations:

a axis

10-125 K: $$\alpha_a\,(K^{-1}) = 1.35000 \times 10^{-6}\,T - 1.85724 \times 10^{-8}\,T^{2} + 1.27598 \times 10^{-10}\,T^{3} - 3.35405 \times 10^{-13}\,T^{4} - 9.29678 \times 10^{-6} \quad (80a)$$

125-234.321 K: $$\alpha_a\,(K^{-1}) = 1.91620 \times 10^{-7}\,T + 1.53713 \times 10^{-9}\,T^{2} - 2.01125 \times 10^{-11}\,T^{3} + 5.55128 \times 10^{-14}\,T^{4} + 1.42981 \times 10^{-5} \quad (80b)$$

c axis

10-25 K: $$\alpha_c\,(K^{-1}) = 2.30000 \times 10^{-6}\,T - 3.33333 \times 10^{-8}\,T^{2} - 1.46667 \times 10^{-5} \quad (80c)$$

25-200 K: $$\alpha_c\,(K^{-1}) = 1.20089 \times 10^{-6}\,T - 1.29936 \times 10^{-8}\,T^{2} + 6.58667 \times 10^{-11}\,T^{3} - 1.18788 \times 10^{-13}\,T^{4} - 9.10434 \times 10^{-7} \quad (80d)$$

200-234.321K: $$\alpha_c\,(K^{-1}) = 3.66347 \times 10^{-7}\,T - 1.65522 \times 10^{-10}\,T^{2} - 1.02485 \times 10^{-5} \quad (80e)$$

Equivalent length change values were derived by three point integration.

Table 80a. Lattice parameter measurements of alpha mercury

References	Temperature K	Rhomb I		Hexagonal		Notes
		a_r nm	α°	a_h nm	c_h nm	
McKeehan and Cioffi 1922	158	0.3031	70.53	0.3500	0.6778	a
Alseń and Aminoff 1924	195	0.299_6	70.53	0.346_0	0.670_0	a, b
Wolf 1928, 1929	193	0.3015	70.55	0.3483	0.6741	a
Terry and Wright 1928	123	0.3002	70.53	0.3467	0.6713	a
Mehl and Barrett 1930	227	0.3003	70.52	0.3467	0.6716	a
Hermann and Ruheman 1932	223	0.3061	70.53	0.3535	0.6845	a
Barrett 1957	5	0.2986	70.74	0.3458	0.6664	
	78	0.2993	70.74	0.3465	0.6678	
Malytin et al. 1973	213	0.3005	70.75	0.3480	0.6706	
Amand and Giessen 1978	83	0.2992	70.61	0.3458	0.6684	c

Notes for Table 80a

a. Assumes cos α = ⅓

b. As re-interpreted by Neuburger 1933

c. Given as Rhomb II structure: a_r = 0.4572 nm α = 98.27°

Rhombohedral and hexagonal conversion equations for alpha mercury

Rhomb I: lattice parameter a_1 angle α_1 Rhomb II: lattice parameter a_2 angle α_2

Hexagonal: lattice parameters a_h and c_h :

Rhomb I basis:

$a_h = 2\, a_1 \sin(\alpha_1/2)$ $c_h = a_1 \sqrt{(3 + 6\cos\alpha_1)}$

$a_2 = a_1 \sqrt{[1 + 4\sin^2(\alpha_1/2)]}$ $\sin(\alpha_2/2) = \sin(\alpha_1/2) / \sqrt{[1/4 + \sin^2(\alpha_1/2)]}$

Hexagonal basis:

$a_1^2 = a_h^2/3 + c_h^2/9$ $\sin(\alpha_1/2) = a_h / (2\, a_1)$ $a_2^2 = 4/3\, a_h^2 + c_h^2/9$;

$\sin(\alpha_2/2) = 3\, a_h / \sqrt{(12\, a_h^2 + c_h^2)}$

Rhomb II basis:

$a_1 = a_2 / \sqrt{[1 + \tan^2(\alpha_2/2)]}$ $\sin(\alpha_1/2) = \sin(\alpha_2/2) / 2\sqrt{[1 - \sin^2(\alpha_2/2)]}$

80.2 Beta Phase: Tetragonal (tI2): 0 K to 79 K

Atoji et al. 1959 determined the lattice parameters at 77 K to be *a* 0.3995 nm *c* 0.2825 nm which leads to a *c*/*a* ratio of $1/\sqrt{2}$. Swenson 1958 established that the molar volume differences between the alpha and beta phases at both 0 K and 50 K were the same at a value of – 0.206 $cm^3\ mol^{-1}$ and therefore crystallographic properties for the beta phase over the whole range were generated on this basis using the *c*/ *a* ratio as $1/\sqrt{2}$. The actual *a* axis determination of Atoji et al. 1959 is therefore 0.0008 nm lower than the tabulated value and the *c* axis value 0.0006 nm lower. The beta phase undergoes a superconducting transition at 3.95 (1) K (Schirber and Swenson 1962).

80.3 A comparison with other evaluations

Bodryakov and Babintsev 2015 did not correlate the density of the solid and the liquid at the melting point and as a result their values for density are on average 14 $kg\ m^{-3}$ lower than the selected values. Their selected values for volume thermal expansion, when corrected to linear thermal expansion, show a sinusoidal difference varying from 15.5% high at 20 K to 1.3% low at 130 K to 2.3% high at 200K to 1.1% low at the melting point.

Table 80b. Crystallographic properties of beta mercury

T K	*a* nm	*c* nm	*d*2 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.3996	0.2826	0.3159	13.586	14765
10	0.3996	0.2826	0.3159	13.586	14764
20	0.3996	0.2826	0.3159	13.590	14760
30	0.3997	0.2826	0.3160	13.597	14753
40	0.3998	0.2827	0.3161	13.606	14743
50	0.3999	0.2828	0.3162	13.617	14731
60	0.4000	0.2829	0.3163	13.630	14717
70	0.4002	0.2830	0.3164	13.643	14703
79	0.4003	0.2831	0.3165	13.656	14689

$$d1 = c \quad d2 = (a^{2}/2 + c^{2}/4)^{1/2}$$

Table 80c. Crystallographic properties of alpha mercury

T K	$\alpha_{ah} \times 10^6\ K^{-1}$	$\alpha_{ch} \times 10^6\ K^{-1}$	$\alpha_{avr} \times 10^6\ K^{-1}$	$100\ \varepsilon_0\ a$	$100\ \varepsilon_0\ c$	$100\ \varepsilon_0$ avr
0	0	0	0	0	0	0
10	2.5	5.0	3.3	0.001	0.002	0.001
20	11.2	18.0	13.5	0.008	0.014	0.010
30	17.7	25.1	20.1	0.022	0.036	0.027
40	22.3	30.2	24.9	0.043	0.063	0.050
50	25.6	34.1	28.4	0.067	0.096	0.077
60	28.1	37.1	31.0	0.093	0.131	0.106
70	29.9	39.2	33.0	0.122	0.170	0.138
79	31.3	40.7	34.4	0.150	0.206	0.169
80	31.4	40.9	34.6	0.153	0.210	0.172
90	32.8	42.1	35.9	0.185	0.251	0.207
100	34.0	43.2	37.1	0.219	0.294	0.244
110	35.2	44.2	38.2	0.254	0.338	0.282
120	36.2	45.3	39.2	0.289	0.383	0.320
130	36.9	46.4	40.1	0.326	0.429	0.360
140	37.4	47.6	40.8	0.363	0.476	0.401
150	37.9	49.0	41.6	0.401	0.525	0.442
160	38.3	50.5	42.4	0.439	0.575	0.484
170	38.8	52.1	43.2	0.478	0.626	0.527
180	39.6	53.7	44.3	0.518	0.680	0.572
190	40.6	55.2	45.5	0.558	0.734	0.617
200	42.0	56.4	46.8	0.599	0.790	0.663
210	44.0	59.4	49.1	0.643	0.849	0.712
220	46.7	62.3	51.9	0.688	0.910	0.762
230	50.3	65.3	55.3	0.737	0.974	0.816
234.3210	52.2	66.5	57.0	0.759	1.010	0.843

Table 80c. Crystallographic properties of alpha mercury

T K	a_h nm	c_h nm	a_r nm	α°	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.34502	0.66646	0.29838	70.641	13.792	14544
10	0.34502	0.66648	0.29839	70.640	13.792	14544
20	0.34505	0.66656	0.29842	70.638	13.796	14540
30	0.34509	0.66670	0.29847	70.634	13.803	14533
40	0.34517	0.66688	0.29854	70.632	13.812	14523
50	0.34528	0.66710	0.29863	70.628	13.824	14511
60	0.34534	0.66734	0.29872	70.624	13.836	14498
70	0.34544	0.66760	0.29883	70.619	13.849	14484
79	0.34554	0.66784	0.29892	70.616	13.862	14471
80	0.34555	0.66786	0.29893	70.615	13.863	14469
90	0.34566	0.66814	0.29904	70.611	13.878	14454
100	0.34577	0.66842	0.29916	70.607	13.893	14438
110	0.34589	0.66872	0.29928	70.603	13.909	14422
120	0.34602	0.66902	0.29940	70.599	13.925	14405
130	0.34614	0.66932	0.29953	70.595	13.941	14388
140	0.34627	0.66964	0.29965	70.590	13.958	14371
150	0.34640	0.66996	0.29978	70.585	13.975	14353
160	0.34653	0.67030	0.29992	70.580	13.993	14335
170	0.34667	0.67064	0.30005	70.575	14.011	14317
180	0.34681	0.67100	0.30020	70.568	14.030	14298
190	0.34694	0.67136	0.30034	70.561	14.049	14278
200	0.34708	0.67173	0.30049	70.555	14.068	14259
210	0.34724	0.67213	0.30064	70.549	14.088	14238
220	0.34739	0.67253	0.30080	70.542	14.109	14217
230	0.34756	0.67296	0.30097	70.535	14.137	14194
234.3210	0.34764	0.67320	0.30106	70.529	14.143	14183

$d1 = a_r \qquad d2 = a_h$

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81 THALLIUM Tl

Atomic Weight: 204.382 to 204.385 (Meija 2017)
Select 2007 value 204.3833 (2) (Wieser and Berglund 2009).

Structure: Alpha phase: Hexagonal close-packed (hP2)
Beta phase: Body-centered cubic (cI2)

Gurvich et al. 1994 select 507 (1) K for the alpha beta transition and 577 (1) K for the melting point. Roberts 1976 selects 2.38 (4) K for the superconducting transition temperature of the alpha phase.

81.1 Alpha Phase: Hexagonal close packed (hP2): 0 K to 507 K

After correction from a 273.2 K base to a 298.15 K base, length change values of Meyeroff and Smith 1962 (0-273.2 K) were selected to represent the thermal expansion up to 293.15 K.

Possibly because of orientation effects, dilatometric measurements of Swenson 1955 (0-300 K) show poor agreement with the selected values. On the basis $100\Delta\varepsilon$ they are initially 0.17 high and then trend towards the selected values with increasing temperature. Thermal expansion coefficients values of Larikov et al. 1966 (124-529 K) were shown only graphically with actual data points being given by Touloukian et al. 1975. Again on a length change basis, in the low temperature region they are initially 0.055 high and then trend towards towards the selected values.

In the high temperature region the direct density values of Stankus and Khairulin 1988 (293-507 K in the alpha phase) were selected which lead to an average length change value of $100\varepsilon = 0.669_9$ at 507 K. Together with the selected expansion coefficients at 293.15 K, the assumption that $d\alpha_a = d\alpha_c = 0$ at 293.15 K and that based on the behavior of the α_c / α_a ratio at low temperatures then it is assumed that the ratio α_c^* / α_a^* is constant at 1.3893 above 293.15 K then these combinations lead to the following equations to represent the thermal expansion from 293.15 K to 507 K:

$$\varepsilon_T\, a = 3.45078 \times 10^{-5}\, T - 2.81164 \times 10^{-8}\, T^2 + 3.19706 \times 10^{-11}\, T^3 - 8.50514 \times 10^{-3} \quad (81a)$$

$$\varepsilon_T\, c = 4.79420 \times 10^{-5}\, T - 3.90630 \times 10^{-8}\, T^2 + 4.44175 \times 10^{-11}\, T^3 - 1.18162 \times 10^{-2} \quad (81b)$$

On the basis $100\Delta\varepsilon$ length change values of Larikov et al. 1966 (124-529 K) as given by Touloukian et al. 1975 trend to 0.023 low. Lattice parameter measurements of Schneider and Heymer 1956 (291-465 K) show very poor agreement with equivalent length change values at 465 K being 0.25 high along the *a* axis and 0.49 low along the *c* axis. Lattice parameter values of Shinoda 1933 (305-364 K) can be interpreted as equivalent thermal expansion coefficients of 72×10^{-6} K^{-1} along the *a* axis and for the *c* axis 9×10^{-6} K^{-1}, which are in poor agreement with selected values while lattice parameter values of Meyeroff and Nitteberg 1960 lead to values in the room temperature region of 27.5×10^{-6} K^{-1} for the *a* axis and 40.0×10^{-6} K^{-1} for the *c* axis, which are in satisfactory agreement.

Table 81a. Lattice parameter values of alpha thallium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm	Note
Suganuma 1960	305	0.34576	0.55249	a
Meyeroff and Smith 1963	RT	0.34575	0.55269	a
Lipson and Stokes 1941	291	0.34569	0.55256	
Morris et al. 1979	298	0.34563	0.55249	
	Selected	0.34566 (3)	0.55252 (5)	

Note for Table 81a

a. Not included in the average

Values at 293.15 K: Density 11873 (2) kg m^{-3} Molar volume 17.215 (2) cm^3 mol^{-1}.

81.2 Beta Phase: Body-centered cubic (cI2): 507 K to 577 K

Sekito 1930 and Schneider and Haymer 1956 both suggested that the structure was face-centered cubic but both Lipson and Stokes 1941 and Ponyatovskii and Zakharova 1962 indexed the structure as being body-centered cubic which is accepted. Direct density measurements of Stankus and Khairulin 1988 (507-577 K) were converted to length change values while lattice parameter values were calculated by directly referring to the selected values at 293.15 K:

$$a\ (\text{nm}) = 1.58082 \times 10^{-5}\, T + 0.379656 \qquad (81c)$$

$$\varepsilon_T = 4.10353 \times 10^{-5}\, T - 1.44806 \times 10^{-2} \qquad (81d)$$

The derived thermal expansion coefficient is 40.7 x 10^{-6} K^{-1}. The derived volume contraction on transition of – 0.020 cm^3 mol^{-1} agrees with the value determined by both Jayaraman et al. 1963c and Adler and Margolin 1964 as – 0.019 cm^3 mol^{-1}. The lattice parameter values determined by Lipson and Stokes 1941 at 535 K and by Ponyatovskii and Zakharova 1962 at 523 K agree with the selected values to better than 0.0001 nm. A dilatometric value determined by Larikov et al. 1966 at 529 K must be considered as being in the beta range and if so on the basis $100\Delta\varepsilon$ differs from the selected value by only 0.003.

Table 81b. Crystallographic properties of alpha thallium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
0	0	0	0	- 0.647	- 0.863	- 0.719
5	0.8	3.3	1.6	- 0.647	- 0.862	- 0.719
10	1.9	8.5	4.1	- 0.646	- 0.860	- 0.718
15	3.4	13.7	6.8	- 0.645	- 0.854	- 0.715
20	4.9	17.0	9.0	- 0.643	- 0.846	- 0.711
25	10.6	19.2	13.5	- 0.639	- 0.837	- 0.705
30	15.2	21.0	17.1	- 0.633	- 0.827	- 0.697
40	20.5	23.1	21.4	- 0.614	- 0.805	- 0.678
50	21.5	24.7	22.6	- 0.593	- 0.781	- 0.656
60	22.2	26.1	23.5	- 0.572	- 0.756	- 0.633
70	22.7	27.0	24.2	- 0.549	- 0.730	- 0.609
80	23.0	27.9	24.6	- 0.526	- 0.703	- 0.585
90	23.2	28.7	25.0	- 0.503	- 0.675	- 0.560
100	23.3	29.3	25.3	- 0.480	- 0.646	- 0.535
110	23.5	29.9	25.6	- 0.457	- 0.616	- 0.510
120	23.7	30.4	25.9	- 0.433	- 0.586	- 0.484
130	23.9	30.9	26.2	- 0.410	- 0.556	- 0.458
140	24.1	31.4	26.5	- 0.386	- 0.525	- 0.432
150	24.2	31.9	26.8	- 0.362	- 0.493	- 0.406
160	24.3	32.3	27.0	- 0.338	- 0.461	- 0.379
170	24.5	32.7	27.2	- 0.313	- 0.429	- 0.352
180	24.7	33.1	27.5	- 0.289	- 0.396	- 0.325
190	24.8	33.5	27.7	- 0.264	- 0.363	- 0.297
200	25.0	33.9	28.0	- 0.239	- 0.329	- 0.269
210	25.2	34.3	28.2	- 0.214	- 0.295	- 0.241
220	25.3	34.6	28.4	- 0.189	- 0.261	- 0.213
230	25.5	35.0	28.7	- 0.164	- 0.226	- 0.185
240	25.7	35.3	28.9	- 0.138	- 0.191	- 0.156
250	25.8	35.6	29.1	- 0.112	- 0.156	- 0.127
260	25.9	35.9	29.3	- 0.087	- 0.120	- 0.098
270	26.1	36.2	29.4	- 0.061	- 0.089	- 0.068
280	26.2	36.3	29.6	- 0.034	- 0.048	- 0.039
290	26.2	36.5	29.7	- 0.008	- 0.011	- 0.009
293.15	26.3	36.5	29.7	0	0	0
300	26.3	36.5	29.7	0.018	0.025	0.020
320	26.3	36.6	29.7	0.071	0.098	0.080
340	26.4	36.7	29.9	0.123	0.171	0.139
360	26.6	37.0	30.1	0.177	0.245	0.199
380	26.9	37.4	30.4	0.230	0.320	0.260
400	27.3	37.9	30.8	0.285	0.395	0.321
420	27.7	38.5	31.3	0.340	0.472	0.384
440	28.2	39.1	31.9	0.396	0.550	0.447
460	28.8	39.9	32.5	0.453	0.629	0.512
480	29.5	40.9	33.3	0.512	0.711	0.578
500	30.2	41.9	34.1	0.572	0.794	0.646
507	30.5	42.2	34.4	0.593	0.824	0.670

Table 81c. Crystallographic properties of alpha thallium

T K	*a* nm	*c* nm	*c*/*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.34342	0.54775	1.5950	0.33811	16.846	12133
5	0.34342	0.54776	1.5950	0.33812	16.846	12132
10	0.34343	0.54777	1.5950	0.33812	16.847	12132
15	0.34343	0.54780	1.5951	0.33814	16.848	12131
20	0.34344	0.54785	1.5952	0.33816	16.850	12129
25	0.34345	0.54789	1.5953	0.33818	16.853	12127
30	0.34347	0.54795	1.5953	0.33821	16.857	12125
40	0.34354	0.54807	1.5954	0.33828	16.867	12117
50	0.34361	0.54820	1.5954	0.33836	16.878	12109
60	0.34368	0.54834	1.5955	0.33844	16.890	12101
70	0.34376	0.54849	1.5955	0.33853	16.902	12092
80	0.34384	0.54864	1.5956	0.33861	16.914	12084
90	0.34392	0.54879	1.5957	0.33870	16.927	12075
100	0.34400	0.54895	1.5958	0.33880	16.940	12065
110	0.34408	0.54911	1.5959	0.33889	16.953	12056
120	0.34416	0.54928	1.5960	0.33898	16.966	12047
130	0.34424	0.54945	1.5961	0.33908	16.979	12037
140	0.34433	0.54962	1.5962	0.33918	16.992	12028
150	0.34441	0.54979	1.5963	0.33928	17.006	12018
160	0.34449	0.54997	1.5965	0.33937	17.020	12009
170	0.34458	0.55015	1.5966	0.33948	17.034	11999
180	0.34466	0.55033	1.5967	0.33958	17.048	11989
190	0.34475	0.55051	1.5969	0.33968	17.062	11979
200	0.34483	0.55070	1.5970	0.33979	17.076	11969
210	0.34492	0.55089	1.5972	0.33989	17.090	11959
220	0.34501	0.55108	1.5973	0.34000	17.105	11949
230	0.34509	0.55197	1.5974	0.34010	17.119	11939
240	0.34518	0.55146	1.5976	0.34021	17.134	11928
250	0.34527	0.55166	1.5978	0.34032	17.149	11918
260	0.34536	0.55186	1.5979	0.34043	17.164	11908
270	0.34545	0.55206	1.5981	0.34054	17.179	11897
280	0.34554	0.55226	1.5982	0.34066	17.195	11887
290	0.34563	0.55246	1.5984	0.34077	17.210	11876
293.15	0.34566	0.55252	1.5984	0.34080	17.215	11873
300	0.34572	0.55266	1.5986	0.34088	17.225	11865
320	0.34590	0.55306	1.5989	0.34110	17.256	11844
340	0.34609	0.55347	1.5992	0.34133	17.287	11823
360	0.34627	0.55388	1.5995	0.34156	17.318	11802
380	0.34646	0.55429	1.5999	0.34179	17.349	11780
400	0.34664	0.55470	1.6002	0.34202	17.381	11759
420	0.34683	0.55513	1.6006	0.34226	17.414	11737
440	0.34703	0.55556	1.6009	0.34250	17.447	11715
460	0.34723	0.55600	1.6013	0.34274	17.480	11692
480	0.34743	0.55645	1.6016	0.34299	17.515	11669
500	0.34764	0.55691	1.6020	0.34325	17.550	11646
507	0.34771	0.55707	1.6021	0.34334	17.563	11637

$$d1 = [a^2/3 + c^2/4] \qquad d2 = a$$

Table 81d. Crystallographic properties of beta thallium

T K	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
507	0.632	0.3877	0.3357	17.54	11650
510	0.645	0.3877	0.3358	17.56	11650
520	0.686	0.3879	0.3359	17.57	11630
530	0.727	0.3880	0.3360	17.59	11620
540	0.768	0.3882	0.3362	17.61	11600
550	0.809	0.3884	0.3363	17.64	11590
560	0.850	0.3885	0.3365	17.66	11580
570	0.891	0.3887	0.3366	17.68	11560
577	0.920	0.3888	0.3367	17.69	11550

$$d = \sqrt{3}a/2$$

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82 LEAD Pb

Atomic weight: 207.2 (1) (CIAAW 2015)
The 2017 atomic weight was not available (Meija 2017) but since it would be given only as interval values then these extreme values would not be used for calculating the density values.

Structure: Face-centered cubic (cF4)

The superconducting transition temperature at 7.1997 (25) K and the freezing point at 600.612 (1) K are secondary fixed points on ITS-90 (Bedford et al. 1996).

82.1 Crystallographic properties at low temperature

Thermal expansion coefficients of White 1962 (3-11 K), in both the superconducting and normal states, were combined with measurements of Rubin et al. 1962 (17-292 K). These measurements together with the specific heat values selected by Arblaster 2012 were fitted to Equation A with an overall standard deviation of ± 1.4 x 10^{-7} K^{-1} and are used to represent the thermal expansion up to 293.15 K:

$$\alpha\ (K^{-1}) = C_p\ (1.02990 \times 10^{-6} + 1.99262 \times 10^{10}\, T - 6.36559 \times 10^{-7}/T) \qquad (82a)$$

On the basis 100Δε dilatometric measurements of Nix and MacNair 1942 (85-298 K) show an average bias of only 0.001 lower than the selected values while when converted from thermal expansion coefficients to length change values the measurements of Channing and Weintroub 1965 (11-267 K) agree to within 0.002. Dilatometric measurements of Dorsey 1908 (113-273 K) average 0.003 low. In the low temperature region measurements of Asay et al. 1968 (173-473 K) as given by Touloukian et al. 1975 trend from an initial 0.058 high while an isolated low temperature measurement of Richards 1942 (83, 300-598 K) is 0.065 high at 83 K.

82.2 Crystallographic and bulk properties at high temperature

Dilatometric measurements of d'Heurle et al. 1963 (435-600 K) and Feder and Nowick 1967 (293-600 K) were combined. The measurements of d'Heurle et al. 1963 were only shown graphically with actual data points being given by Touloukian et al. 1975:

$$\varepsilon_T = 2.79319 \times 10^{-5}\, T - 4.57804 \times 10^{-9}\, T^{\,2} + 1.35069 \times 10^{-11}\, T^{\,3} - 8.13509 \times 10^{-3} \qquad (82b)$$

The dilatometric measurements of Feder and Nowick 1967 were combined with lattice parameter measurements of d'Heurle et al. 1963 (433-599 K) which were shown only graphically and given as length change values by Touloukian et al. 1975 leading to a coefficient of vacancy formation (c_V) of 1.68 x 10^{-4}, an enthalpy of vacancy formation (H_V) of 0.49 (10) eV and an entropy of vacancy formation (S_V) of S_V/k = 0.7 (2.0). The value of H_V is in excellent agreement with the value of 0.50 (3) eV obtained by McKee et al. 1972 from positron annihilation. Up to 420 K the dilatometric and crystallographic thermal expansion values are assumed to be the identical but above this temperature the

divergence is given by the following equations which are used to calculate crystallographic properties above this temperature:

$3\,(\varepsilon_T L - \varepsilon_T a) = \exp(0.7 - 5641/T)$ $\quad \alpha_L - \alpha_a = (1880.3/T^2)\exp(0.7 - 5641/T)$

Dilatometric and lattice parameter measurements of both Van Duijn and Van Galen 1957 and Feder and Nowick 1958 were only shown graphically with actual data points given by Touloukian et al. 1975. Deviations of experimental dilatometric and lattice parameter values from the selected values are given in Part 82.3.

Table 82a. Lattice parameter values of lead at 293.15 K

References	Original Temperature K	*a* nm 293.15 K
Owen and Iball 1932	289.7	0.49501
Obinata and Schmid 1933	293	0.49492
Owen and Yates 1933a	291	0.49501
Ölander 1934	291	0.49487
Straumanis and Ievinš 1936	291	0.49500
Chiswik and Hultgren 1940a, 1940b	298	0.49494
Lu and Chang 1941	294	0.49495
Foote and Jette 1941	298	0.49501
Stokes and Wilson 1941	293	0.49499
Klug 1946	298	0.49503
Straumanis 1949	298	0.49496
Swanson and Tatge 1953	298	0.49501
Tyzack and Raynor 1954	293	0.49496
Feder and Nowick 1958	298	0.49505
	Selected	0.49498 (5)

At 293.15: Density 11348 (8) kg m^{-3} Molar volume 18.258 (9) cm^3 mol^{-1}.

82.3 Deviations of experimental values from the selected values

Table 82b. Dilatometric values on the basis 100Δε

References	Temperature Range K	Deviations 100Δε
Uffelmann 1930	353-553	Trend to 0.029 low
Hidnert and Sweeney 1932	294-577	Trend to 0.015 low
Richards 1942	83, 300-598	In the high temperature region scatter 0.040 low to 0.013 high
Van Duijn and Van Galen 1957	323-572	Trends to 0.039 low
Feder and Nowick 1958	293-592	Maximum deviation 0.010 low at 480 K
Asay et al. 1968	173-473	Trends to 0.16 low above room temperature
Balasundaram and Sinha 1971	293-398	0.003 low at 398 K

Table 82c. Lattice parameter values on the basis 100Δε

References	Temperature Range K	Deviations 100Δε
Stokes and Wilson 1941	286-594	Trends to 0.014 high
Van Duijn and Van Galen 1957	313-559	Trends to 0.034 low
Feder and Nowick 1958	293-595	Maximum deviation 0.010 high at 541 K

Table 82d. Bulk properties of lead

$3\,(\varepsilon_T L - \varepsilon_T a) = \exp(0.7 - 5641/T)$ $\quad \alpha_L - \alpha_a = (1880.3/T^2)\exp(0.7 - 5641/T)$

T K	α x 10^6 K^{-1}	100 ε	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
420	31.12	0.379	18.466	11220
440	31.61	0.442	18.501	11199
460	32.13	0.506	18.537	11178
480	32.69	0.571	18.573	11156
500	33.27	0.638	18.609	11134
520	33.89	0.705	18.647	11112
540	34.54	0.774	18.685	11089
560	35.21	0.844	18.724	11066
580	35.92	0.916	18.764	11042
600	36.66	0.989	18.805	11018
600.612	36.69	0.992	18.807	11017

This Table is considered to be identical to Table 82e below 420 K.

Table 82e. Crystallographic properties of lead

T K	$\alpha \times 10^6$ K^{-1}	$100\ \varepsilon_T$	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0	- 0.7064	0.49148	0.34753	17.874	11592
5	0.22	- 0.7064	0.49148	0.34753	17.874	11592
10	2.88	- 0.7057	0.49149	0.34753	17.874	11592
15	7.63	- 0.7032	0.49150	0.34754	17.876	11591
20	10.98	- 0.6985	0.49152	0.34756	17.878	11590
25	13.92	- 0.6923	0.49155	0.34758	17.881	11587
30	16.34	- 0.6848	0.49159	0.34761	17.886	11585
40	19.85	- 0.6667	0.49168	0.34767	17.895	11578
50	22.04	- 0.6458	0.49178	0.34774	17.907	11571
60	23.34	- 0.6231	0.49190	0.34782	17.919	11563
70	24.09	- 0.5995	0.49201	0.34791	17.932	11555
80	24.58	- 0.5753	0.49213	0.34799	17.945	11547
90	24.99	- 0.5507	0.49225	0.34808	17.958	11538
100	25.36	- 0.5256	0.49238	0.34816	17.972	11529
110	25.68	- 0.5002	0.49250	0.34825	17.985	11520
120	25.97	- 0.4745	0.49263	0.34834	17.999	11512
130	26.22	- 0.4485	0.49276	0.34842	18.013	11503
140	26.45	- 0.4222	0.49289	0.34853	18.028	11493
150	26.65	- 0.3959	0.49302	0.34862	18.042	11484
160	26.83	- 0.3692	0.49315	0.34871	18.057	11475
170	26.99	- 0.3424	0.49329	0.34881	18.071	11466
180	27.15	- 0.3154	0.49342	0.34890	18.086	11456
190	27.29	- 0.2883	0.49355	0.34899	18.101	11447
200	27.42	- 0.2610	0.49369	0.34909	18.115	11438
210	27.54	- 0.2336	0.49382	0.34919	18.130	11428
220	27.68	- 0.2061	0.49396	0.34928	18.145	11419
230	27.82	- 0.1784	0.49410	0.34938	18.160	11409
240	27.96	- 0.1505	0.49424	0.34948	18.176	11400
250	28.11	- 0.1225	0.49437	0.34957	18.191	11390
260	28.25	- 0.0944	0.49451	0.34967	18.206	11381
270	28.39	- 0.0661	0.49465	0.34977	18.222	11371
280	28.54	- 0.0376	0.49479	0.34987	18.237	11361
290	28.68	- 0.0090	0.49494	0.34997	18.253	11351
293.15	28.73	0	0.49498	0.35000	18.258	11348
300	28.83	0.020	0.49508	0.35007	18.269	11342
320	29.13	0.078	0.49536	0.35028	18.301	11322
340	29.46	0.136	0.49565	0.35048	18.333	11302
360	29.83	0.196	0.49595	0.35069	18.365	11282
380	30.23	0.256	0.49625	0.35090	18.399	11262
400	30.66	0.317	0.49655	0.35111	18.432	11241
420	31.12	0.379	0.49686	0.35133	18.466	11220
440	31.56	0.442	0.49717	0.35155	18.501	11199
460	32.05	0.506	0.49748	0.35177	18.536	11178
480	32.56	0.571	0.79780	0.35200	18.572	11156
500	33.08	0.637	0.49813	0.35223	18.609	11134
520	33.62	0.704	0.49846	0.35247	18.646	11112
540	34.16	0.772	0.49880	0.35271	18.684	11090
560	34.71	0.841	0.49915	0.35295	18.723	11067
580	35.26	0.912	0.49949	0.35320	17.762	11043
600	35.80	0.984	0.49985	0.35345	18.802	11020
600.612	35.82	0.986	0.49986	0.35346	18.803	11019

Interatomic distance calculations for Table 82e: $d = a/\sqrt{2}$

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83 BISMUTH Bi

Atomic weight: 208.98040 (1) (Meija 2017)

Structure: Rhombohedral (hR2)

The freezing point is a secondary fixed point on ITS-90 at 544.552 (1) K (Bedford et al. 1996).

83.1 Crystallographic properties of bismuth

Above 293.15 K selected values are based on the precision lattice parameter measurements of Matsuno 1977 (323-533 K) which can be expressed as length change values for the equivalent hexagonal cell. Values were selected to establish the thermal expansion coefficients at 293.15 K and the crystallographic thermal expansion up to the freezing point:

$$\varepsilon_T a = 1.10630 \times 10^{-5} T + 3.38843 \times 10^{-10} T^2 - 3.27224 \times 10^{-3} \quad (83a)$$

$$\varepsilon_T c = 1.64861 \times 10^{-5} T + 4.32434 \times 10^{-10} T^2 - 4.87007 \times 10^{-3} \quad (83b)$$

In the low temperature region thermal expansion coefficients of White 1972 (2-85, 283 K) were accepted up to 85 K. These supersede earlier measurements of White 1964 and White 1969. For the *a* axis various fits to the data of White 1972 in the range 58 to 85 K were combined with the value of thermal expansion at 293.15 K derived from Equation 83a and fitted to Equation A using values of specific heat as given in Part 83.3. In view of the large intervals between actual specific heat values above 200 K as given in Part 83.3 then calculated thermal expansion values were further refined between 110 K to 293.15 K as given by Equation 83c below. In view of the very small rise for the thermal expansion of the *c* axis between 85 K and 293.15 K (1.1×10^{-7} K^{-1}) intermediate values were initially estimated graphically and then further refined between 90 K and 293.15 K as given in Equation 83d below:

$$\alpha_a\ (K^{-1}) = 1.06001 \times 10^{-7} T - 6.10206 \times 10^{-10} T^2 + 1.63060 \times 10^{-12} T^3 - 1.66892 \times 10^{-15} T^4 + 3.86680 \times 10^{-6} \quad (83c)$$

$$\alpha_c\ (K^{-1}) = 2.04331 \times 10^{-9} T - 1.34543 \times 10^{-11} T^2 + 4.79005 \times 10^{-14} T^3 - 5.99641 \times 10^{-17} T^4 + 1.65329 \times 10^{-5} \quad (83d)$$

The *c* axis mean thermal expansion measurements of Jacob and Goetz 1937 were interpreted as length change values by Touloukian et al. 1975 as were the mean thermal expansion coeffcients of Roberts 1924. Touloukian et al. 1975 also derived length change values from the lattice parameter values of Zubenko and Umanskii 1956 and Klemm et al. 1960. X-ray *d*-spacing d_{111} values determined by Goetz and Hergenrother 1931, 1932 were interpreted as *c* axis thermal expansion, while similar *d*-spacing d_{100} measurements of Jay 1934 were interpreted as *a* axis thermal expansion. Lattice parameter measurements of Schiferl and Barrett 1969 superseded earlier measurements of Cucka

and Barrett 1962. Although of high quality the lattice parameter measurements of Fischer et al. 1978 (5-500 K) were unfortunately shown only in the form of small graphs and could not be interpreted. Deviations of experimental values from the selected values are given in Part 83.3.

The positional parameter z

Values of z determined by Fischer et al. 1978 (5-516 K) were selected because they virtually covered the whole temperature range. Values above 180 K were fitted to a smooth curve in order to remove the effect of a sharp change in slope at 293 K. In order to improve the fit above 180 K graphically values were combined with experimental values:

0-180 K: $z = -1.83622 \times 10^{-6} T + 0.23384$ (83e)

180-544.552 K: $z = 1.82170 \times 10^{-5} T - 1.02716 \times 10^{-7} T^{2} + 2.31736 \times 10^{-10} T^{3} - 2.03161 \times 10^{-13} T^{4} + 0.23242$ (83f)

Measurements of z by Schiferl and Barrett 1969 at 4.2 K, 78 K and 298 K trend from 0.0002 to 0.0006 higher than the above selected values. At 298 K this is equivalent to differences for the interatomic distances of 0.0008 nm for $d1$ and 0.0010 nm for $d2$.

Table 83a. Lattice parameter measurements of bismuth at 293.15 K

References	Original Temperature K	Hexagonal		Notes
		a_h nm	c_h nm	
Jay 1934	291.7	0.45460	1.18612	
Jette and Foote 1935	298	0.45464	1.18617	
Ievinš et al. 1938	298	0.45459	1.18620	
Chiswik and Hultgren 1940a, 1940b	298	0.45459	1.18617	
Zubenko and Umansky 1956	293	0.45467	1.18636	a, b
Dismukes et al. 1968	298	0.45465	1.18613	
Schiferl and Barrett 1969	298	0.45460	1.18617	
Matsumo 1977	298	0.45451	1.18591	c
Berger et al. 1982	298	0.45463	1.18622	
	Selected	0.45462 (3)	1.18617 (4)	

Notes for Table 83a

a. Values given by Touloukian et al. 1975

b. *c* axis not included in the average

c. Values derived from equations. Not included in the averages

Equivalent selected rhombohedral cell: a_r 0.47458 (2) α 57.236 (4) °

At 293.15: Density 9807 (1) kg m^{-3} Molar volume 21.310 (3) cm^3 mol^{-1}.

83.2 Bulk properties of bismuth

From precision dilatometry and lattice parameter measurements Matsuno 1977 (323-533 K) determined a vacancy concentration parameter (c_V) of 6.17 x 10^{-4}, an enthalpy of vacancy formation (H_V) of 0.35 eV and an entropy of vacancy formation (S_V/k) of 0.3. For self-consistency the value of H_V was slightly adjusted until c_V was exactly reproduced. Direct density measurements of Stankus et al. 2005 (337-539 K) lead to a value at the freezing point which is only 0.1% higher than the selected bulk value.

83.3 Deviations of experimental values from the selected values

Table 83b. Thermal expansion coefficients

References	Temperature Range K	Percentage Deviation
Bunton and Weintroub 1969	10-200	Average 11% high along the *a* axis above 80 K and 1.7% high along the *c* axis above 60 K
Cave and Holroyd 1960	100, 150, 540	Trends from 10% to 4% high along the *a* axis and 0.3% low to 4% high along the *c* axis.

Table 83c. Dilatometric values on the basis 100Δε

References	Temperature Range K	Deviations 100Δε
Roberts 1924	315-506	Trends to 0.015 high along the *a* axis and 0.013 low along the *c* axis
Jacobs and Goetz 1937	30-537	*c* axis values generally scattering 0.006 low to 0.011 high except foranomaly in the region 258 to 348 K
Gachkovskii and Strelkov 1937	286-527	The *a* axis averages only 0.003 high and the *c* axis trends to only 0.008 low
Erfling 1939	20-333	Below 90 K average only 0.005 low along the *a* axis 0.015 high along the *c* axis and then both trend to agree with selected values

Table 83d. Lattice parameter values on the basis 100Δε

References	Temperature Range K	Deviations 100Δε
Goetz and Hergenrother 1931, 1932	294-535	*c* axis values trending to a maximum low of 0.027 at 390 K before trending to 0.008 high
Jay 1934	292-541 (*a* axis) 294-413 (*c* axis)	*a* axis values trending to a maximum of 0.016 high at 512 K before trending to 0.002 low while *c* axis values trend 0.005 low to 0.005 high
Zubenko and Umanskii 1956	293-365	Trends to 0.023 high along the *a* axis and to 0.018 low along the *c* axis
Klemm et al. 1960	293-537	Scatters 0.036 low to 0.028 high along the *a* axis and 0.050 low to 0.010 high along the *c* axis
Schiferl and Barrett 1969	4.2-298	Trends from 0.014 low along the *a* axis and 0.088 low along the *c* axis

83.4 Low temperature specific heat of bismuth

The Table incorporates the specific heat values determined and selected by Archer 1995 with other values selected by interpolation. C_p values in units of J mol^{-1} K^{-1}:

T K	20	30	40	50	60	70	80	90
C_p	7.392	11.885	15.41	17.92	19.67	20.91	21.82	22.49
T K	100	110	120	130	140	150	160	170
C_p	23.00	21.42	23.74	24.01	24.25	24.44	24.61	24.76
T K	180	190	200	210	220	230	240	250
C_p	24.89	25.01	25.11	25.21	25.31	25.40	25.49	25.58
T K	260	270	280	290	293.15			
C_p	25.66	25.75	25.83	25.91	25.94			

Table 83b. Crystallographic properties of bismuth

T K	α_{ah} x 10^6 K^{-1}	α_{ch} x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr	z
0	0	0	0	- 0.266	- 0.452	- 0.328	0.2338
5	0.03	0.23	0.09	- 0.266	- 0.452	- 0.328	0.2338
10	0.20	2.07	0.82	- 0.266	- 0.452	- 0.328	0.2338
15	0.63	5.82	2.36	- 0.266	- 0.450	- 0.327	0.2338
20	1.26	9.33	3.95	- 0.266	- 0.446	- 0.326	0.2338
25	1.95	11.83	5.24	- 0.265	- 0.441	- 0.324	0.2338
30	3.32	13.51	6.72	- 0.264	- 0.434	- 0.321	0.2338
40	5.46	15.36	8.76	- 0.259	- 0.420	- 0.313	0.2338
50	6.82	16.07	9.90	- 0.253	- 0.404	- 0.303	0.2337
60	7.77	16.34	10.63	- 0.246	- 0.388	- 0.293	0.2337
70	8.49	16.51	11.16	- 0.238	- 0.372	- 0.282	0.2337
80	9.05	16.61	11.57	- 0.229	- 0.355	- 0.271	0.2337
90	9.48	16.64	11.87	- 0.220	- 0.338	- 0.259	0.2337
100	9.81	16.64	12.09	- 0.210	- 0.322	- 0.247	0.2337
110	10.07	16.65	12.26	- 0.200	- 0.305	- 0.235	0.2336
120	10.27	16.65	12.40	- 0.190	- 0.289	- 0.223	0.2336
130	10.44	16.66	12.51	- 0.179	- 0.272	- 0.210	0.2336
140	10.58	16.66	12.61	- 0.169	- 0.255	- 0.198	0.2336
150	10.70	16.67	12.69	- 0.158	- 0.239	- 0.185	0.2336
160	10.79	16.67	12.75	- 0.148	- 0.222	- 0.172	0.2335
170	10.87	16.68	12.81	- 0.137	- 0.206	- 0.160	0.2335
180	10.93	16.68	12.85	- 0.126	- 0.189	- 0.147	0.2335
190	10.99	16.69	12.89	- 0.115	- 0.172	- 0.134	0.2335
200	11.03	16.69	12.92	- 0.104	- 0.156	- 0.121	0.2335
210	11.07	16.70	12.95	- 0.093	- 0.139	- 0.108	0.2335
220	11.11	16.70	12.97	- 0.082	- 0.122	- 0.095	0.2334
230	11.14	16.71	13.00	- 0.071	- 0.106	- 0.082	0.2334
240	11.16	16.71	13.01	- 0.060	- 0.089	- 0.069	0.2334
250	11.19	16.72	13.03	- 0.048	- 0.072	- 0.056	0.2334
260	11.21	16.72	13.05	- 0.037	- 0.055	- 0.043	0.2334
270	11.23	16.73	13.06	- 0.026	- 0.039	- 0.030	0.2333
280	11.24	16.73	13.07	- 0.015	- 0.022	- 0.017	0.2333
290	11.25	16.74	13.08	- 0.004	- 0.005	- 0.004	0.2333
293.15	11.26	16.74	13.09	0	0	0	0.2333
300	11.27	16.74	13.09	0.008	0.011	0.009	0.2333
320	11.28	16.76	13.10	0.030	0.045	0.035	0.2332
340	11.29	16.77	13.11	0.053	0.078	0.061	0.2331
350	11.29	16.77	13.12	0.064	0.095	0.075	0.2331
360	11.30	16.78	13.13	0.075	0.112	0.088	0.2331
380	11.31	16.79	13.14	0.098	0.146	0.114	0.2330
400	11.32	16.80	13.15	0.121	0.179	0.140	0.2329
420	11.33	16.81	13.16	0.143	0.213	0.167	0.2328
440	11.34	16.83	13.17	0.166	0.247	0.193	0.2327
450	11.35	16.83	13.18	0.177	0.264	0.206	0.2326
460	11.35	16.84	13.18	0.189	0.281	0.219	0.2325
480	11.36	16.85	13.19	0.212	0.314	0.246	0.2323
500	11.38	16.86	13.20	0.234	0.348	0.272	0.2321
520	11.39	16.87	13.21	0.257	0.382	0.299	0.2318
540	11.40	16.88	13.23	0.280	0.416	0.325	0.2315
544.552	11.40	16.89	13.23	0.285	0.424	0.331	0.2314

Table 83c. Crystallographic properties of bismuth

T K	a_h nm	c_h nm	a_r nm	α°	$d1$ nm	$d2$ nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.45341	1.18080	0.47270	57.317	0.3061	0.3518	21.100	9904
5	0.45341	1.18081	0.47270	57.317	0.3061	0.3518	21.100	9904
10	0.45341	1.18081	0.47271	57.317	0.3061	0.3518	21.100	9904
15	0.45341	1.18083	0.47271	57.316	0.3061	0.3518	21.101	9904
20	0.45341	1.18088	0.47273	57.315	0.3061	0.3518	21.102	9903
25	0.45342	1.18094	0.47274	57.313	0.3060	0.3519	21.103	9903
30	0.45342	1.18102	0.47277	57.311	0.3060	0.3519	21.105	9902
40	0.45344	1.18119	0.47282	57.306	0.3060	0.3519	21.110	9899
50	0.45347	1.18138	0.47288	57.302	0.3060	0.3520	21.116	9897
60	0.45350	1.18157	0.47295	57.298	0.3061	0.3521	21.123	9894
70	0.45354	1.18176	0.47301	57.295	0.3061	0.3521	21.130	9890
80	0.45358	1.18196	0.47308	57.291	0.3061	0.3522	21.137	9887
90	0.45362	1.18215	0.47315	27.288	0.3061	0.3523	21.144	9884
100	0.45367	1.18235	0.47322	27.585	0.3061	0.3524	21.152	9880
110	0.45371	1.18255	0.47328	57.282	0.3061	0.3524	21.260	9876
120	0.45376	1.18275	0.47335	57.279	0.3061	0.3525	21.167	9873
130	0.45380	1.18294	0.47342	57.277	0.3061	0.3526	21.175	9869
140	0.45385	1.18314	0.47349	57.274	0.3062	0.3527	21.183	9865
150	0.45390	1.18334	0.47356	57.271	0.3062	0.3527	21.191	9862
160	0.45395	1.18353	0.47363	57.269	0.3062	0.3528	21.199	9858
170	0.45400	1.18373	0.47370	57.266	0.3062	0.3529	21.268	9854
180	0.45405	1.18393	0.47378	57.264	0.3062	0.3530	21.216	9850
190	0.45410	1.18413	0.47385	57.261	0.3062	0.3530	21.224	9846
200	0.45415	1.18432	0.47392	57.259	0.3063	0.3531	21.232	9843
210	0.45420	1.18452	0.47399	57.256	0.3063	0.3532	21.240	9839
220	0.45425	1.18472	0.47406	57.254	0.3063	0.3533	21.249	9835
230	0.45430	1.18492	0.47413	57.252	0.3063	0.3533	21.257	9831
240	0.45435	1.18512	0.47420	57.249	0.3063	0.3534	21.265	9827
250	0.45440	1.18531	0.47427	57.246	0.3063	0.3535	21.274	9823
260	0.45445	1.18551	0.47434	57.244	0.3063	0.3536	21.282	9820
270	0.45450	1.18571	0.47441	57.242	0.3064	0.3537	21.290	9816
280	0.45455	1.18591	0.47449	57.240	0.3064	0.3538	21.299	9812
290	0.45460	1.18611	0.47456	57.237	0.3064	0.3539	21.307	9808
293.15	0.45462	1.18617	0.47458	57.236	0.3064	0.3539	21.310	9807
300	0.45466	1.18631	0.47463	57.235	0.3064	0.3540	21.315	9804
320	0.45476	1.18670	0.47477	57.230	0.3064	0.3541	21.332	9797
340	0.45486	1.18710	0.47492	57.225	0.3064	0.3543	21.349	9789
350	0.45491	1.18730	0.47499	57.223	0.3064	0.3544	21.357	9785
360	0.45496	1.18750	0.47506	57.220	0.3064	0.3545	21.366	9781
380	0.45507	1.18790	0.47520	57.216	0.3064	0.3548	21.382	9773
400	0.45517	1.18830	0.47535	57.211	0.3063	0.3550	21.399	9766
420	0.45527	1.18870	0.47549	57.206	0.3063	0.3553	21.416	9758
440	0.45538	1.18910	0.47568	57.201	0.3062	0.3556	21.433	9750
450	0.45543	1.18930	0.47571	57.199	0.3062	0.3557	21.442	9746
460	0.45548	1.18950	0.47578	57.197	0.3061	0.3560	21.450	9743
480	0.45558	1.18990	0.47592	57.192	0.3060	0.3563	21.467	9735
500	0.45569	1.19030	0.47607	57.187	0.3058	0.3568	21.484	9727
520	0.45579	1.19070	0.47621	57.182	0.3055	0.3573	21.501	9720
540	0.45589	1.19110	0.47636	57.178	0.3052	0.3579	21.518	9712
544.552	0.45592	1.19119	0.47639	57.177	0.3051	0.3581	21.522	9710

Interatomic distance calculations for Table 83c: $d1 = [\, a_h{}^2/3 + c_h{}^2 (2z - \tfrac{1}{3})^2 \,]^{\frac{1}{2}}$
$d2 = [\, a_h{}^2/3 + c_h{}^2 (2z - \tfrac{2}{3})^2 \,]^{\frac{1}{2}}$

Table 83d. Bulk properties of bismuth

$3\,(\varepsilon_T L - \varepsilon_T \mathrm{avr}) = \exp(0.3 - 4188/T)$ $\quad \alpha_L - \alpha_{avr} = (1396/T^2) \exp(0.3 - 4188/T)$

T K	α x 10^6 K^{-1}	100 ε	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
350	13.21	0.075	21.357	9785
360	13.26	0.088	21.366	9781
380	13.35	0.115	21.383	9773
400	13.48	0.141	21.400	9765
420	13.66	0.169	21.418	9757
440	13.89	0.196	21.435	9749
450	14.02	0.210	21.444	9745
460	14.17	0.224	21.453	9741
480	14.52	0.253	21.472	9733
500	14.93	0.283	21.491	9724
520	15.43	0.313	21.510	9715
540	16.00	0.344	21.531	9706
544.552	16.12	0.352	21.536	9704

This Table is considered to be identical to Tables 83b and 83c below 350 K.

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84 POLONIUM Po

Atomic mass ^{209}Po: 208.9824303 (19) (Wang et al. 2017)
Atomic mass ^{210}Po: 209.9828736 (12) (Wang et al. 2017)

^{209}Po is the longest living isotope with a half life of 124 y (Audi et al. 2017) while ^{210}Po with a half life of 138.376 d is considered to be the most useful. However, both isotopes have been used in determining lattice parameter values.

Allotropy: Alpha phase: Simple cubic (cP1)
Beta phase: Rhombohedral (hR1)

Maxwell 1949 determined the melting point to be 527 K and obtained a transition temperature of 338 to 358 K for samples over 4000 atoms in thickness. However, Goode 1957 obtained a repeatable hysteresis with 327 K on heating and 291 K on cooling and while the median of 309 K could be considered as being the "equilibrium" transition temperature, because of the very poor agreement for the determination of lattice parameters for the beta phase, then the average measuring temperature of 319 K is taken as a tentative transition temperature.

84.1 Alpha Phase: Simple cubic (cP1): 0 K to 319 K

Brocklehurst et al. 1957 determined a thermal expansion coefficient of 23 x 10^{-6} K^{-1} over the range 179 to 297 K.. Based on this determination, an estimated value in the room temperature region and above is considered to be 30 x 10^{-6} K^{-1} and lattice parameter values were adjusted using this value.

Table 84a. Lattice parameter values for alpha polonium at 293.15 K

References	Original Temperature K	*a* nm
Beamer and Maxwell 1949	283	0.3353
Goode 1953	312	0.3365
De Sando and Lange 1966	298	0.3359
	Selected	0.3359 (6)

At 293.15 K: Density: ^{209}Po 9157 (49) kg m^{-3} ^{210}Po 9200 (49) kg m^{-3}
Molar volume: 22.82 (12) cm^3 mol^{-1}.

84.2 Beta Phase: Rhombohedral (hR1): 319 K to 527 K

Because of the relatively poor agreement no estimate has been made of the possible variation of the lattice parameters with temperature and only average values have been selected.

Table 84b. Lattice parameter values for beta polonium

References	Temperature K	Rhombohedral Cell		Hexagonal Cell	
		a_r	α°	a_h	c_h
De Sando and Lange 1966	298	0.3368	98.24	0.5093	0.4927
Goode 1953	312	0.3373	98.08	0.5094	0.4953
Beamer and Maxwell 1949	348	0.3366	98.22	0.5089	0.4927
Average	319	0.3369 (4)	98.18 (9)	0.5092 (3)	0.4936 (15)

At 319 K: Density: ^{209}Po 9393 (29) kg m^{-3} ^{210}Po 9438 (29) kg m^{-3}
Molar volume: 22.249 (69) cm^3 mol^{-1}.

Table 84c. Crystallographic properties of alpha polonium

T K	$a = d$ nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3} ^{209}Po	Density kg m^{-3} ^{210}Po
293.15	0.3359	22.81	9157	9204
300	0.3360	22.84	9151	9195
305	0.3360	22.85	9147	9191
310	0.3361	22.86	9143	9186
315	0.3361	22.87	9139	9182
319	0.3362	22.88	9135	9179

Table 84d. Crystallographic properties of beta polonium

T K	Rhombohedral Cell		Hexagonal Cell		Molar Volume cm^3 mol^{-1}	Density kg m^{-3} ^{209}Po	Density kg m^{-3} ^{210}Po
	$a_r = d$	α°	a_h	c_h			
319	0.3369	98.18	0.5092	0.4936	22.25	9393	9438

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85 ASTATINE At

Atomic mass ^{210}At: 209.987147 (8) (Wang 2017)
Atomic mass ^{211}A: 210.9874961 (29) (Wang 2017)

^{210}At is the longest living isotope with an half-life of only 8.1 h (Audi et al. 2017). while ^{211}At is the "most useful" isotope with an half-life of 7.214 h.

The melting point is estimated to be 573 K by Stull 1972.

A number of physical properties have been determined on the microscopic scale but not for the solid. At ambient pressure the analogues chlorine, bromine and iodine are all molecular and crystallize in the orthorhombic (oC8) structure, space group Cmca, but at high pressures molecular dissociation to a monatomic state takes place at an estimated 220 GPa in the case of chlorine (Fujihisa et al. 1995), 80 GPa in the case of bromine (Fujii et al. 1989) and at 21 GPa in the case of iodine (Takemura et al. 1980). The structure changes to body-centered orthorhombic (oI4), space group Immm. This rapid periodic decrease in the transition pressure suggests that solid astatine should exist in the monatomic metallic form. By combining density functional theory and structural selection methods and accounting for relativistics physics Hermann et al. 2013 have indicated that the correct room temperature structure is the metallic form and is probably face-centered cubic (cF4) with an estimated lattice parameter of 0.539 nm (Hermann 2014) which leads to the estimated crytallographic properties given in Table 85. The molar volume is notably lower than the range of 33.9 to 34.5 cm^3 mol^{-1} estimated by Bonchev and Kamenska 1981 using the technique of information indices.

Table 85. Estimated crystallographic properties of astatine

T K	*a* nm	*d* nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3} ^{210}At	Density kg m^{-3} ^{211}At
RT	0.539	0.381	23.6	8910	8950

$$d = a/\sqrt{2}$$

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86 RADON Rn

Atomic mass ^{222}Rn: 222.0175763 (21) (Wang et al. 2017)

The half-life of ^{222}Rn is 3.8215 d (Audi et al. 2017),

Structure: Face-centered cubic (cF4)

The structure has not been determined but is considered to be isostructual with lower analogues. Ferreira and Lobo 2008 estimate the triple point to be 207.7 K.

Radon has been obtained in coherent form and a number of physical properties measured but not properties for the solid. In consideration of the best correlation in order to estimate periodic trends it is found that the lattice parameters of argon, krypton and xenon at their triple points can be correlated to within ± 2 x 10^{-5} nm by relating to the period number n (where n = 3 for argon and n = 6 for radon):

$$a(\text{nm}) = 7.32729 \times 10^{-3} (n - 1)^{2} + 0.51761 \quad (86)$$

The derived lattice parameter for radon is 0.7008 nm which is used to estimate the crystallographic properties in Table 86 below. It is found that below the triple point that the above relationship begins to deteriorate and was therefore not applied to lower temperatures. It is noted that the derived density at the triple point as given in Table 86 is notably lower than the value of 4680 kg m^{-3} estimated by Grosse 1965. However, it is also noted that the value of 5250 kg m^{-3} at 0 K estimated by Grosse 1964, 1965 differs considerable from the value of 4450 ± 50 kg m^{-3} estimated by Bonchev and Kamenska 1981 who used the technique of information indices. If this difference could be transferred to the triple point then the average value would be similar to that estimated here.

The density of the solid at the melting point is notably lower than estimated values for the liquid at the selected triple point of 4359 kg m^{-3} estimated by Herreman 1980 and 4348 kg m^{-3} estimated by Mick et al. 2016. The difference between the molar volumes of liquid argon, krypton and xenon at their triple points as given by Terry et al. 1969 and the molar volumes of the crystallographic solids at their triple points (V_S) is given by the equation $\Delta V = 0.1488\ V_S$ $cm^3\ mol^{-1}$ which for radon based on the selected molar volume of the solid would be equal to 7.71 $cm^3\ mol^{-1}$, so the estimated molar volume for the liquid would be 59.53 $cm^3\ mol^{-1}$ and the density 3730 kg m^{-3}, which is similar to values estimated by Miller 1960 and Gopal 1962 but not by Grosse 1965 who estimated 4070 kg m^{-3}. These differences clearly indicate the widespread values estimated for the density of liquid radon.

Table 86. Estimated crystallographic properties of radon at the triple pont

T K	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
207.7	0.7008	0.4955	51.82	4285

$$d = a/\sqrt{2}$$

References for Radon

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87 FRANCIUM Fr

Atomic mass ^{223}Fr: 223.0197343 (21) (Wang et al. 2017)

The half-life of ^{223}Fr is 22.00 min (Audi et al. 2017)

Structure: Body-centered cubic (cI2)

The structure has not been determined but is considered to be isostructual with lower analogues. The melting point is estimated to be 296 K (see Part 87.2).

87.1 Crystallographic properies of francium

Because the half-life of the longest living isotope is only 22.00 min then it is unlikely that francium will ever to be obtained in coherent form and therefore, values are estimated. In consideration of the best correlation in order to estimate periodic trends, it is found that the lattice parameters of potassium, rubidium and cesium at 293.15 K can be correlated to within a standard deviation of ± 3 x 10^{-4} nm by relating to the periodic number n (where n = 4 for potassium and n = 7 for francium) by the equation:

$$a \text{ (nm)} = 4.17673 \times 10^{-3} n^2 + 0.46573 \qquad (87)$$

The derived lattice parameter for francium is 0.6704 nm which was used to estimate the crystallographic properties in Table 87 below. Eberle 1983 summarized a number of previous estimates of the density of solid francium in the room temperature region and these varied from 2350 to 2480 kg m^{-3} and therefore agree with the present estimate of 2458 kg m^{-3}. Kazragis et al. 1974 estimated a much higher value of 2974 kg m^{-3} but this is based on an estimated lattice parameter of 0.629 nm which appears to be far too small when considering periodic trends.

87.2 An estimate of the melting point of francium

Eberle 1983 summarized various estimates which vary from 282 to 297 K while Stull 1972 estimated 300 K. Periodic trends are found for both atomic number (Z) and atomic weight (A_r) using values of the melting points of sodium, potassium, rubidium and cesium slected in the present evaluation. The agreement for francium is excellent and a value of 296 K is selected.

T_M (K) = 991.410 / Z + 282.550 (87c) Fr: T_M = 295.9 (1.5) K

T_M (K) = 1884.96 / A_r + 288.769 (87d) Fr: T_M = 297.2 (2.1) K

Table 87. Estimated crystallographic properties of francium at room temperature

T K	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
RT	0.6704	0.5806	90.72	2458

$$d = \sqrt{3}a/2$$

References for Francium

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88 RADIUM Ra

Atomic mass of ^{226}Ra: 226.0254085 (21) (Wang et al. 2017)

The half life of ^{226}Ra is 1600 y (Audi et al. 2017)

Structure: Body-centered cubic (cI2)

Stull and Sinke 1956 estimate the melting point to be 973 K.

Weigel and Trinkl 1968 determined the lattice parameter at room temperature to be 0.5148 (15) nm, equivalent to a density value of 5502 (48) kg m^{-3} and a molar volume of 41.08 (36) cm^3 mol^{-1}.

Table 88. Crystallographic properties of radium at room temperature

T K	*a* nm	*d* nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
RT	0.5148	0.4458	41.08	5502

$$d = \sqrt{3}a/2$$

References for Radium

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89 ACTINIUM Ac

Atomic mass of ^{227}Ac: 227.0277507 (21) (Wang et al. 2017)

The half life of ^{227}Ac is 21.772 y (Audi et al. 2017)

Allotropy

It is uncertain if actinium shows the same allotropic sequence as lanthanum, i.e. double close-packed hexagonal (hP4) – face-centered cubic (cF4) – body-centered cubic (cI2). If the double close-packed hexagonal structure is present then it probably exists only at low temperatures. Farr et al. 1961 obtained the face-centered cubic structure at room temperature which was confirmed by Baybarz et al. 1976. As with the other light lanthanides and actinides it is likely that there is a transformation to a body-centered cubic structure at high temperature and Arblaster 1995 estimated the transformation temperature as 1400 K and the melting point as 1500 K. The latter is considered to be more realistic than the value of 1323 (50) K determined by Stites et al. 1955 on highly impure metal.

Farr et al. 1961 obtained a lattice parameter for the face-centered cubic structure on a highly impure sample to be 0.5311 (10) nm. Baybarz et al. 1976 established on samples of the purified metal that this identification was correct with lattice parameters on two samples determined as 0.5317 (9) nm and 0.5314 (1) nm with a weighted average of 0.5315 nm which is selected.

Table 89. Crystallographic properties of actinium at room temperature

T K	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
RT	0.5315	0.3758	22.60	10040

$$d = a/\sqrt{2}$$

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90 THORIUM Th

Atomic weight: 232.0377 (4) (Meija 2017)

Allotropy: Alpha: Face-centered cubic (cF4)
Beta: Body-centered cubic (cI2)

Rand et al. 2009 select 1633 (20) K for the transition temperature and 2023 (10) K for the melting point in agreement with previous reviews by Oetting et al. 1976 and Ward et al. 1986.

90.1 Alpha Phase: Face-centered cubic (cF4): 0 K to 1633 K

Length change values derived from the lattice parameter measurements of Chiotti and White 1967 (298-1573 K but also including the metastable extrapolated values 1673 to 1873 K) were fitted to the following equation with an accuracy on the basis ± $100\varepsilon_T$ given as ± 0.007:

$$\varepsilon_T = 1.10073 \times 10^{-5} T + 9.69418 \times 10^{-10} T^2 - 1.52369 \times 10^{-13} T^3 - 3.30627 \times 10^{-3} \quad (90a)$$

Although the lattice parameters are only accurate to 0.0001 nm the molar volume and density have been given to five significant figures for interpolation purposes. The derived thermal expansion at 293.15 K, 11.54 x 10^{-6} K^{-1}, agrees satisfactorily with the value of 11.6 x 10^{-6} K^{-1} obtained by James and Straumanis 1956 (283-333 K) from precision lattice parameter measurements. On the basis $100\Delta\varepsilon$ lattice parameter measurements in the high temperature region by Harris and Raynor 1964 (298-692 K) trend 0.028 low to 0.059 high while those of Wilson et al. 1958 (293-1523 K in the alpha phase region) show marked scatter from 0.26 low to 0.12 high. Dilatometric measurements by Armstrong et al. 1959 (347-655 K), as given by Touloukian et al. 1975, trend 0.023 to 0.045 low while those of Danielson et al. 1952 (298-1098 K), which were also given by Touloukian et al. 1975, scatter from 0.08 low to 0.10 high when not including outlying values but if these are included the scatter is 0.17 low to 0.14 high.

In the low temperature region selected values are based on the unpublished lattice parameter values of Marples 1988 (4-295 K) (see Part 90.3) which were combined with the enthalpy values as given in Part 90.5 and fitted to equation B. It is found that if the value at 295 K as given by Marples 1988 is adjusted from 5.0856 Å to 5.0859 Å, which is still within the assigned error of ± 0.0004 Å, then exact agreement is obtained with equation 90a:

$$\ln (L_T) = (H_T - H_0) (4.55599 \times 10^{-7} - 2.98108 \times 10^{-11} T + 9.78223 \times 10^{-7} / T) - 2.80707 \times 10^{-3} \quad (90b)$$

On the basis $100\Delta\varepsilon$ the lattice parameter value of Waber et al. 1964 at 93 K agrees with the selected values to within 0.004 while the dilatometric measurements of Erfling 1942 (57-303 K) initially average 0.021 high below 90 K but agree with the selected values above this temperature. Lattice parameter values of Benedict et al. 1979 (50-300 K) were

shown only in the form of a small graph with actual data points given by Benedict 1986 (55-315 K) as given in Part 90.4. When corrected to length change values these scatter 0.043 low to 0.067 high.

Table 90a. The lattice parameters of alpha thorium at 293.15 K

Refererences	Original Temperature K	*a* nm	Note
James and Straumanis 1956	298	0.50844	
Wilson et al. 1958	RT	0.50848	
Evans and Raynor 1959	298	0.50844	
Evans et al. 1960	RT	0.50844	
Evans and Raynor 1960, 1962	298	0.50847	
Eash and Carlson 1960	RT	0.50849	
Evans and Raynor 1961a, 1961b	298	0.50848	
Johnson and Honeycombe 1961	291	0.50856	a
McMasters and Larson 1961	RT	0.50857	a
Harris and Raynor 1964	298	0.50861	a
Waber et al. 1964	RT	0.50861	a
Thomson 1964	RT	0.50866	a
Norman et al. 1966, 1967b	295	0.50859	a
Norman et al. 1967a	298	0.50858	a
Blumenthal and Sanacke 1967	295.7	0.50842	
Bohet and Müller 1978	295	0.50841	
Benedict et al. 1979	293	0.50851	
Benedict 1986	298, 300	0.50846	
Marples 1988	295	0.50858	a
	Selected	0.50845 (5)	

Note for Table 90a

a. Not included in the average

At 293.15 K: Density 11725 (3) kg m^{-3} Molar volume 19.790 (6) cm^3 mol^{-1}.

90.2 Beta Phase: Body-centered cubic (cI2): 1633 K to 2023 K

Lattice parameter measurements of Chiotti and White 1967 (1698-1773 K) were fitted to the following equations which were extended to the melting point:

$$a \text{ (nm)} = 5.26346 \times 10^{-6} T + 0.402601 \quad (90c)$$

$$\varepsilon_T = 1.30427 \times 10^{-5} T - 2.36901 \times 10^{-3} \quad (90d)$$

The derived overall thermal expansion coefficient is 12.8 x 10^{-6} K^{-1}. Based on an accuracy for the lattice parameters of ± 0.0002 nm then the derived accuracy of the molar volumes is ± 0.031 cm^3 mol^{-1} leading to a molar volume change from the alpha to beta phases of 0.69 (16) %. Wilson et al. 1958 obtained low accuracy lattice parameters of 0.410 nm at 1598 K and 0.411 nm at 1673 K confirming the body-centered cubic structure originally identified by Chiotti 1954.

90.3 Lattice parameter values of Marples 1988

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Table 90b. Low temperature lattice parameter values of alpha thorium

T K	4	24	44	52	62	77	77
a Å	5.0715 (3)	5.0717 (3)	5.07235(30)	5.0725 (3)	5.0730 (3)	5.0737 (4)	5.0734 (3)
T K	107	133	158	193	224	295	
a Å	5.0753 (4)	5.07675(40)	5.0780 (4)	5.0800 (3)	5.0817 (4)	5.0856 (4)	

90.4 Lattice parameter values of Benedict 1986

These values are unpublished and are reproduced by permission of the author.

T K	300	55	65	75	85	95	105	115
a Å	5.0854	5.0714	5.0714	5.0737	5.0738	5.0716	5.0734	5.0760
T K	125	135	145	155	175	195	220	245
a Å	5.0750	5.0763	5.0780	5.0804	5.0789	5.0787	5.0803	5.0826
T K	270		298	75	85	155	175	315
a Å	5.0851		5.0840	5.0705	5.0723	5.0762	5.0781	5.0861

90.5 Low temperature specific heat and enthalpy of alpha thorium

Selected values are based on a combination of the specific heat measurements of Gordon et al. 1966 (1.0-4.2 K), Griffel and Skochdopole 1953 (20-300 K) and Nakamura et al. 1980 (80-1000K) with an interpolation in the region 4 to 20 K and with the values of Nakamura et al. being preferred above 80 K. C_p values are in units of J mol^{-1} K^{-1} and enthalpy values as $H_T - H_0$ in units of J mol^{-1}.

Table 90d. Low temperature specific heat and enthalpy values for alpha thorium

T K	5	10	15	20	25	30	35	40	45
C_p	0.083	0.679	2.119	4.626	7.533	10.026	12.171	14.032	15.613
$H_T - H_0$	0.128	1.93	8.33	24.70	55.27	99.31	154.92	220.55	294.77
T K	50	60	70	80	90	100	110	120	130
C_p	16.931	19.033	20.541	21.490	22.130	22.690	23.166	23.570	23.908
$H_T - H_0$	376.21	556.52	754.86	965.27	1183.4	1407.6	1637.0	1870.7	2108.1
T K	140	150	160	170	180	190	200	210	220
C_p	24.190	24.427	24.630	24.815	24.980	25.127	25.260	25.384	25.500
$H_T - H_0$	2348.6	2591.8	2837.1	3084.3	3333.3	3583.8	3835.8	4089.0	4343.4
T K	230	240	250	260	270	280	290	293.15	298.15
C_p	25.608	25.710	25.807	25.900	25.991	26.080	26.168	26.196	26.242
$H_T - H_0$	4599.0	4855.6	5113.2	5371.7	5631.2	5891.5	6152.8	6235.2	6366.3

Table 90e. Crystallographic properties of alpha thorium

T K	α x 10^6 K^{-1}	100 ε_T	*a* nm	*d* nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
0	0	- 0.280	0.50702	0.35852	19.624	11824
10	0.36	- 0.280	0.50703	0.35852	19.624	11824
20	2.27	- 0.279	0.50703	0.35853	19.624	11824
30	4.77	- 0.275	0.50705	0.35854	19.626	11823
40	6.58	- 0.270	0.50708	0.35856	19.630	11821
50	7.86	- 0.263	0.50712	0.35858	19.634	11818
60	8.78	- 0.254	0.50716	0.35861	19.639	11815
70	9.43	- 0.245	0.50720	0.35865	19.644	11812
80	9.83	- 0.236	0.50725	0.35868	19.650	11809
90	10.09	- 0.226	0.50730	0.35872	19.656	11805
100	10.31	- 0.215	0.50735	0.35875	19.662	11801
110	10.50	- 0.205	0.50741	0.35879	19.668	11798
120	10.66	- 0.194	0.50746	0.35883	19.674	11794
130	10.79	- 0.184	0.50752	0.35887	19.681	11790
140	10.90	- 0.173	0.50757	0.35891	19.687	11786
150	10.99	- 0.162	0.50763	0.35895	19.694	11782
160	11.06	- 0.151	0.50768	0.35899	19.700	11779
170	11.13	- 0.140	0.50774	0.35903	19.707	11775
180	11.18	- 0.129	0.50780	0.35907	19.713	11771
190	11.23	- 0.118	0.50785	0.35911	19.720	11767
200	11.27	- 0.106	0.50791	0.35915	19.726	11763
210	11.31	- 0.095	0.50797	0.35919	19.733	11759
220	11.35	- 0.084	0.50802	0.35923	19.740	11755
230	11.38	- 0.072	0.50808	0.35927	19.747	11751
240	11.41	- 0.061	0.50814	0.35931	19.753	11747
250	11.43	- 0.050	0.50820	0.35935	19.760	11743
260	11.46	- 0.038	0.50826	0.35939	19.767	11739
270	11.48	- 0.027	0.50831	0.35943	19.774	11735
280	11.51	- 0.015	0.50837	0.35947	19.781	11731
290	11.53	- 0.004	0.50843	0.35952	19.787	11727
293.15	11.54	0	0.50845	0.35953	19.790	11725
300	11.55	0.008	0.50849	0.35956	19.974	11723
400	11.70	0.124	0.50908	0.35997	19.863	11682
500	11.83	0.242	0.50968	0.36040	19.934	11641
600	11.96	0.361	0.51029	0.36083	20.005	11599
700	12.08	0.482	0.51090	0.36126	20.077	11557
800	12.19	0.604	0.51152	0.36170	20.150	11515
900	12.29	0.727	0.51215	0.36214	20.225	11473
1000	12.38	0.852	0.51278	0.36259	20.300	11431
1100	12.47	0.977	0.51342	0.36304	20.375	11388
1200	12.54	1.104	0.51406	0.36350	20.452	11346
1300	12.60	1.231	0.51471	0.36395	20.529	11303
1400	12.65	1.359	0.51538	0.36441	20.607	11260
1500	12.70	1.487	0.51601	0.36488	20.686	11217
1600	12.73	1.612	0.51667	0.36534	20.765	11175
1633	12.74	1.659	0.51689	0.36549	20.791	11161

$$d = a/\sqrt{2}$$

Table 90f. Crystallographic properties of beta thorium

T K	100 ε_T	a nm	d nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1633	1.893	0.4112	0.3561	20.93	11080
1650	1.915	0.4113	0.3562	20.95	11080
1700	1.980	0.4115	0.3564	20.99	11050
1750	20.46	0.4118	0.3566	21.03	11030
1800	2.111	0.4121	0.3569	21.07	11010
1850	2.176	0.4123	0.3571	21.11	10990
1900	2.241	0.4126	0.3573	21.15	10970
1950	2.306	0.4129	0.3576	21.19	10950
2000	2.372	0.4131	0.3578	21.23	10930
2023	2.402	0.4132	0.3579	21.25	10920

$$d = \sqrt{3}a/2$$

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91 PROTACTINIUM Pa

Atomic weight: 231.03588 (2) (Meija 2017)

Allotropy: Alpha: Body-centered tetragonal (tI2)
Beta: Body-centered cubic (cI2)

The room temperature structure is body-centered tetragonal and because all other of the light lanthanides and actinides crystallize in a body-centered cubic structure just below the melting point then this structure is also adopted for protactinium. However, initially Asprey et al. 1971 and then later Bohet and Müller 1978, quenched out a face-centered cubic (cF4) structure which it was suggested was the real high temperature phase although the derived molar volume, 27% larger than the alpha phase, appeared to be highly suspicious and also this phase did not spontaneously transform to the alpha phase but could only be made do so by heating to high temperatures and cooling slowly. Blank 2002 considered the existence of this structure and concluded that holding samples at a temperature of 1773 K for prolonged periods caused saturation with tungsten from the container, especially because the Pa-W eutectic temperature is estimated as being 1785 (20) K. Quenching of the body-centered cubic structure saturated with tungsten would then cause a matensitic transformation to the face-centered cubic structure.

Both Oetting et al. 1976 and Ward et al. 1986 select 1845 (20) K for the melting point while based on the lattice parameter thermal expansion coefficients of Marples 1965 (291-1328 K) it was suggested that the alpha phase would lose its tetragonal structure at 1443 K. However, this is based on the actual lattice parameters determined by Marples 1965 and if it is assumed that the derived thermal expansion coefficients are independent of the lattice parameter values then the selected lattice parameters below would lead to the same effect at 1670 K, although the selected transition temperature of 1500 K is much lower for the reasons given in Part 91.2.

91.1 Alpha Phase: Body-centered tetragonal (tI2): 0 K to 1500 K

Length change values derived from the lattice parameter values of Marples 1965 (291-1328 K), less the *a* axis value at 615 K, were selected. Derived as an accuracy on the basis ± 100ε_T the the *a* axis equation is accurate to ± 0.021 and the *c* axis equation to ± 0.014. The equations were extrapolated to 1500 K:

$$\varepsilon_T a = 4.72215 \times 10^{-5} T - 9.53442 \times 10^{-8} T^2 + 9.56590 \times 10^{-11} T^3 - 3.84860 \times 10^{-14} T^4 - 7.77505 \times 10^{-3} \quad (91a)$$

$$\varepsilon_T c = -3.05509 \times 10^{-5} T + 1.18970 \times 10^{-7} T^2 - 1.34020 \times 10^{-10} T^3 + 6.36062 \times 10^{-14} T^4 + 1.63863 \times 10^{-3} \quad (91b)$$

Length changes derived from lattice parameter measurements of Dod 1972 (303-773 K) show poor agreement with the above equations. On the basis 100$\Delta\varepsilon$ a first sample trending to 0.09 low along the *a* axis and 0.37 low along the *c* axis while a second sample

trends 0.11 low along the *a* axis and 0.27 low along the *c* axis. Low temperature lattice parameter measurements of Benedict et al. 1979 (55-293 K) were only shown in the form of a small graph but do not appear to agree with the high temperature data with the thermal expansion appearing to be negligible along the *a* axis down to about 150 K and then the derived thermal expansion coefficient appearing to be negative below this temperature. For the *c* axis a mean thermal expansion coefficient of 3.4 x 10^{-6} K^{-1} between 60 and 293 K also does not appear to agree with the selected values.

Table 91a. The lattice parameters of alpha protactinium at 293.15 K

References	Original Temperature K	*a* nm	*c* nm
Zachariasen 1952	RT	0.3925	0.3238
Zachariasen 1959	RT	0.3932	0.3238
Marples 1965	291	0.3924	0.3239
Cunningham 1966	RT	0.3929	0.3241
Dod 1972	303	0.3931	0.3246
Baybarz et al. 1976	RT	0.3922	0.3236
Brown et al. 1977	RT	0.3931	0.3236
Bohet and Müller 1978	RT	0.3921	0.3235
	Selected	0.3921 (1)	0.3235 (1)

The selected values are based on a very close agreement between the measurements of Baybarz et al. 1976 and Bohet and Müller 1978.

At 293.15 K: Density 15427 (9) kg m^{-3} Molar volume 14.976 (9) cm^3 mol^{-1}.

91.2 Beta Phase: Body-centered cubic (cI2): 1500 K to 1845 K

A value of 1500 K is selected for the transition temperature because above this temperature the extrapolations of equations 91a and 91b are likely to be increasingly unreliable beyond the experimental limit of 1328 K. The volume change from alpha to beta thorium at 0.69 (16) % and from beta to gamma uranium at 0.73 (11) % are the same within experimental accuracy and suggests a value of 0.7 % for protactinium leading to a molar volume for the beta phase at the transition temperature of 15.721 cm^3 mol^{-1}. Because the melting points of thorium and uranium are considerably different then the molar volumes are averaged at reduced temperatures T/T_M . In order to match the selected molar volume at 1500 K then this would lead to weighting factors of 0.3113 for beta thorium and 0.6887 for gamma uranium and these factors have been used to weight the molar volumes at reduced temperatures from 0.80 to 1.00 at 0.02 intervals. Derived lattice parameter and length change values were then fitted to the equations:

$$a \text{ (nm)} = 5.81498 \times 10^{-6} T + 0.365034 \quad (91c)$$

$$\varepsilon_T = 1.58122 \times 10^{-5} T - 7.39302 \times 10^{-3} \quad (91d)$$

The derived overall thermal expansion coefficient is 15.5 x 10^{-6} K^{-1}. Marples 1965 determined a highly tentative value of 0.381 nm at 1443 K but this would lead to a large volume expansion on transition of 6.8%.

Table 91b. Crystallographic properties of alpha protactinium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
293.15	12.1	11.0	11.8	0	0	0
300	11.7	11.5	11.6	0.008	0.008	0.008
400	7.0	16.6	10.2	0.100	0.150	0.117
500	4.8	19.7	9.5	0.155	0.333	0.214
600	2.9	22.4	9.4	0.197	0.542	0.308
700	1.6	26.3	9.8	0.213	0.785	0.403
800	0.5	32.7	10.6	0.220	1.077	0.505
900	- 4.2	43.4	11.7	0.198	1.454	0.615
1000	- 10.4	59.8	13.0	0.128	1.964	0.736
1100	- 20.2	83.3	14.3	- 0.022	2.673	0.868
1200	- 34.4	116	15.6	- 0.291	3.660	1.009
1300	- 53.9	158	16.8	- 0.728	5.021	1.153
1400	- 79.7	213	17.8	- 1.390	6.865	1.288
1500	- 113	280	18.4	- 2.345	9.318	1.397

Table 91c. Crystallographic properties of alpha protactinium

T K	*a* nm	*c* nm	*c*/*a*	*d*1 nm	Molar Volume cm^3 mol^{-1}	Density kg m^{-3}
293.15	0.3921	0.3235	0.8250	0.3210	14.98	15430
300	0.3921	0.3235	0.8250	0.3210	14.98	15420
400	0.3925	0.3240	0.8255	0.3214	15.03	15370
500	0.3927	0.3246	0.8265	0.3216	15.07	15330
600	0.3928	0.3253	0.8279	0.3219	15.11	15290
700	0.3929	0.3260	0.8298	0.3221	15.16	15240
800	0.3930	0.3270	0.8321	0.3224	15.20	15200
900	0.3929	0.3282	0.8354	0.3227	15.25	15150
1000	0.3926	0.3299	0.8402	0.3229	15.31	15090
1100	0.3920	0.3321	0.8473	0.3231	15.37	15030
1200	0.3910	0.3353	0.8577	0.3233	15.43	14970
1300	0.3892	0.3397	0.8728	0.3234	15.50	14910
1400	0.3867	0.3457	0.8941	0.3235	15.56	14850
1500	0.3829	0.3536	0.9236	0.3234	15.61	14800

$$d1 = [\, a^{\,2}/2 + c^{\,2}/4 \,]^{\,½} \qquad d2 = c$$

Table 91d. Estimated crystallographic properties of beta protactinium

T K	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1500	1.633	0.3738	0.3237	15.72	14700
1550	1.712	0.3740	0.3239	15.76	14660
1600	1.791	0.3743	0.3242	15.80	14630
1650	1.870	0.3746	0.3244	15.83	14590
1700	1.948	0.3749	0.3247	15.87	14560
1750	2.028	0.3752	0.3249	15.90	14530
1800	2.107	0.3755	0.3252	15.94	14490
1845	2.178	0.3758	0.3254	15.98	14460

$$d = \sqrt{3}a/2$$

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92 URANIUM U

Atomic Weight: 238.02891 (3) (Meija 2017)

Allotropy: Alpha: Orthorhombic (oS4)
Beta: Tetragonal (tP30)
Gamma: Body-centered cubic (cI2)

Transition temperatures determined by Blumenthal 1960 corrected to ITS-90 as 941 (1) K for the alpha-beta transformation temperature, 1049 (2) K for the beta-gamma transformation temperature and 1407 (1) K for the melting point on ITS-90.

92.1 Alpha Phase: Orthorhombic (oS4): 0 K to 941 K

Below 43 K the alpha phase exists in a second order incommensurate charge-density wave (CDW) mode (Smith et al. 1980) with two additional transformations at 22 K and 37 K as detected by both specific heat measurements by Crangle and Temporal 1973 and dilatometric measurements by Steinitz et al. 1970. Using high-resolution X-ray and neutron scattering experiments, Grübel et al. 1991 showed that the 37 K transition was due to lock-in of the q_x component of the modulation wave vector to a value of $q_x = ½$ while the 22 K transition was due to lock in of the other two components at $q_y = {}^1/_6$ and $q_z = {}^2/_{11}$, although from neutron diffraction experiments Marmeggi et al. 1990 suggested that $q_z = {}^5/_{27}$. Dilatometric measurements by both Steinitz et al. 1970 and Tindall and Steinitz 1984 and neutron diffraction measurements by Fournier et al. 1979 showed that the two transitions were first order. Lattice parameter values determined by Barrett et al. 1963 (4.2-298.0 K) were only given at 4.2 K, 50 K, 78 K and 298 K although a large number of diffraction angles were also determined which allowed Lloyd and Barrett 1966 to develop thermal expansion equations to cover the whole range up to 923 K. These equations were selected over the range 43 K to 293.15 K after correcting from a 4.2 K base to a 293.15 K base:

$$\varepsilon_T a = 2.4150 \times 10^{-5} T - 5.0804 \times 10^{-9} T^2 + 1.5915 \times 10^{-11} T^3 - 7.0439 \times 10^{-3} \quad (92a)$$

$$\varepsilon_T b = 2.9608 \times 10^{-6} T + 1.9287 \times 10^{-9} T^2 - 1.2907 \times 10^{-11} T^3 - 7.0855 \times 10^{-4} \quad (92b)$$

$$\varepsilon_T c = 8.6843 \times 10^{-6} T + 1.8322 \times 10^{-8} T^2 + 3.5810 \times 10^{-12} T^3 - 4.2105 \times 10^{-3} \quad (92c)$$

Below 43 K these equations were modified so as to eliminate the abrupt changes at 20 K and measurements over the range 25 to 40 K were adjusted so that length changes at 43 K exactly matched those obtained from equations 92a to 92c. The scatter in the measurements were such that the abrupt changes at 22 K and 37 K were not evidenced in the actual equations and were therefore not included. Similarly, the thermal expansion coefficients below 5 K given by Andres 1968 were not included because they could not be linked up with measurements above this temperature.

Lattice parameter measurements of Marples 1970 (4-107 K) were only shown graphically with actual data points as length change values given by Touloukian et al. 1975. On the

basis 100Δε these measurements show only poor agreement with those of Lloyd and Barrett 1966. For the *a* axis being on average 0.073 lower below 30 K and 0.012 lower above 40 K, for the *b* axis trending 0.025 to 0.042 high and for the *c* axis trending 0.050 to 0.026 high. Lattice parameter measurements obtained by Bridge et al. 1956 in the low temperature region, 20 to 188 K, show a significant scatter with the *a* axis varying from 0.12 low to 0.058 high, the *b* axis varying 0.044 low to 0.041 high and the *c* axis varying 0.12 low to 0.016 high.

In the high temperature region Lloyd and Barrett 1966 selected the anisotropic dilatometric measurements on single crystals obtained by Lloyd 1961 (298-923 K) and considered that the results differed from those obtained by Bridge et al. 1956 and Chiotti et al. 1959 because elastic strains in the polycrystalline samples used caused distortion of the derived thermal expansion. However, the measurements of Lloyd 1961 differ significantly from all other measurements including those on single crystals by Lehr and Langeron 1955, 1957 and Ibrahim 1964-1965 and were apparently rejected by Touloukian et al. 1975 and were therefore also rejected here. However, the thermal expansion coefficients at 293.15 K derived from the equations of Lloyd and Barrett 1966 were retained and combined with length change values derived from the dilatometric measurements of Ibrahim 1964 (323-773 K) and lattice parameter measurements of Lawson et al. 1988 (298-919 K), as well as three high temperature measurements of the *a* axis from lattice parameter measurements of Chiotti et al. 1959 (273-935 K in the alpha phase region) to give the following equations to cover the range from 293.15 K to 941 K:

$$\varepsilon_T a = 1.98738 \times 10^{-5} T + 1.18387 \times 10^{-8} T^2 - 1.12788 \times 10^{-11} T^3 + 1.35690 \times 10^{-14} T^4 - 6.65946 \times 10^{-3} \quad (92d)$$

$$\varepsilon_T b = 8.53542 \times 10^{-6} T - 2.02650 \times 10^{-8} T^2 + 2.31677 \times 10^{-11} T^3 - 1.84868 \times 10^{-14} T^4 - 1.20777 \times 10^{-3} \quad (92e)$$

$$\varepsilon_T c = -3.62703 \times 10^{-6} T + 6.74180 \times 10^{-8} T^2 - 7.64622 \times 10^{-11} T^3 + 4.13054 \times 10^{-14} T^4 - 3.10921 \times 10^{-3} \quad (92f)$$

On the basis 100Δε the marked difference between the selected values and the measurements of Lloyd 1961, as included in the review by Lloyd and Barrett 1966, is indicated by the differences of 0.07 high along the *a* axis, 0.07 low along the *b* axis and 0.14 high along the *c* axis. The scatter amongst the older determinations can be shown by deviations from the presently accepted values. The dilatometric measurements of Lehr and Langeron 1955, 1957 (473-873 K) trend to 0.24 low along the *a* axis, 0.06 high along the *b* axis and 0.04 low to 0.04 high along the *c* axis. Values derived from the lattice parameter measurements of Bridge et al. 1956 (300-913 K) show a marked scatter from 0.15 low to 0.10 high along the *a* axis, 0.06 low to 0.07 high along the *b* axis and 0.21 low to 0.09 high along the *c* axis. The measurements of Konobeevsky et al. 1958 (273-773 K) trend to 0.05 high along the *a* axis, 0.06 high to 0.03 low along the *b* axis, and biases 0.05 low along the *c* axis. The values of Chiotti et al. 1959 (273-935 K in the alpha phase) trend 0.04 low to 0.01 high along the *a* axis, 0.04 high to 0.04 low along the *b* axis and trends to 0.12 low along the *c* axis. Preferences amongst the scattered data may explain the differences between the presently selected values and those of Touloukian et

al. 1975 which bias 0.06 low along the *a* axis, trends to 0.10 high along the *b* axis and trends to 0.11 low along the *c* axis, but certainly the inclusion of the later measurements of Lawson et al. 1988 influenced the present evaluation.

Table 92a. The lattice parameters of alpha uranium at 293.15 K

References	Original Temperature K	*a* nm	*b* nm	*c* nm	Notes
Schramm et al. 1950	RT	0.28542	0.58687	0.49579	a
Bridge et al. 1956	300	0.28528	0.58680	0.49559	a
Chiotti et al. 1959	298	0.28533	0.58651	0.49541	a
Cooper 1962	297.8	0.28535	0.58702	0.49554	
Berndt 1963	298	0.28534	0.58691	0.49556	
Barrett et al. 1963	298.0	0.28535	0.58698	0.49546	
Lawson et al. 1988	298	0.28537	0.58681	0.49552	b
	Selected	0.28535 (1)	0.58697 (5)	0.49552 (5)	

Notes for Table 92a

a. Not included in the average

b**.** The *b* axis value not included in the average

At 293.15 K: Density 19050 (3) kg m^{-3} Molar volume 12.495 (2) cm^3 mol^{-1}.

The *y* positional parameter for the alpha phase as determined by Sturcken and Post 1960 (298 K), Mueller et al. 1962 (298-898 K) and by Barrett et al. 1963 (4.2-298.0 K) were fitted to the following equations where the measurements below 43 K were constrained to avoid a discontinuity at this temperature.

0 – 43 K: $y = -1.28130 \times 10^{-5} T + 0.10242$ (92g)

43 – 293.15 K: $y = 2.08106 \times 10^{-6} T + 0.10178$ (92h)

293.15 – 941 K: $y = -4.82338 \times 10^{-6} T + 1.45422 \times 10^{-8} T^2 - 6.29009 \times 10^{-12} T^3 + 0.102715$ (92i)

Calculation of interatomic distance for alpha uranium

$d1 = 0.5\,[(4\,y\,b)^2 + c^2]^{½}$ $d2 = a$ $d3 = 0.5\,[a^2 + b^2]^{½}$

$d4 = 0.5\,[a^2 + (1 - 4\,y)^2 b^2 + c^2]^{½}$

92.2 Beta Phase: Tetragonal (tP30): 941 K to 1049 K

Chiotti et al. 1959 determined the lattice parameters at 954 K, 1009 K and 1038 K which were averaged to selected values at 1000 K. These average values were then combined

with thermal expansion coefficients derived from a large number of *d* spacing measurements which lead to the following equations:

a (nm) = 2.29 x 10^{-5} T + 1.05324 (92j)

c (nm) = 5.0 x 10^{-6} T + 0.560241 (92k)

The accuracies of equations 92j and 92k were considered to be only ± 0.0005 nm in each case but were extended in Table 92e for interpolation purposes.

The overall thermal expansion coefficients are α_a = 21.3 x 10^{-6} K^{-1} α_c = 8.84 x 10^{-6} K^{-1} α_{avr} = 17.1 x 10^{-6} K^{-1}. The accuracies assigned to the lattice parameters are equivalent to a molar volume accuracy of ± 0.013 cm^3 mol^{-1} so that the volume expansion involved in the alpha beta transformation is 0.89 (10) %

The earlier measurements of Thewlis 1952 at 993 K show excellent agreement with the *a* axis value agreeing exactly and the *c* axis value differing by only 0.0002 nm. However, the later measurements by Lawson et al. 1988 at 955 K and 1030 K show relatively poor agreement with the *a* axis values averaging 0.0009 nm high and the *c* axis values averaging 0.0004 nm high.

Postional parameters for beta uranium

These are the average values for measurements obtained at 955 K and 1030 K by Lawson et al. 1988 on powdered samples.

	I	II	III	IV	V
x	[0]	0.1028	0.3188	0.5624	0.3655
y	[0]	0.1028	0.3188	0.2344	0.0391
z	[0.5]	[0]	0.7463	[0]	[0]

In Table 92f, in which interatomic distances have been calculated with the above positional parameters, it is noted that although these values specifically apply to the lattice parameter measurements of Lawson et al. 1988 they have been used together with the selected lattice parameter values to produce a set of interatomic distance at 1000 K.

Calculation of interatomic distances in beta uranium using the order given by Donohue 1974

U I – U IV: $d1 = a\,[\,(x_{IV} - 0.5)^2 + (y_{IV} - 0.5)^2\,]^{½}$

U I – U III: $d2 = [\,2\,a^2(0.5 - x_{III})^2 + c^2(1 - z_{III})^2\,]^{½}$

U I – U II: $d3 = [\,2\,x_{II}^2\,a^2 + 0.25\,c^2\,]^{½}$

U II – U V: $d4 = a\,[\,(x_V - x_{II})^2 + (y_V - y_{II})^2\,]^{½}$

U II – U II: $d5 = 8^{½}\,a\,x_{II}$

U II – U IV: $d6 = [\,a^2(0.5 + x_{II} - x_{IV})^2 + a^2(0.5 - y_{II} - y_{IV})^2 + 0.25\,c^2\,]^{½}$

U II – U III: $d7 = [\,a^2(x_{III} - x_{II} - 0.5)^2 + a^2(y_{III} + y_{II} - 0.5)^2 + c^2(z_{III} - 0.5)^2\,]^{½}$

U II – U III: $d8 = [\,2\,a^2(x_{III} - x_{II})^2 + c^2(1 - z_{III})^2\,]^{½}$

U III – U III: $d9 = c\,(2\,z_{III} - 1)$

U III – U IV: $d10 = [\,a^2(x_{IV} - x_{III})^2 + a^2(y_{IV} - y_{III})^2 + c^2(1 - z_{III})^2\,]^{½}$

U III – U IV: $d11 = [\,a^2(x_{III} - x_{IV} + 0.5)^2 + a^2(y_{III} + y_{IV} - 0.5)^2 + c^2(z_{III} - 0.5)^2\,]^{½}$

U III – U V: $d12 = [\,a^2(x_V - x_{III})^2 + a^2(y_V - y_{III})^2 + c^2(1 - z_{III})^2\,]^{½}$

U III – U V: $d13 = [\,a^2(x_V + x_{III} - 0.5)^2 + a^2(y_V - y_{III} + 0.5)^2 + c^2(z_{III} - 0.5)^2\,]^{½}$

U IV – U V: $d14 = a\,[\,(x_V - x_{IV})^2 + (y_V - y_{IV})^2\,]^{½}$

U IV – U V: $d15 = a\,[\,(1 - x_{IV} - x_V)^2 + (y_{IV} + y_V)^2\,]^{½}$

U IV – U V: $d16 = [\,a^2(x_{IV} - y_V - 0.5)^2 + a^2(x_V + y_{IV} - 0.5)^2 + 0.25\,c^2\,]^{½}$

U IV – U IV: $d17 = 2^{½}\,a\,(1 - x_{IV} - y_{IV})$

U V – U V: $d18 = a\,[\,(1 - 2\,x_V)^2 + 4\,y_V^2\,]^{½}$

U V – U V: $d19 = [\,a^2(0.5 + y_V - x_V)^2 + a^2(0.5 - y_V - x_V)^2 + 0.25\,c^2\,]^{½}$

92.3 Gamma Phase: Body-centered cubic (cI2): 1049 K to 1407 K

Lattice parameter measurements of Chiotti et al. 1959 (1073-1333 K) were fitted to the following equations. The overall thermal expansion coefficient is 21.8 x 10^{-6} K^{-1}:

$$a \text{ (nm)} = 7.72335 \times 10^{-6} T + 0.345151 \quad (92l)$$

$$\varepsilon_T = 2.23082 \times 10^{-5} T - 3.06604 \times 10^{-3} \quad (92m)$$

Assuming an accuracy of ± 0.00005 nm for the lattice parameters then the equivalent molar volume accuracy is ± 0.006 cm^3 mol^{-1} and the volume expansion at the beta-gamma transition temperature is 0.73 (11) %.

The measurement of Lawson et al. 1988 at 1060 K shows excellent agreement being only 0.00003 nm higher. Extrapolation of equation 92i into the room temperature region leads to 0.3474 nm in exact agreement with the value obtained by Wilson and Rundle 1949 by extrapolating the lattice parameters of molybdenum–uranium alloys to zero molybdenum content.

Table 92b. Crystallographic properties of alpha uranium

T K	α_a x 10^6 K^{-1}	α_b x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	100 ε_T *a*	100 ε_T *b*	100 ε_T *c*	100 ε_T avr
0	0	0	0	0	- 0.298	- 0.007	- 0.461	- 0.256
17	0	0	0	0	- 0.298	- 0.007	- 0.461	- 0.256
20	- 48.5	- 6.92	11.7	-14.6	- 0.305	- 0.008	- 0.459	- 0.258
25	- 115	- 18.6	35.6	-32.5	- 0.347	- 0.014	- 0.448	- 0.270
30	- 133	- 21.6	36.7	-39.2	- 0.408	- 0.025	- 0.430	- 0.288
35	- 151	- 24.7	37.9	-45.8	- 0.479	- 0.036	- 0.411	- 0.309
40	- 169	- 27.8	39.0	-52.5	- 0.558	- 0.049	- 0.392	- 0.333
43	- 180	- 29.6	39.7	-56.5	- 0.610	- 0.058	- 0.380	- 0.351
43	23.95	3.06	10.32	12.44	- 0.610	- 0.058	- 0.380	- 0.351
45	23.93	3.06	10.39	12.46	- 0.597	- 0.057	- 0.378	- 0.344
50	23.90	3.06	10.58	12.51	- 0.585	- 0.056	- 0.373	- 0.338
60	23.85	3.05	10.96	12.62	- 0.561	- 0.053	- 0.362	- 0.326
70	23.80	3.04	11.34	12.73	- 0.537	- 0.050	- 0.351	- 0.313
80	23.76	3.02	11.72	12.84	- 0.514	- 0.047	- 0.340	- 0.301
90	23.74	3.00	12.11	12.95	- 0.490	- 0.044	- 0.328	- 0.287
100	23.72	2.96	12.50	13.06	- 0.466	- 0.041	- 0..16	- 0.274
110	23.72	2.92	12.88	13.17	- 0.443	- 0.038	- 0.303	- 0.261
120	23.72	2.87	13.27	13.29	- 0.419	- 0.035	- 0.290	- 0.248
130	23.73	2.81	13.67	13.40	- 0.396	- 0.032	- 0.276	- 0.235
140	23.75	2.74	14.06	13.52	- 0.372	- 0.029	- 0.263	- 0.221
150	23.78	2.67	14.46	13.64	- 0.348	- 0.026	- 0.248	- 0.208
160	23.82	2.59	14.86	13.76	- 0.324	- 0.024	- 0.234	- 0.194
170	23.87	2.50	15.26	13.88	- 0.301	- 0.021	- 0.219	- 0.180
180	23.93	2.40	15.66	14.00	- 0.277	- 0.019	- 0.203	- 0.166
190	24.00	2.30	16.06	14.12	- 0.254	- 0.017	- 0.187	- 0.152
200	24.08	2.18	16.47	14.25	- 0.229	- 0.014	- 0.171	- 0.138
210	24.17	2.06	16.88	14.37	- 0.205	- 0.012	- 0.155	- 0.124
220	24.27	1.94	17.29	14.50	- 0.181	- 0.010	- 0.138	- 0.109
230	24.38	1.80	17.70	14.63	- 0.156	- 0.008	- 0.120	- 0.095
240	24.49	1.66	18.12	14.76	- 0.132	- 0.007	- 0.102	- 0.080
250	24.62	1.51	18.53	14.89	- 0.108	- 0.005	- 0.084	- 0.065
260	24.76	1.35	18.95	15.02	- 0.083	- 0.004	- 0.165	- 0.050
270	24.90	1.18	19.37	15.15	- 0.058	- 0.002	- 0.046	- 0.035
280	25.06	1.01	19.79	15.28	- 0.033	- 0.001	- 0.026	- 0.020
290	25.22	0.82	20.22	15.42	- 0.008	- 0.000	- 0.006	- 0.005
293.15	25.27	0.76	20.35	15.46	0	0	0	0
300	25.39	0.64	20.64	15.55	0.017	0.000	0.014	0.011
350	26.30	- 0.31	22.52	16.17	0.147	0.001	0.122	0.090
400	27.33	- 1.29	24.12	16.72	0.281	- 0.003	0.239	0.172
450	28.50	- 2.37	25.56	17.23	0.421	- 0.012	0.364	0.257
500	29.87	- 3.60	26.96	17.74	0.568	- 0.027	0.426	0.345
550	31.46	- 5.04	28.45	18.29	0.722	- 0.048	0.635	0.436
600	33.33	- 6.74	30.15	18.91	0.885	- 0.077	0.782	0.529
650	35.50	- 8.76	32.17	19.64	1.059	- 0.116	0.939	0.626
700	38.01	- 11.16	34.65	20.50	1.244	- 0.165	1.108	0.727
750	40.91	- 13.99	37.69	21.53	1.444	- 0.228	1.290	0.833
800	44.22	- 17.32	41.41	22.77	1.660	- 0.306	1.491	0.944
850	47.98	- 21.20	45.93	24.24	1.894	- 0.402	1.712	1.063
900	52.22	- 25.68	51.36	25.97	2.150	- 0.518	1.959	1.190
941	56.08	- 29.86	56.57	27.60	2.377	- 0.631	2.185	1.301

Table 92c. Crystallographic properties of alpha uranium

T K	*a* nm	*b* nm	*c* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
0	0.28450	0.58693	0.49324	12.400	19196
17	0.28450	0.58693	0.49324	12.400	19196
20	0.28448	0.58692	0.49324	12.399	19198
25	0.28436	0.58688	0.49330	12.394	19205
30	0.28418	0.58683	0.49339	12.388	19215
35	0.28398	0.58676	0.49348	12.380	19227
40	0.28376	0.58668	0.49358	12.371	19241
43	0.28361	0.58663	0.49364	12.365	19251
45	0.28365	0.58663	0.49365	12.367	19248
50	0.28368	0.58664	0.49367	12.369	19244
60	0.28375	0.58666	0.49372	12.374	19237
70	0.28382	0.58668	0.49378	12.378	19229
80	0.28388	0.58670	0.49384	12.383	19222
90	0.28395	0.58671	0.49390	12.388	19215
100	0.28402	0.58673	0.49396	12.393	19207
110	0.28409	0.58675	0.49402	12.398	19200
120	0.28415	0.58677	0.49408	12.403	19192
130	0.28422	0.58678	0.49415	12.407	19184
140	0.28429	0.58680	0.49422	12.413	19177
150	0.28436	0.58681	0.49429	12.418	19169
160	0.28442	0.58683	0.49436	12.423	19161
170	0.28449	0.58685	0.49444	12.428	19153
180	0.28456	0.58686	0.49451	12.433	19145
190	0.28463	0.58687	0.49459	12.438	19137
200	0.28470	0.58689	0.49467	12.444	19129
210	0.28477	0.58690	0.49475	12.449	19120
220	0.28483	0.58691	0.49484	12.454	19112
230	0.28490	0.58692	0.49493	12.460	19104
240	0.28497	0.58693	0.49501	12.465	19095
250	0.28504	0.58694	0.49510	12.471	19087
260	0.28511	0.58695	0.49520	12.476	19078
270	0.28518	0.58696	0.49529	12.482	19070
280	0.28526	0.58696	0.49539	12.488	19061
290	0.28533	0.58697	0.49549	12.493	19052
293.15	0.28535	0.58697	0.49552	12.495	19050
300	0.28540	0.58697	0.49559	12.499	19043
350	0.28577	0.58698	0.49613	12.529	18998
400	0.28615	0.58695	0.49670	12.560	18951
450	0.28655	0.58690	0.49732	12.592	18903
500	0.28697	0.58681	0.49798	12.625	18854
550	0.28741	0.58669	0.49867	12.659	18803
600	0.28788	0.58652	0.49940	12.695	18750
650	0.28837	0.58629	0.50017	12.731	18696
700	0.28890	0.58600	0.50101	12.770	18640
750	0.28947	0.58563	0.50191	12.810	18581
800	0.29009	0.58517	0.50291	12.853	18520
850	0.29076	0.58461	0.50400	12.898	18455
900	0.29148	0.58393	0.50523	12.947	18385
941	0.29213	0.58327	0.50635	12.989	18325

Table 92d. Interatomic distances in alpha uranium

T K	*y*	*d*1 nm	*d*2 nm	*d*3 nm	*d*4 nm
0	0.10242	0.27436	0.28450	0.32612	0.33327
10	0.10229	0.27430	0.28450	0.32612	0.33334
17	0.10220	0.27425	0.28450	0.32612	0.33340
20	0.10216	0.27423	0.28448	0.32612	0.33342
25	0.10210	0.27423	0.28436	0.26607	0.33345
30	0.10204	0.27423	0.28419	0.32601	0.33348
35	0.10197	0.27423	0.28398	0.32593	0.33350
40	0.10191	0.27423	0.28376	0.32585	0.33351
43	0.10187	0.27423	0.28361	0.32579	0.33352
45	0.10187	0.27424	0.28365	0.32581	0.33353
50	0.10188	0.27426	0.28368	0.32582	0.33354
60	0.10190	0.27429	0.28375	0.32584	0.33356
70	0.10193	0.27433	0.28382	0.32586	0.33359
80	0.10195	0.27437	0.28388	0.32588	0.33361
90	0.10197	0.27441	0.28395	0.32591	0.33364
100	0.10199	0.27445	0.28402	0.32593	0.33366
110	0.10201	0.27449	0.28409	0.32595	0.33369
120	0.10203	0.27453	0.28415	0.32597	0.33372
130	0.10205	0.27457	0.28422	0.32600	0.33375
140	0.10207	0.27458	0.28429	0.32602	0.33378
150	0.10209	0.27466	0.28436	0.32604	0.33381
160	0.10211	0.27470	0.28442	0.32606	0.33384
170	0.10213	0.27475	0.28449	0.32608	0.33387
180	0.10215	0.27479	0.28456	0.32610	0.33390
190	0.10218	0.27484	0.28463	0.32613	0.33394
200	0.10220	0.27489	0.28470	0.32615	0.33397
210	0.10222	0.27494	0.28477	0.32617	0.33400
220	0.10224	0.27499	0.28483	0.32619	0.33404
230	0.10226	0.27504	0.28490	0.32621	0.33408
240	0.10228	0.27509	0.28497	0.32623	0.33411
250	0.10230	0.27514	0.28504	0.32625	0.33415
260	0.10232	0.27520	0.28511	0.32627	0.33419
270	0.10234	0.27525	0.28518	0.32629	0.33423
280	0.10236	0.27530	0.28526	0.32630	0.33427
290	0.10268	0.27536	0.28533	0.32632	0.33431
293.15	0.10239	0.27538	0.28535	0.32633	0.33432
300	0.1024	0.27542	0.28540	0.32634	0.33435
350	0.1025	0.27573	0.28577	0.32642	0.33455
400	0.1027	0.27607	0.28615	0.32650	0.33473
450	0.1029	0.27645	0.28655	0.32656	0.33492
500	0.1031	0.27686	0.28697	0.32661	0.33509
550	0.1034	0.27729	0.28741	0.32665	0.33527
600	0.1037	0.27775	0.28788	0.32668	0.33544
650	0.1040	0.27823	0.28837	0.32669	0.33562
700	0.1043	0.27874	0.28890	0.32667	0.33582
750	0.1046	0.27928	0.28947	0.32663	0.33604
800	0.1049	0.27984	0.29009	0.32657	0.33629
850	0.1053	0.28045	0.29076	0.32646	0.33657
900	0.1056	0.28109	0.29148	0.32632	0.33691
941	0.1058	0.28166	0.29213	0.32617	0.33723

Table 92e. Crystallographic properties of beta uranium

T K	100 ε_T avr	*a* nm	*c* nm	*c*/*a*	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
941	1.600	1.07479	0.56513	0.5258	13.105	18164
950	1.615	1.07500	0.56517	0.5257	13.111	18155
960	1.633	1.07522	0.56522	0.5257	13.117	18146
970	1.650	1.07545	0.56527	0.5256	13.124	18137
980	1.668	1.07568	0.56532	0.5255	12.131	18127
990	1.685	1.07591	0.53537	0.5255	13.138	18118
1000	1.702	1.07614	0.56542	0.5254	13.144	18109
1010	1.720	1.07637	0.56547	0.5253	13.151	18100
1020	1.737	1.07660	0.56552	0.5253	13.158	18090
1030	1.755	1.07683	0.56557	0.5252	13.165	18081
1040	1.772	1.07706	0.52562	0.5252	13.171	18072
1049	1.788	1.07726	0.56567	0.5251	13.177	18063

Table 92f. Interatomic distances in beta uranium at 1000 K

In the Table *d* refers to the equation number and *N* to the number of nearest neighbors.

First Type	Second Type	*d*	Distance nm	*N*	First Type	Second Type	*d*	Distance nm	*N*
I	IV	*d*1	0.2936	4	IV	I	*d*1	0.2936	1
	III	*d*2	0.3108	4		V	*d*14	0.2984	1
	II	*d*3	0.3231	4		V	*d*16	0.3035	1
			Total	**12**		V	*d*15	0.3044	2
II	V	*d*4	0.2909	2		III	*d*10	0.3123	2
	II	*d*5	0.3129	1		III	*d*11	0.3143	2
	I	*d*3	0.3231	2		IV	*d*17	0.3092	1
	IV	*d*6	0.3354	4		II	*d*6	0.3354	2
	III	*d*7	0.3463	4				Total	**12**
	III	*d*8	0.3587	2	V	II	*d*4	0.2909	1
			Total	**15**		IV	*d*14	0.2984	1
III	III	*d*9	0.2785	2		V	*d*18	0.3015	1
	I	*d*2	0.3108	1		IV	*d*16	0.3035	1
	IV	*d*10	0.3123	2		IV	*d*15	0.3044	2
	IV	*d*11	0.3143	2		III	*d*12	0.3372	2
	V	*d*12	0.3372	2		III	*d*13	0.3390	2
	V	*d*13	0.3390	2		V	*d*19	0.3541	4
	II	*d*7	0.3463	2				Total	**4**
	II	*d*8	0.3587	2					
			Total	**14**					

Table 92g. Crystallographic properties of gamma uranium

T K	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1049	2.034	0.35325	0.30593	13.273	17933
1050	2.036	0.35326	0.30593	13.274	17932
1075	2.092	0.32345	0.30610	13.296	17903
1100	2.147	0.35365	0.30627	13.318	17873
1125	2.204	0.35384	0.30643	13.339	17844
1150	2.259	0.35403	0.30660	13.361	17815
1175	2.315	0.35422	0.30677	13.383	17786
1200	2.370	0.35442	0.30694	13.405	17757
1225	2.426	0.35461	0.30710	13.427	17728
1250	2.482	0.35480	0.30727	13.449	17699
1275	2.538	0.35500	0.30744	13.471	17670
1300	2.593	0.35519	0.30760	13.493	17641
1325	2.649	0.35538	0.30777	13.515	17612
1350	2.705	0.35558	0.30794	13.537	17584
1375	2.761	0.35577	0.30811	13.559	17555
1400	2.817	0.35596	0.30827	13.581	17527
1407	2.832	0.35602	0.30831	13.587	17519

$$d = \sqrt{3}a/2$$

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93 NEPTUNIUM Np

Atomic mass ^{237}Np: 237.0481717 (12) (Wang et al. 2017)

Half-life of ^{237}Np: 2.144 x 10^6 y (Audi et al. 2017)

Allotropy: Alpha: Orthorhombic (oP8)
Beta: Tetragonal (tP4)
Gamma: Body-centered cubic (cI2)

Lemire et al. 2001 selected 553 (3) K for the alpha-beta transformation, 849 (3) K for the beta-gamma transformation and 912 (3) K for the melting point.

93.1 Alpha Phase: Orthorhombic (oP8): 0 K to 553 K

Certain publications transpose the *a* and *c* values but following Donohue 1974 the original lattice parameter sequence as given by Zachariasen 1952a, 1952b was retained. Length change values derived from the lattice parameter measurements of Zachariasen 1952a, 1952b (293-548 K) were fitted to the following equations which were extrapolated to the transition temperature:

$\varepsilon_T a = 2.45439 \times 10^{-5} T - 7.19504 \times 10^{-3}$ (93a)

$\varepsilon_T b = 2.53830 \times 10^{-5} T - 7.44103 \times 10^{-3}$ (93b)

$\varepsilon_T c = 3.37567 \times 10^{-5} T - 9.89578 \times 10^{-3}$ (93c)

The derived thermal expansion coefficients are:

$\alpha_a = 24.5 \times 10^{-6} K^{-1}$ $\alpha_b = 25.3 \times 10^{-6} K^{-1}$ $\alpha_c = 33.6 \times 10^{-6} K^{-1}$ $\alpha_{avr} = 27.8 \times 10^{-6} K^{-1}$

The average value agrees with the dilatometric value of 27.0 x 10^{-6} K^{-1} over the range 300 to 525 K obtained by Cort 1987 who also determined a mean thermal expansion coefficient of 16.2 x 10^{-6} K^{-1} over the range 100 to 300 K.

Table 93a. Lattice parameter of alpha neptunium at 293.15 K

References	Original Temperature K	*a* nm	*b* nm	*c* nm
Zachariasen 1952a, 1952b	293	0.4723	0.4887	0.6663
Lee et al. 1959	RT	0.4721	0.4888	0.6661
	Selected	0.4723 (2)	0.4887 (2)	0.6663 (3)

At 293.15 K: Density 20476 (15) kg m^{-3} Molar Volume 11.577 (9) cm^3 mol^{-1}.

Positional parameters for alpha neptunium

Values at 293.15 K determined by Zachariasen 1952 a:

$y1 = 0.208\ (6)$ $z1 = 0.036\ (6)$ $y2 = 0.842\ (6)$ $z2 = 0.319\ (6)$

Calculation of interatomic distances in alpha neptunium

NpI – NpII: $d1 = [\ b^2(1 + y1 - y2)^2 + c^2(z2 - z1)^2\ ]^{½}$

NpI – NpII: $d2 = [\ b^2(1½ - y1 - y2)^2 + c^2(½ + z1 - z2)^2\ ]^{½}$

NpI – NpII: $d3 = [\ a^2/4 + b^2(y2 - y1 - ½)^2 + c^2(½ - z1 - z2)^2\ ]^{½}$

NpI – NpII: $d4 = [\ b^2(y2 + y1 - ½)^2 + c^2(½ + z1 - z2)^2\ ]^{½}$

NpI – NpI: $d5 = [\ a^2/4 + 4\,b^2y1^2 + 4\,c^2z1^2\ ]^{½}$

NpI – NpII: $d6 = [\ a^2/4 + b^2(y2 + y1 - 1)^2 + c^2(z1 + z2)^2\ ]^{½}$

NpI – NpII: $d7 = [\ b^2(½ - 2\,y1)^2 + c^2/4\ ]^{½}$

NpII – NpII: $d8 = [\ b^2(2\,y2 - 1½)^2 + c^2/4\ ]^{½}$

NpII – NpII: $d9 = [\ a^2/4 + b^2/4 + c^2(2\,z2 - ½)^2\ ]^{½}$

93.2 Beta Phase: Tetragonal (tP4): 553 K to 849

Lattice parameter values of Zachariasen 1952 b (555-773 K) were fitted to the following equations except for the *a* axis value at 698 K which was rejected:

$a\ (\text{nm}) = 3.69486 \times 10^{-5}\,T + 0.467822$ (93d)

$c\ (\text{nm}) = 0.3389$ (93e)

The derived overall *a* axis thermal expansion coefficient is 75.0 x 10^{-6} K^{-1} while that for the *c* axis is zero leading to an average value of 50.0 x 10^{-6} K^{-1}. Cort 1987 obtained a dilatometric value of 60.5 x 10^{-6} K^{-1} over the range 550 to 870 K where the difference may be explainable in terms of the marked anisotropic effects. Lee et al. 1959 obtained lattice parameters at 585 K which are 0.0001 nm lower than the selected values along the *a* axis and 0.0003 nm lower along the *c* axis. The same differences were obtained by McKay et al. 1958 at the same temperature. On these grounds the *a* axis values are considered to be accurate to ± 0.0002 nm and the *c* axis values to ± 0.0003 nm, leading to a molar volume accuracy of ± 0.015 cm^3 mol^{-1} and a molar volume expansion from the alpha phase to the beta phase at the transition temperature at 2.82 (14) %.

Calculation of interatomic distances in beta neptunium

Zachariasen 1952b determined the positional parameter to be z = 0.375 (15) at 586 K.

NpI – NpII: $d1 = [\, a^{2}/4 + c^{2} z^{2} \,]^{½}$

NpI – NpII: $d2 = [\, a^{2}/4 + c^{2} (1 - z)^{2} \,]^{½}$

NpI – NpI: $d3 = c$

NpI – NpI: $d4 = a / \sqrt{2}$

NpI – NpII: $d5 = [\, a^{2}/2 + c^{2} (1 - 2z)^{2} \,]^{½}$

93.3 Gamma Phase: Body-centered cubic (cI2): 849 K to 912 K

Zachariasen 1952b tentatively identified the structure to be body-centered cubic and obtained a low accuracy value for the lattice parameter. The structure is now well established (Sheldon and Peterson 1985a, 1985b). By extrapolating Np-Pu alloy lattice parameters to pure neptunium a lattice parameter of 0.3512 nm at a metastable temperature of 823 K was derived by Mardon et al. 1961. Lee and Hall 1961 derived a thermal expansion coefficient of 33 x 10^{-6} K^{-1}. These values were combined to give the equation:

$$a \text{ (nm)} = 1.15903 \times 10^{-5} T + 0.341679 \qquad (93f)$$

This equation reproduces values of 0.3515 nm at 853 K and 0.3518 nm at 873 K as reported by Poole et al. 1961 and therefore, the accuracy of ± 0.0003 nm assigned to these values is also applied to equation 93f leading to a molar volume accuracy of ± 0.033 cm^3 mol^{-1} and a molar volume expansion from the beta phase to the gamma phase at the transition temperature of 2.87 (28) %.

Table 93b. Crystallographic properties of alpha neptunium

T K	100 ε_T *a*	100 ε_T *b*	100 ε_T *c*	100 ε_T avr
293.15	0	0	0	0
300	0.017	0.017	0.023	0.019
350	0.140	0.144	0.192	0.159
400	0.262	0.271	0.361	0.298
450	0.385	0.398	0.529	0.438
500	0.508	0.525	0.698	0.577
550	0.630	0.651	0.867	0.716
553	0.638	0.660	0.877	0.725

Table 93c. Crystallographic properties of alpha neptunium

T K	*a* nm	*b* nm	*c* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
293.15	0.4723	0.4887	0.6663	11.58	20480
300	0.4724	0.4888	0.6665	11.59	20460
350	0.4730	0.4894	0.6676	11.63	20380
400	0.4735	0.4900	0.6687	11.68	20290
450	0.4741	0.4906	0.6698	11.73	20210
500	0.4747	0.4913	0.6710	11.78	20120
550	0.4753	0.4919	0.6721	11.83	20040
553	0.4753	0.4919	0.6721	11.83	20040

Table 93d. Inter-atomic distances in alpha neptunium at 293.15 K

d is the equation number and N is the number of nearest neighbors.

First Type	Second Type	*d*	Distance nm	*N*	First Type	Second Type	*d*	Distance nm	*N*
I	II	*d1*	0.2599	1	II	I	*d*1	0.2599	1
	II	*d*2	0.2632	1		I	*d*2	0.2632	1
	II	*d*3	0.2634	2		I	*d*3	0.2634	2
	II	*d*4	0.3052	1		I	*d*4	0.3052	1
	I	*d*5	0.3153	2		I	*d*6	0.3351	2
	II	*d*6	0.3351	2		II	*d*8	0.3451	2
	I	*d*7	0.3357	2		II	*d*9	0.3520	4

Table 93e. Crystallographic properties of beta neptunium

T K	100 ε_{avr}	*a* nm	*c* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
553	1.661	0.4883	0.3389	12.16	19490
600	1.902	0.4900	0.3389	12.25	19350
650	2.158	0.4918	0.3389	12.34	19210
700	2.414	0.4937	0.3389	12.44	19060
750	2.669	0.4955	0.3389	12.53	18920
800	2.924	0.4974	0.3389	12.62	18780
849	3.174	0.4992	0.3389	12.71	18640

Table 93e. Inter-atomic distances in beta neptunium

d is the equation number and N is the number of nearest neighbors. The positional parameter $z = 0.375$ (15) is assumed to be temperature independent.

First Type	Second Type	*d*	Distance nm 553 K	Distance nm 849 K	*N*
I	II	*d*1	0.2752	0.2801	4
	II	*d*2	0.3232	0.3274	4
	I	*d*3	0.3389	0.3389	2
	I	*d*4	0.3453	0.3530	4
II	I	*d*1	0.2752	0.2801	4
	I	*d*2	0.3232	0.3274	4
	I	*d*3	0.3389	0.3389	2
	II	*d*5	0.3555	0.3630	4

Table 93f. Crystallographic properties of gamma neptunium

T K	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
849	4.150	0.3515	0.3044	13.08	18120
850	4.153	0.3515	0.3044	13.08	18120
875	4.239	0.3518	0.3047	13.11	18080
900	4.325	0.3521	0.3049	13.15	18030
913	4.370	0.3523	0.3051	13.16	18010

$$d = \sqrt{3}a/2$$

References for Neptunium

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94 PLUTONIUM Pu

Atomic mass ^{239}Pu: 239.0521617 (12) (Wang et al. 2017)
Atomic mass ^{244}P: 244.0642044 (25) (Wang et al. 2017)

The longest living isotope, ^{244}Pu, has a half-life of 8.00 x 10^7 y while the "most useful" isotope ^{239}Pu has a half-life of 24110 y (Audi et al. 2017).

Allotropy: Alpha: Monoclinic (mP16)
Beta: Body-centered monoclinic (mI34)
Gamma: Orthorhomic (oF8)
Delta: Face-centered cubic (cF4)
Delta Prime: Body-centered tetragonal (tI2)
Epsilon: Body-centered cubic (cI2)

The transition temperatures and melting point were selected by Oetting and Adams 1983 as Alpha-Beta: 397.6 K Beta-Gamma: 487.9 K Gamma-Delta: 593.1 K Delta-Delta Prime: 736.0 K Delta Prime – Epsilon: 755.7 K Melting point: 913.0 K.

A review of the thermal expansion behavior of plutonium was also given by Schonfeld and Tate 1996 using a different approach.

94.1 Alpha Phase: Monoclinic (mP16): 0 K to 397.6 K

Length changes derived from the lattice parameter measurements of Lee et al. 1967 (8–300 K) on a higher purity sample and by Zachariasen and Ellinger 1963b (294-377 K) were combined with enthalpy measurements of Gordon et al. 1976 (6-298 K) and Oerting and Adams 1983 (331.7-389.4 K) and fitted to Equation B. The measurements of Lee et al. 1967 were only shown graphically with actual data points being given by Touloukian et al. 1975 while the two sets of enthalpy measurements were amalgamated as described in Part 94.7. The angle β thermal expansion was based on a combination of values derived from the graphical represention of Lee et al. 1967 on a higher purity sample, the selected value at 293.15 K (see below) and the high temperature values of Zachariasen and Ellinger 1963b:

$$\ln (L_a) = (H_T - H_0) (1.25130 \times 10^{-6} + 9.99575 \times 10^{-10} T - 7.98017 \times 10^{-6}/T) - 1.02498 \times 10^{-2} \quad (94a)$$

$$\ln (L_b) = (H_T - H_0) (1.53651 \times 10^{-6} + 1.11874 \times 10^{-9} T - 1.43370 \times 10^{-5}/T) - 1.22662 \times 10^{-2} \quad (94b)$$

$$\ln (L_c) = (H_T - H_0) (8.41747 \times 10^{-7} + 1.18940 \times 10^{-10} T - 4.55335 \times 10^{-5}/T) - 4.87314 \times 10^{-3} \quad (94c)$$

$$\beta \text{ (rads)} = - 7.94125 \times 10^{-6} T + 1.77893 \quad (94d)$$

The sharp change in slope in the region of 60 K exhibited by all three axes is considered to be due to the build up of the daughter americium isotope because of the use of ^{239}Pu for these measurements. These anomalies have been smoothed out in the above equations because the specific heat measurements of Gordon et al. 1976 were made on ^{242}Pu which did not show this anomaly. Above 293.15 K these equations can be represented by:

$$\varepsilon_T a = 2.20994 \times 10^{-5} T + 4.41348 \times 10^{-8} T^2 + 2.65215 \times 10^{-11} T^3 - 1.09394 \times 10^{-2} \quad (94e)$$

$$\varepsilon_T b = 2.69866 \times 10^{-5} T + 5.21111 \times 10^{-8} T^2 + 3.06825 \times 10^{-11} T^3 - 1.31623 \times 10^{-2} \quad (94f)$$

$$\varepsilon_T c = 1.30112 \times 10^{-5} T + 2.29701 \times 10^{-8} T^2 + 1.77094 \times 10^{-12} T^3 - 5.83282 \times 10^{-3} \quad (94g)$$

$$\beta \text{ (rads)} = - 7.94125 \times 10^{-6} T + 1.77893 \quad (94h)$$

The principal thermal expansion coefficients are α_1 , α_2 and α_3 where $\alpha_2 = \alpha_b$ and α_1 and α_3 are given by: $\alpha_1 - \alpha_3 = - \Delta / \sin \beta \cos (2\varphi - \beta)$ and $\alpha_1 + \alpha_3 = \alpha_a + \alpha_c + \Delta / \tan \beta$, where $\tan (2\varphi - \beta) = (\alpha_a - \alpha_c) / \Delta$ and $\alpha_{avr} = (\alpha_1 + \alpha_2 + \alpha_3)/3$. Δ = the thermal expansion coefficient of the angle $\beta = - 7.94 \times 10^{-6}$ rads K^{-1} and φ is the angle between the *x* axis of the principal tensor ellipsoid and the crystallographic *a* axis.

Table 94a. Lattice parameter of alpha plutonium at 293.15 K

References	Original Temperature K	*a* nm	*b* nm	*c* nm	β°
Zachariasen and Ellinger 1957	291	0.6185	0.4825	1.0974	101.80
Čebotarev and Beznosikova 1959	RT	0.6181	0.4821	1.0966	101.82
Zachariasen and Ellinger 1963b	294	0.6183	0.4822	1.0963	101.79
Lallement and Solent 1967	300	0.6181	0.4820	1.0962	101.74
Lee at al 1967	293	0.6182	0.4822	1.0965	101.80
	296-299	0.6184	0.4823	1.0966	101.79
Fournier 1972	293	0.6181	0.4822	1.0967	-
	Selected	0.6183 (1)	0.4822 (2)	1.0964 (2)	101.79 (1)

In the cases of Lee et al. 1967 and Fournier 1972 the measurements were only shown graphically with actual data points given by Touloukian et al. 1975.

At 293.15 K: Density: ^{239}Pu 19848 (11) kg m^{-3} ^{244}Pu 20265 (11) kg m^{-3}
Molar volume: 12.044 (7) cm^3 mol^{-1}.

Postional parameters for alpha plutonium

Values determined by Zachariasen and Ellinger 1963b at 294 K

	I	II	III	IV	V	VI	VII	VIII
x	0.345(4)	0.767(4)	0.128(4)	0.657(5)	0.025(5)	0.473(4)	0.328(4)	0.569(4)
z	0.162(2)	0.168(2)	0.340(3)	0.457(3)	0.618(3)	0.653(2)	0.926(2)	0.894(2)

Calculation of interatomic distances in alpha plutonium

The order is that given by Zachariasen and Ellinger 1963b.

$d = [(a \text{ L} \cos(\beta - 90))^2 + (c \text{ M} - a \text{ L} \sin(\beta - 90))^2 + (\text{N } b)^2/4]^{1/2}$

Order	Bond	L	M	N
*d*1	I –VII	$x_{I} - x_{VII}$	$1 + z_{I} - z_{VII}$	0
*d*2	I – III	$x_{III} - x_{I}$	$z_{III} - z_{I}$	0
*d*3	I – II	$x_{II} - x_{I}$	$z_{II} - z_{I}$	0
*d*4	I – VIII	$1 - x_{I} - x_{VIII}$	$1 - z_{I} - z_{VIII}$	1
*d*5	I – VI	$1 - x_{I} - x_{VI}$	$1 - z_{I} - z_{VI}$	1
*d*6	I – IV	$x_{IV} - x_{I}$	$z_{IV} - z_{I}$	0
*d*7	I – VII	$1 - x_{I} - x_{VII}$	$1 - z_{I} - z_{VII}$	1
*d*8	I – II	$1 + x_{I} - x_{II}$	$z_{I} - z_{II}$	0
*d*9	I - VIII	$1 + x_{I} - x_{VIII}$	$1 + z_{I} - z_{VIII}$	0
*d*10	II-III	$1 + x_{III} - x_{II}$	$Z_{III} - z_{II}$	0
*d*11	II – VII	$1 - x_{I\,I} - x_{VII}$	$1 - z_{II} - z_{VII}$	1
*d*12	II – VIII	$x_{II} - x_{VIII}$	$1 + z_{II} - z_{VIII}$	0
*d*13	II – IV	$x_{II} - x_{IV}$	$z_{II} - z_{IV}$	0
*d*14	II – VII	$x_{II} - x_{VII}$	$1 + z_{II} - z_{VII}$	0
*d*15	II – V	$1 - x_{II} - x_{V}$	$1 - z_{II} - z_{V}$	1
*d*16	II – VIII	$2 - x_{I\,I} - x_{VIII}$	$1 - z_{II} - z_{VIII}$	1
*d*17	II - VI	$1 - x_{I\,I} - x_{VI}$	$1 - z_{II} - z_{VI}$	1
*d*18	III – V	$0 - x_{III} - x_{V}$	$1 - z_{III} - z_{V}$	1
*d*19	III – V	$x_{III} - x_{V}$	$z_{III} - z_{V}$	0
*d*20	III – IV	$x_{IV} - x_{III}$	$z_{IV} - z_{III}$	0
*d*21	III – IV	$1 - x_{III} - x_{IV}$	$1 - z_{III} - z_{IV}$	1
*d*22	III – IV	$1 + x_{III} - x_{IV}$	$z_{III} - z_{IV}$	0
*d*23	III – VI	$1 - x_{III} - x_{VI}$	$1 - z_{III} - z_{VI}$	1
*d*24	III – VIII	$1 - x_{III} - x_{VIII}$	$1 - z_{III} - z_{VIII}$	1
*d*25	III - VI	$x_{VI} - x_{III}$	$z_{VI} - z_{III}$	0
*d*26	IV – V	$1 + x_{V} - x_{IV}$	$z_{V} - z_{IV}$	0
*d*27	IV – VI	$x_{IV} - x_{VI}$	$z_{IV} - z_{VI}$	0
*d*28	IV – VI	$1 - x_{IV} - x_{VI}$	$1 - z_{IV} - z_{VI}$	1
*d*29	IV – V	$1 - x_{IV} - x_{V}$	$1 - z_{IV} - z_{V}$	1
*d*30	IV - IV	$2\,x_{IV} - 1$	$2\,z_{IV} - 1$	1
*d*31	V – VI	$x_{VI} - x_{V}$	$z_{VI} - z_{V}$	0
*d*32	V – VIII	$1 + x_{V} - x_{VIII}$	$z_{V} - z_{VIII}$	0
*d*33	V – V	$2\,x_{V}$	$2\,z_{V} - 1$	1
*d*34	V – VI	$1 + x_{V} - x_{VI}$	$z_{V} - z_{VI}$	0
*d*35	V - VII	$x_{VII} - x_{V}$	$z_{VII} - z_{V}$	0
*d*36	VI – VIII	$x_{VIII} - x_{VI}$	$z_{VIII} - z_{VI}$	0
*d*37	VI - VII	$x_{VI} - x_{VII}$	$z_{VI} - z_{VII}$	0
*d*38	VII – VIII	$1 + x_{VII} - x_{VIII}$	$z_{VII} - z_{VIII}$	0
*d*39	VII – VII	$1 - 2\,x_{VII}$	$2 - 2\,z_{VII}$	1
*d*40	VII – VIII	$x_{VIII} - x_{VII}$	$z_{VIII} - z_{VII}$	0
*d*41	VII - VIII	$1 - x_{VII} - x_{VIII}$	$2 - z_{VII} - z_{VIII}$	1
*d*42	VIII - VIII	$2 - 2\,x_{VIII}$	$2 - 2\,z_{VIII}$	1

Comparison with other length change values for the alpha phase

Lattice parameter values were reduced to length change values and on the basis $100\Delta\varepsilon$ the measurements of Lallement and Solente 1967 (20-300 K) scatter 0.02 low to 0.02 high along the *a* axis, bias 0.10 high along the *b* axis and bias 0.06 high along the *c* axis. Those of Lee et al. 1967, on a second less pure sample, were shown only graphically with actual data points as length change values over the range 11 K to 360 K were given by Touloukian et al. 1975. Below room temperature these bias 0.04 high along the *a* axis, 0.10 high along the *b* axis and 0.05 high along the *c* axis. The measurements in the region of 360 K show very poor agreement with the selected values being 0.14 low averaged over the three axes. The measurements of Fournier 1972 (10-300 K) show a bias 0.12 low along the *a* axis, 0.08 high along the *b* axis and 0.04 high along the *c* axis.

94.2 Beta Phase: Body-centered monoclinic (mI34): 397.6 K to 487.9 K

Lattice parameter measurements of Zachariasen and Ellinger 1959, 1963a at 366 K and 463 K were fitted to the following equations:

$$a \text{ (nm)} = 5.87662 \times 10^{-5} T + 0.901235 \quad (94i)$$

$$b \text{ (nm)} = 1.44338 \times 10^{-5} T + 1.039674 \quad (94k)$$

$$c \text{ (nm)} = 3.60845 \times 10^{-5} T + 0.769232 \quad (94l)$$

$$\beta \text{ (rads)} = -7.37716 \times 10^{-5} T + 1.64213 \quad (94m)$$

Using the defintions for thermal expansion coefficients given in the review on alpha plutonium then for beta plutonium:

$\alpha_a = 63.5 \times 10^{-6} K^{-1}$ $\alpha_b = 13.8 \times 10^{-6} K^{-1}$ $\alpha_c = 46.0 \times 10^{-6}$ $\Delta = d\beta/dT = -73.8 \times 10^{-6}$ rads K^{-1}

$\alpha_1 = 94.1 \times 10^{-6} K^{-1}$ $\alpha_2 = 13.8 \times 10^{-6} K^{-1}$ $\alpha_3 = 18.2 \times 10^{-6} K^{-1}$ $\alpha_{avr} = 42.1 \times 10^{-6} K^{-1}$ $\varphi = 39.4°$

Based on the accuracy of the lattice parameters then the accuracy of the molar volume is $\pm$ 0.008 cm^3 mol^{-1} and the volume change from the alpha to beta phases is an expansion of 9.37 (9) %.

Postional parameters beta plutonium

Values determined by Zachariasen and Ellinger 1963a. In calculating the inter-atomic distances at the median temperature of 443 K of the thermodynamically stable range the positional parameters are considered to be temperature independent.

	I	II	III	IV	V	VI	VII
x	0	0.146(4)	0.337(4)	0.434(5)	0.500	0.145(3)	0.167(3)
y	0	0	0	0	0.220(3)	0.268(2)	0.150(2)
z	0	0.387(5)	0.082(5)	0.672(5)	0	0.108(3)	0.753(4)

Calculation of interatomic distances in beta plutonium

$d = [(a \text{ L} \cos(\beta - 90))^2 + (c \text{ M} - a \text{ L} \sin(\beta - 90))^2 + (\text{N } b)^2 / 4]^{1/2}$

Order	Bond	L	M	N
*d*1	I –VII	x_{VII}	$z_{VII} - 1$	y_{VII}
*d*2	I – III	x_{III}	z_{III}	0
*d*3	I – VI	x_{VI}	z_{VI}	y_{VI}
*d*4	I – II	x_{II}	z_{II}	0
*d*5	II – III	$x_{III} - x_{II}$	$z_{III} - z_{II}$	0
*d*6	II – VI	$0.5 - x_{II} - x_{VI}$	$0.5 - z_{II} - z_{VI}$	$0.5 - y_{VI}$
*d*7	II – VII	$x_{VII} - x_{II}$	$z_{VII} - z_{II}$	y_{VII}
*d*8	II – II	$2\ x_{II}$	$2\ z_{II} - 1$	0
*d*9	II – V	$-\ x_{II}$	$0.5 - z_{II}$	$0.5 - y_{V}$
*d*10	II – IV	$x_{IV} - x_{II}$	$z_{IV} - z_{II}$	0
*d*11	II – VII	$-x_{II} - x_{VII}$	$1 - z_{II} - z_{VII}$	y_{VII}
*d*12	II - VI	$x_{II} - x_{VI}$	$z_{II} - z_{VI}$	y_{VI}
*d*13	III – IV	$1 - x_{III} - x_{IV}$	$1 - z_{III} - z_{IV}$	0
*d*14	III – V	$0.5 - x_{III}$	$-z_{III}$	y_{V}
*d*15	III – III	$2\ x_{III} - 1$	$2\ z_{III}$	0
*d*16	III – VI	$x_{III} - x_{VI}$	$z_{III} - z_{VI}$	y_{VI}
*d*17	III – VII	$x_{III} - x_{VII}$	$1 + z_{III} - z_{VII}$	y_{VII}
*d*18	III – IV	$x_{III} - x_{IV}$	$1 + z_{III} - z_{IV}$	0
*d*19	III - VI	$0.5 - x_{III} - x_{VI}$	$0.5 - z_{III} - z_{VI}$	$0.5 - y_{VI}$
*d*20	IV – IV	$1 - 2\ x_{IV}$	$1 - 2\ z_{IV}$	0
*d*21	IV – VII	$x_{IV} - x_{VII}$	$z_{IV} - z_{VII}$	y_{VII}
*d*22	IV – VI	$0.5 + x_{VI} - x_{IV}$	$0.5 + z_{VI} - z_{IV}$	$0.5 - y_{VI}$
*d*23	IV – VI	$0.5 - x_{IV} - x_{VI}$	$0.5 - z_{IV} - z_{VI}$	$0.5 - y_{VI}$
*d*24	IV - V	$0.5 - x_{IV}$	$1 - z_{IV}$	y_{V}
*d*25	V – VII	x_{VII}	$z_{VII} - 0.5$	$0.5 - y_{V} - y_{VII}$
*d*26	V – VI	x_{VI}	$z_{VI} - 0.5$	$0.5 - y_{V} - y_{VI}$
*d*27	V - VI	$x_{VI} - 0.5$	z_{VI}	$y_{V} - y_{VI}$
*d*28	V - VII	$0.5 - x_{VII}$	$1 - z_{VII}$	$y_{V} - y_{VII}$
*d*29	VI – VI	$0.5 - 2\ x_{VI}$	$0.5 - 2\ z_{VI}$	$0.5 - 2\ y_{VI}$
*d*30	VI – VII	$x_{VI} - x_{VII}$	$1 + z_{VI} - z_{VII}$	$y_{VI} - y_{VII}$
*d*31	VI – VI	$2\ x_{VI}$	$2\ z_{VI}$	0
*d*32	VI – VII	$-x_{VI} - x_{VII}$	$1 - z_{VI} - z_{VII}$	$y_{VI} - y_{VII}$
*d*33	VI - VII	$0.5 - x_{VI} - x_{VII}$	$0.5 - z_{VI} - z_{VII}$	$0.5 - y_{VI} - y_{VII}$
*d*34	VII – VII	$0.5 - 2\ x_{VII}$	$1.5 - 2\ z_{VII}$	$0.5 - 2\ y_{VII}$
*d*35	VII - VII	0	0	$2\ y_{VII}$

94.3 Gamma Phase: Orthorhombic (oF8): 487.9 K to 593.1 K

Lattice parameter values of Zachariasen and Ellinger 1955 (486-585 K) were fitted to the equations:

a (nm) = $-6.21891 \times 10^{-6} T + 0.319056 \pm 0.00004$ (94n)

b (nm) = $2.27484 \times 10^{-5} T + 0.565280 \pm 0.00005$ (94o)

c (nm) = $8.54482 \times 10^{-5} T + 0.972877 \pm 0.00024$ (94p)

These equations reproduce the reported lattice parameter values given at 508 K to within the stated accuracies. Derived overall thermal expansion coefficients are:

$\alpha_a = -19.7 \times 10^{-6}$ K $\alpha_b = 39.4 \times 10^{-6}$ K $\alpha_c = 83.8 \times 10^{-6}$ K $\alpha_{avr} = 34.5 \times 10^{-6}$ K

Based on the standard deviations obtained for equations 94n to 94p then the accuracy of the molar volume values are ± 0.004 $cm^3 mol^{-1}$ and the volume change from the beta to the gamma phase is an expansion of 2.62 (7) %.

94.4 Delta Phase: Face-centered cubic (cF4): 593.1 K to 736.0 K

Lattice parameter measurements of Ellinger 1956 (590-712 K) were shown only graphically and by an equation which was refitted as:

a (nm) = $-4.01022 \times 10^{-6} T + 0.466114$ (94q)

The overall thermal expansion coefficient is -8.6×10^{-6} K^{-1}. Based on the accuracy assigned to the lattice parameters of ± 0.00004 nm then the accuracy of the molar volumes are ± 0.004 $cm^3 mol^{-1}$ and the volume change from the gamma to the delta phase is an expansion of 6.76 (4) %. A lattice parameter determination by Marples 1964 at 673 K is only 0.0003 nm lower than the selected values.

94.5 Delta Prime Phase: Body-centered tetragonal (tI2): 736.0 K to 755.7 K

Lattice parameter measurements of Ellinger 1956 (738-757 K) were superseded by later measurements of Elliott and Larsen 1961 which included measurement of the lattice parameters at 723 K and determination of the thermal expansion coefficients using a diffractometer leading to the following equations:

a (nm) = $1.47953 \times 10^{-4} T + 0.225637$ (94r)

c (nm) = $-4.74667 \times 10^{-4} T + 0.789581$ (94s)

The mean thermal expansion coefficients are 445 (12) x 10^{-6} K^{-1} along the a axis and

– 1064 (18) x 10^{-6} K^{-1} along the *c* axis with an average value of – 66 (10) x 10^{-6} K^{-1}. Based on the accuracies assigned to the lattice parameters at 723 K of ± 0.00008 nm along the *a* axis and ± 0.00014 nm along the *c* axis then the accuracy of the molar volumes are ± 0.013 cm^3 mol^{-1} and the volume change from the delta to the delta prime phase is a contraction of 0.83 (9) %.

94.6 Epsilon Phase: Body-centered cubic (cI2): 755.7 K to 913 K

Lattice parameter measurements of Ellinger 1956 (759-825 K) were shown only graphically and by an equation which was refitted as:

$$a\ (\text{nm}) = 1.32507 \times 10^{-5}\ T + 0.353519 \qquad (94t)$$

The overall thermal expansion coefficient is 36.5 x 10^{-6} K^{-1}. Based on the accuracy assigned to the lattice parameters of ± 0.00004 nm then the accuracy of the molar volumes are ± 0.005 cm^3 mol^{-1} and the volume change from the delta prime to the epsilon phase is a contraction of 2.08 (10) %.

94.7 High temperature specific heat and enthalpy values of alpha plutonium

A compromise between the relatively incompatible specific heat measurements of Gordon et al. 1976 (6-298 K) and Oetting and Adams 1983 (331.7-389.4 K) was obtained by combining to produce a smooth curve which above 298.15 K can be represented by the equations:

$$C_p\ (\text{J mol}^{-1}\ \text{K}^{-1}) = 18.1258 + 0.04482\ T \qquad (94u)$$

$$H_T - H_0\ (\text{J mol}^{-1}) = 18.1258\ T + 0.02241\ T^2 - 483.279 \qquad (94v)$$

Table 94b. High temperature specific heat and enthalpy values for alpha plutonium

T K	260	270	280	290	293.15	298.15	300	310	320
C_p	29.899	30.272	30.684	31.123	31.264	31.489	31.572	32.020	32.468
$H_T - H_0$	5743.3	6044.1	6348.9	6657.9	6756.2	6913.0	6971.4	7289.3	7611.8
T K	330	340	350	360	370	380	390	397.6	
C_p	32.916	33.365	33.813	34.261	34.709	35.157	35.606	35.946	
$H_T - H_0$	7938.7	8270.1	8606.0	8946.4	9291.2	9640.5	9999.3	10266.2	

The selected values of Gordon et al. 1976 were accepted below 260 K.

Table 94c. Crystallographic properties of alpha plutonium

T K	α_a x 10^6 K^{-1}	α_b x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_1 x 10^6 K^{-1}	α_3 x 10^6 K^{-1}	α_{avr} x 10^6 K^{-1}	φ°
0	0	0	0	0	0	0	50.96
10	0.4	0.4	- 1.3	4.6	- 3.7	0.4	44.81
20	3.8	4.0	- 3.1	6.6	- 4.2	2.1	30.28
30	9.8	11.1	- 1.7	12.1	- 2.2	7.0	23.23
40	15.7	18.2	1.7	17.7	1.3	12.4	20.78
50	20.2	23.8	5.3	22.2	5.0	17.0	19.97
60	23.9	28.4	8.4	25.8	8.1	20.8	19.52
70	26.9	32.1	10.9	29.0	10.7	23.9	19.14
80	29.4	35.2	13.0	31.3	12.7	26.4	18.88
90	31.3	37.6	14.7	33.3	14.4	28.4	18.70
100	32.9	39.6	16.1	34.9	15.8	30.1	18.54
110	34.4	41.3	17.2	36.3	17.0	31.5	18.34
120	35.6	42.9	18.1	37.6	17.9	32.8	18.14
130	36.8	44.3	18.9	38.7	18.7	33.9	17.93
140	37.8	45.5	19.6	39.7	19.4	34.9	17.70
150	38.9	46.8	20.3	40.8	20.1	35.9	17.46
160	39.9	48.0	20.8	41.8	20.6	36.8	17.20
170	41.0	49.3	21.4	42.8	21.2	37.8	16.94
180	42.0	50.5	21.9	43.9	21.7	38.7	16.67
190	43.1	51.7	22.4	44.9	22.2	39.6	16.40
200	44.1	53.0	22.8	45.9	22.7	40.5	16.13
210	45.2	54.2	23.3	47.0	23.2	41.5	15.86
220	46.3	55.5	23.7	48.1	23.6	42.4	15.60
230	47.3	56.7	24.1	49.1	24.0	43.3	15.35
240	48.5	58.0	24.6	50.2	24.5	44.2	15.10
250	49.6	59.3	25.0	51.3	24.9	45.2	14.86
260	50.7	60.6	25.4	52.4	25.3	46.1	14.62
270	51.9	62.0	25.8	53.6	25.8	47.1	13.39
280	53.1	63.5	26.3	54.8	26.3	48.2	14.15
290	54.4	65.0	26.8	59.1	26.7	49.3	13.92
293.15	54.8	65.4	26.9	59.5	26.9	49.6	13.84
300	55.7	66.5	27.3	57.4	27.2	50.4	13.69
310	57.1	68.1	27.8	58.7	27.7	51.5	13.47
320	58.4	69.6	28.2	60.1	28.2	52.6	13.26
330	59.8	71.2	28.7	31.4	28.7	53.8	13.06
340	61.1	72.8	29.2	62.8	29.2	54.9	12.87
350	62.5	74.4	29.7	64.2	29.7	56.1	12.68
360	63.9	76.1	30.2	65.6	30.2	57.3	12.50
370	65.3	77.7	30.7	67.0	30.7	58.5	12.33
380	66.8	79.3	31.2	68.4	31.2	59.7	12.16
390	68.2	81.1	31.6	68.9	31.6	60.9	12.00
397.6	69.3	82.3	32.0	71.0	32.0	61.8	11.88

$\alpha_2 = \alpha_b$

Table 94d. Crystallographic properties of alpha plutonium

T K	100 ε_T *a*	100 ε_T *b*	100 ε_T *c*	100 ε_T avr
0	- 1.020	- 1.219	- 0.486	- 0.925
10	- 1.020	- 1.219	- 0.487	- 0.925
20	- 1.018	- 1.217	- 0.489	- 0.924
30	- 1.011	- 0.210	- 0.492	- 0.919
40	- 0.999	- 1.195	- 0.492	- 0.910
50	- 0.981	- 1.174	- 0.488	- 0.895
60	- 0.959	- 1.149	- 0.481	- 0.876
70	- 0.934	- 1.119	- 0.472	- 0.854
80	- 0.906	- 1.085	- 0.460	- 0.829
90	- 0.876	- 1.049	- 0.446	- 0.802
100	- 0.844	- 1.011	- 0.431	- 0.773
110	- 0.810	- 0.971	- 0.414	- 0.742
120	- 0.775	- 0.929	- 0.396	- 0.710
130	- 0.740	- 0.886	- 0.378	- 0.667
140	- 0.702	- 0.842	- 0.359	- 0.643
150	- 0.664	- 0.796	- 0.339	- 0.608
160	- 0.625	- 0.749	- 0.318	- 0.572
170	- 0.585	- 0.700	- 0.297	- 0.535
180	- 0.544	- 0.651	- 0.276	- 0.497
190	- 0.501	- 0.600	- 0.254	- 0.458
200	- 0.458	- 0.548	- 0.231	- 0.418
210	- 0.413	- 0.495	- 0.208	- 0.377
220	- 0.368	- 0.440	- 0.185	- 0.335
230	- 0.321	- 0.384	- 0.161	- 0.292
240	- 0.273	- 0.327	- 0.137	- 0.249
250	- 0.225	- 0.268	- 0.112	- 0.204
260	- 0.175	- 0.209	- 0.087	- 0.159
270	- 0.123	- 0.147	- 0.061	- 0.112
280	- 0.071	- 0.085	- 0.035	- 0.064
290	- 0.017	- 0.021	- 0.008	- 0.016
293.15	0	0	0	0
300	0.038	0.045	0.019	0.034
310	0.094	0.113	0.046	0.085
320	0.152	0.181	0.074	0.137
330	0.211	0.252	0.103	0.190
340	0.272	0.324	0.132	0.245
350	0.334	0.398	0.161	0.301
360	0.397	0.474	0.191	0.358
370	0.462	0.551	0.222	0.416
380	0.529	0.630	0.253	0.475
390	0.597	0.711	0.284	0.535
397.6	0.649	0.773	0.308	0.582

Table 94e. Crystallographic properties of alpha plutonium

T K	*a* nm	*b* nm	*c* nm	β °	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$ ^{239}Pu	Density $kg\ m^{-3}$ ^{244}Pu
0	0.6120	0.4763	1.0911	101.93	11.713	20410	20838
10	0.6120	0.4763	1.0911	101.92	11.713	20409	20837
20	0.6120	0.4763	1.0910	101.92	11.713	20409	20837
30	0.6120	0.4764	1.0910	101.91	11.715	20406	20834
40	0.6122	0.4764	1.0910	101.91	11.718	20400	20828
50	0.6122	0.4765	1.0910	101.90	11.723	20391	20819
60	0.6124	0.4767	1.0911	101.90	11.730	20380	20807
70	0.6125	0.4768	1.0912	101.89	11.738	20366	20793
80	0.6127	0.4770	1.0914	101.89	11.747	20351	20777
90	0.6129	0.4771	1.0915	101.88	11.756	20334	20760
100	0.6131	0.4773	1.0917	101.88	11.767	20316	20742
110	0.6133	0.4775	1.0919	101.87	11.778	20297	20723
120	0.6135	0.4777	1.0921	101.87	11.789	20278	20703
130	0.6137	0.4779	1.0923	101.87	11.801	20257	20682
140	0.6140	0.4781	1.0925	101.86	11.813	20236	20661
150	0.6142	0.4784	1.0927	101.86	11.826	20215	20639
160	0.6144	0.4786	1.0929	101.85	11.838	20193	20616
170	0.6147	0.4788	1.0931	101.85	11.852	20170	20593
180	0.6149	0.4791	1.0934	101.84	11.865	20147	20570
190	0.6152	0.4793	1.0936	101.84	11.879	20124	20545
200	0.6155	0.4796	1.0939	101.83	11.894	20099	20521
210	0.6157	0.4798	1.0941	101.83	11.908	20075	20496
220	0.6160	0.4801	1.0944	101.82	11.923	20049	20470
230	0.6163	0.4803	1.0946	101.82	11.939	20024	20443
240	0.6166	0.4806	1.0949	101.82	11.954	19997	20417
250	0.6169	0.4809	1.0952	101.81	11.970	19971	20389
260	0.6172	0.4812	10.954	101.81	11.987	19943	20361
270	0.6175	0.4815	1.0957	101.80	12.003	19915	20333
280	0.6179	0.4818	1.0960	101.80	12.021	19887	20304
290	0.6182	0.4821	1.0963	101.79	12.038	19858	20274
293.15	0.6183	0.4822	1.0964	101.79	12.044	19848	20265
300	0.6185	0.4824	1.0966	101.79	12.056	19828	20244
310	0.6189	0.4827	1.0969	101.78	12.075	19798	20213
320	0.6192	0.4831	1.0972	101.78	12.094	19767	20181
330	0.9196	0.4834	1.0975	101.77	12.113	19735	20149
340	0.6200	0.4838	1.0978	101.77	12.133	19703	20116
350	0.6204	0.4841	1.0982	101.77	12.153	19671	20083
360	0.6208	0.4845	1.0985	101.76	12.174	19637	20049
370	0.6212	0.4849	1.0988	101.76	12.195	19603	20014
380	0.6216	0.4852	1.0992	101.75	12.216	19568	19979
390	0.6220	0.4856	1.0995	101.75	12.238	19533	19943
397.6	0.6222	0.4859	1.0998	101.74	12.256	19506	19915

Table 94f . Inter-atomic distances in alpha plutonium at 293.15 K

N is the number of nearest neighbors. Like the beta phase, values are considered to be accurate to ± 0.006 nm. The mean represents a weighted average.

First Type	Second Type	Order	Distance nm	*N*	First Type	Second Type	Order	Distance nm	*N*
I	VII	*d*1	0.257	1	V	IV	*d*26	0.258	1
	III	*d*2	0.258	1		III	*d*18	0.266*	2
	II	*d*3	0.260	1		VI	*d*31	0.272	1
	VIII	*d*4	0.276*	2		III	*d*19	0.324	1
	VI	*d*5	0.320*	2		IV	*d*29	0.332*	2
	VII	*d*7	0.341*	2		VIII	*d*32	0.336	1
	IV	*d*6	0.341	1		II	*d*15	0.343*	2
	II	*d*8	0.359	1		V	*d*33	0.350*	2
	VIII	*d*9	0.371	1		VII	*d*35	0.351	1
		Mean	**0.310**	**12**		VI	*d*34	0.351	1
II	I	*d*3	0.260	1			**Mean**	**0.320**	**14**
	III	*d*10	0.261	1	VI	IV	*d27*	0.263	1
	VII	*d*11	0.264*	2		V	*d*31	0.272	1
	VIII	*d*12	0.319	1		IV	*d*28	0.274*	2
	IV	*d*13	0.337	1		I	*d*5	0.320*	2
	VII	*d*14	0.339	1		VIII	*d*36	0.321	1
	V	*d*15	0.343*	2		VII	*d*37	0.330	1
	VIII	*d*16	0.346*	2		III	*d*23	0.344*	2
	I	*d*8	0.359	1		V	*d*34	0.351	1
	VI	*d*17	0.361*	2		II	*d*17	0.361*	2
		Mean	**0.322**	**14**		III	*d*25	0.365	1
III	I	*d*2	0.258	1			**Mean**	**0.321**	**14**
	II	*d*10	0.261	1	VII	I	*d*1	0.257	1
	V	*d*18	0.266*	2		II	*d*11	0.264*	2
	V	*d*19	0.324	1		VIII	*d*38	0.279	1
	IV	*d*20	0.326	1		VI	*d*37	0.330	1
	IV	*d*21	0.336*	2		II	*d*14	0.339	1
	IV	*d*22	0.341	1		VII	*d*39	0.340*	2
	VI	*d*23	0.344*	2		I	*d*7	0.341*	2
	VIII	*d*24	0.352*	2		VIII	*d*40	0.343	1
	VI	*d*25	0.365	1		VIII	*d*41	0.349*	2
		Mean	**0.320**	**14**		V	*d*35	0.351	1
IV	V	*d*26	0.258	1			**Mean**	**0.320**	**14**
	VI	*d*27	0.263	1	VIII	I	*d*4	0.276*	2
	VI	*d*28	0.274*	2		VII	*d*38	0.279	1
	III	*d*20	0.326	1		II	*d*12	0.319	1
	III	*d*21	0.336*	2		VI	*d*36	0.321	1
	V	*d*29	0.332*	2		V	*d*32	0.336	1
	IV	*d*30	0.335*	2		VII	*d*40	0.343	1
	II	*d*13	0.337	1		II	*d*16	0.346*	2
	I	*d*6	0.341	1		VII	*d*41	0.349*	2
	III	*d*22	0.341	1		VIII	*d*42	0.351*	2
		Mean	**0.316**	**14**		III	*d*24	0.352*	2
						I	*d*9	0.371	1
							Mean	**0.332**	**16**

* Two bonds with atoms lying in adjacent reflection planes

Table 94g. Crystallographic properties of beta plutonium

T K	100 ε_T avr	*a* nm	*b* nm	*c* nm	β °	Molar Volume $cm^3\ mol^{-1}$	Density kg m^{-3} ^{239}Pu	Density kg m^{-3} ^{244}Pu
397.6	3.629	0.9246	1.0454	0.7836	92.41	13.403	17835	18209
400	3.640	0.9247	1.0454	0.7837	92.40	13.407	17830	18204
420	3.727	0.9259	1.0457	0.7844	92.31	13.441	17785	15158
440	3.814	0.9271	1.0460	0.7851	92.23	13.475	17740	18112
460	3.902	0.9283	1.0463	0.7858	92.14	13.509	17695	18066
480	3.989	0.9294	1.0466	0.7866	92.06	13.543	17651	18021
487.9	4.023	0.9299	1.0467	0.7868	92.01	13.557	17633	18003

Table 94h. Inter-atomic distances in beta plutonium at 443 K

First Type	Second Type	Order	Distance nm	*N*	First Type	Second Type	Order	Distance nm	*N*
I	VII	*d*1	0.298	4	V	VII	*d*25	0.282	2
	III	*d*2	0.317	2		III	*d*14	0.284	2
	VI	*d*3	0.321	4		II	*d*9	0.336	2
	II	*d*4	0.328	2		VI	*d*26	0.341	2
		Mean	**0.314**	**12**		VI	*d*27	0.347	2
II	III	*d*5	0.303	1		IV	*d*24	0.349	2
	VI	*d*6	0.311	2		VII	*d*28	0.366	2
	I	*d*4	0.328	1			**Mean**	**0.329**	**14**
	VII	*d*7	0.327	2	VI	VI	*d*29	0.293	1
	II	*d*8	0.329	1		VII	*d*30	0.306	1
	V	*d*9	0.336	2		II	*d*6	0.311	1
	IV	*d*10	0.342	1		VI	*d*31	0.312	1
	VII	*d*11	0.344	2		IV	*d*22	0.317	1
	VI	*d*12	0.356	2		I	*d*3	0.321	1
		Mean	**0.332**	**14**		II	*d*16	0.333	1
III	IV	*d*13	0.281	1		IV	*d*23	0.334	1
	V	*d*14	0.284	2		VIII	*d*32	0.337	1
	II	*d*5	0.303	1		V	*d*26	0.341	1
	I	*d*2	0.317	1		III	*d*19	0.344	1
	III	*d*15	0.333	1		V	*d*27	0.347	1
	VI	*d*16	0.333	2		VII	*d*33	0.349	1
	VII	*d*17	0.336	2		II	*d*12	0.356	1
	IV	*d*18	0.338	1			**Mean**	**0.329**	**14**
	VI	*d*19	0.344	2	VII	VII	*d*34	0.260	1
		Mean	**0.321**	**13**		V	*d*25	0.282	1
IV	III	*d*13	0.281	1		I	*d*1	0.298	1
	IV	*d*20	0.301	1		IV	*d*21	0.302	1
	VII	*d*21	0.302	2		VI	*d*30	0.306	1
	VI	*d*22	0.317	2		VII	*d*35	0.314	1
	VI	*d*23	0.334	2		II	*d*7	0.327	1
	III	*d*18	0.338	1		III	*d*17	0.336	1
	II	*d*10	0.342	1		VI	*d*32	0.337	1
	V	*d*24	0.349	2		II	*d*11	0.344	1
		Mean	**0.322**	**12**		VI	*d*33	0.349	1
						V	*d*28	0.366	1
							Mean	**0.318**	**12**

Values were calculated at the median temperature of 443 K in the thermodynamically sTable region using lattice parameters of *a* 0.9273 nm *b* 1.0461 nm *c* 0.7852 nm and angle β = 92.21°. N is the number of nearest neighbors. Values are considered to be accurate to ± 0.006 nm. The mean represents a weighted average

Table 94i. Crystallographic properties of gamma plutonium

T K	100 ε_T avr	*a* nm	*b* nm	*c* nm	*d*1 nm	*d*3 nm	Molar Volume $cm^3\ mol^{-1}$	Density kg m^{-3} ^{239}Pu	Density kg m^{-3} ^{244}Pu
487.9	4.922	0.31602	0.57638	1.01457	0.30222	0.32866	13.911	17184	17544
490	4.930	0.31601	0.57643	1.01475	0.30227	0.32868	13.914	17180	17591
500	4.966	0.31595	0.57665	1.01560	0.30247	0.32877	13.929	17162	17522
520	5.039	0.31582	0.57711	1.01731	0.30287	0.32894	13.958	17127	17486
540	5.111	0.31570	0.57756	1.01902	0.30328	0.32911	13.987	17091	17450
560	5.184	0.31577	0.57802	1.02073	0.30368	0.32928	14.016	17056	17414
580	5.256	0.31545	0.57847	1.02244	0.30409	0.32945	14.045	17021	17378
590	5.293	0.31539	0.57870	1.02329	0.30429	0.32953	14.059	17003	17360
593.1	5.304	0.31537	0.57877	1.02356	0.30435	0.32956	14.064	16998	17354

$$d1 = [\ a^{\,2}/16 + b^{\,2}/16 + c^{\,2}/16\ ]^{\,½} \quad d2 = a \quad d3 = [\ a^{\,2}/4 + b^{\,2}/4\ ]^{\,½}$$

Table 94j. Crystallographic properties of delta plutonium

T K	100 ε_T avr	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density kg m^{-3} ^{239}Pu	Density kg m^{-3} ^{244}Pu
593.1	7.625	0.46374	0.32791	15.014	15922	16256
600	7.618	0.46371	0.32789	15.012	15925	16258
620	7.600	0.46363	0.32783	15.004	15933	16267
640	7.581	0.46355	0.32778	14.996	15941	16275
660	7.562	0.46347	0.32772	14.988	15949	16284
680	7.544	0.46339	0.37766	14.980	15958	16292
700	7.525	0.46331	0.32761	14.973	15966	16301
720	7.507	0.46323	0.32755	14.965	15974	16309
730	7.497	0.46319	0.32752	14.961	15978	16313
736.0	7.492	0.46316	0.32751	14.959	15981	16316

$$d = a/\sqrt{2}$$

Table 94k. Crystallographic properties of delta prime plutonium

T K	100 ε_T avr	*a* nm	*c* nm	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$ ^{239}Pu	Density $kg\ m^{-3}$ ^{244}Pu
736.0	7.193	0.33453	0.44023	0.32312	14.834	16115	16453
740	7.165	0.33512	0.43833	0.32278	14.823	16127	16466
745	7.129	0.33586	0.43595	0.32236	14.807	16144	16482
750	7.091	0.33660	0.43358	0.32194	14.792	16161	16500
755	7.052	0.33734	0.43121	0.32153	14.776	16179	16518
755.7	7.046	0.33745	0.43088	0.35148	14.773	16181	16521

$$d1 = [\, a^{\,2}/2 + c^{\,2}/4]^{\,½} \qquad d2 = a$$

Table 94l. Crystallographic properties of epsilon plutonium

T K	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$ ^{239}Pu	Density $kg\ m^{-3}$ ^{244}Pu
755.7	6.299	0.36353	0.31483	14.466	16525	16871
760	6.315	0.36359	0.31488	14.473	16517	16864
780	6.393	0.36385	0.31511	14.505	16481	16827
800	6.470	0.36412	0.31534	14.536	16445	16790
820	6.548	0.36438	0.31557	14.568	16409	16753
840	6.625	0.36465	0.31580	14.600	16374	16717
860	6.703	0.36491	0.31603	14.632	16338	16681
880	6.780	0.36518	0.31625	14.664	16302	16644
900	6.858	0.36544	0.31648	14.696	16267	16608
910	6.897	0.36558	0.31660	14.712	16249	16590
913	6.908	0.36562	0.31663	14.716	16244	16585

$$d = \sqrt{3}a/2$$

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95 AMERICIUM Am

Atomic mass ^{241}Am: 241.0568274 (12) (Wang et al. 2017)
Atomic mass ^{243}Am: 243.0613799 (15) (Wang et al. 2017)

^{243}Am is the longest living isotope with a half life of 7364 y (Audi et al. 2017) but this isotope, as well as ^{241}Am with a half life of 432.6 y, have both been used for carrying out experimental work so both are included.

Allotropy: Alpha: Double hexagonal close-packed (hP4)
Beta: Face-centered cubic (cF4)
Gamma: Body-centered cubic (cI2)

Ward et al. 1986, Cordfunke and Konings 1990 and Konings 2003 all selected values of 1042 (10) K for the alpha-beta transformation, 1350 (5) K for the beta-gamma transformation and 1449 (5) K for the melting point.

95.1 Alpha Phase: Double hexagonal close-packed (hP4): 0 K to 1042 K

The expansion coefficients for 293 to 953 K for the *a* axis and 293 to 1073 K for the *c* axis obtained from lattice parameter measurements by Seleznev et al. 1977 differ significantly from values obtained from lattice parameter measurements of McWhan et al. 1962 (153-878 K) but appear to extrapolate to agree with values derived from the unpublished lattice parameter measurements of Marples 1988 (4-293 K) which are summarized in Part 95.4. The values of Seleznev et al. 1977 are selected to be consistent with measurements obtained in the beta phase by Shushakov et al. 1983. By using the procedure adopted in Part 95.5 it is possible to obtain a set of values to cover the whole stability range of the alpha phase. However, above 293.15 K the thermal expansion can be represented by:

$$\varepsilon_T a = 6.5 \times 10^{-6} T - 1.90548 \times 10^{-3} \quad (95a)$$

$$\varepsilon_T c = 8.8 \times 10^{-6} T - 2.57972 \times 10^{-3} \quad (95b)$$

On the basis $100\Delta\varepsilon$, for the *a* axis the measurement of McWhan et al. 1962 trend from 0.02 low initially to 0.12 high while for the *c* axis the trend is from 0.04 high initially trending to 0.02 low at 500 K before increasing to 0.08 high.

Table 95a. The lattice parameters of alpha americium at room temperature

References	*a* nm	*c* nm	Note
McWhan et al. 1962	0.3468	1.1242	
Fuger et al. 1972	0.3471	1.1249	
Spirlet and Müller 1973	0.3470	1.1249	
Kanellakopulos et al. 1976	0.3472	1.1257	a
Seleznev et al. 1978	0.3471	1.1239	
Akella et al. 1980	0.3473	1.1246	
Marples 1988	0.3471	1.1256	a
Selected	0.3471 (2)	1.1245 (5)	

Note for Table 95a

a. The *c* axis value was not included in the average

At room temperature: Density: ^{241}Am 13647 (17) kg m^{-3} ^{243}Am 13760 (17) kg m^{-3}
Molar volume: 17.664 (22) cm^3 mol^{-1}.

95.2 Beta Phase: Face-centered cubic: 1042 K to 1350 K

Baybarz et al. 1976 quenched out the face-centered cubic phase on to tungsten wires with a lattice parameter of 0.48871 (7) nm at room temperature, which is selected. McWhan et al. 1962 using a similar procedure obtained 0.4894 (5) nm at 295 K. Shushakov et al. 1983 determined the lattice parameter in the high temperature region and showed the results graphically as atomic volume against temperature. From this graph it was estimated that for the beta phase the measurements were determined at 1055K, 1075 K and 1200 K and were fitted to a straight line. However, this cannot be correct because a linear extrapolation into the room temperature region indicates that the derived lattice parameter is 0.485 nm which is 0.004 nm lower than the value selected above. Assuming that the thermal expansion coefficients of the alpha and beta phases are similar then extrapolation of the selected value into the beta phase region can easily be accommodated by the scatter in the measurements at 1055 K and 1075 K but the measurements at 1200 K must be too high. The measurements at 1055 K and 1075 K are equivalent to a lattice parameter of 0.4915 (3) nm at 1065 K and this value was joined with the selected room temperature value to give an equation which is considered as representing the thermal expansion for the whole of the beta phase region:

$$a \text{ (nm)} = 3.61469 \times 10^{-6} T + 0.487650 \quad (95c)$$

$$\varepsilon_T = 7.38365 \times 10^{-6} T - 3.88735 \times 10^{-3} \quad (95d)$$

The derived thermal expansion coefficient at 7.3 x 10^{-6} K^{-1} is in exact agreement with the average value obtained for the alpha phase and agrees satisfactorily with a value of 9 (3) x 10^{-6} K^{-1} determined by McWhan et al. 1962 over the range 295 to 633 K. The measurements by Shushakov et al. 1983 at 1200 K would appear to be 0.0006 nm too high while further measurements by Seleznev et al. 1978 at 1123 K would appear to be 0.0004 nm too low but this is within the assigned error of ± 0.0005 nm. Assuming that

the accuracy of the beta phase lattice parameters is equivalent to the scatter in the measurements at 1055 – 1075 K, ± 0.0003 nm, then the molar volume accuracy is ± 0.033 $cm^3\ mol^{-1}$ so that the volume contraction from the alpha to the beta phases is 0.087 (40) $cm^3\ mol^{-1}$ or – 0.49 (22) %. Akella et al. 1980 determined the double hexagonal close-packed – face-centered cubic transition to be 5 (1) GPa at room temperature, which together with an enthalpy of transition of 0.34 (10) kJ mol^{-1} selected by Konings 2003 leads to a molar volume contraction of 0.049 (17) $cm^3\ mol^{-1}$ using the Clausius-Clapeyron equation, and this value is within the limits of the lattice parameter value. Rose et al. 1979 determined the thermal expansion dilatometrically and the volume change at the transition was an increase of 2.8% which completely disagrees with the lattice parameter observations.

95.3 Gamma Phase: Body-centered cubic: 1350 K to 1449 K

The structure is considered to be body-centered cubic by analogy with neighboring elements. Stephens et al. 1968 determined the slope of the transition pressure to be 4.4 K $kbar^{-1}$ which together with the enthalpy of transition value of 5.9 kJ mol^{-1} as determined by Wade and Wolf 1967 leads to a molar volume expansion of 0.192 $cm^3\ mol^{-1}$. However, Konings 2003 selected the enthalpy of transition of 3.8 (4) kJ mol^{-1} as determined by Seleznev et al. 1977 which would lead to a molar volume expansion of 0.124 $cm^3\ mol^{-1}$ and to a molar volume of the gamma phase at the transition temperature as 18.112 $cm^3\ mol^{-1}$. By comparison with the body-centered cubic phases of lanthanum, praseodymium and neodymium a thermal expansion coefficient of 18 (1) x $10^{-6}\ K^{-1}$ is selected which leads to the following equations:

$$a\ (\text{nm}) = 7.05900 \times 10^{-6}\, T + 0.382288 \qquad (95e)$$

$$\varepsilon_T = 1.81661 \times 10^{-5}\, T - 1.61372 \times 10^{-2} \qquad (95f)$$

95.4 Lattice parameter measurements of Marples 1988

The following measurements are reproduced by permission of the author. Values were given only in notebook form and have been averaged for each temperature where N represents the number of determinations at that temperature.

T K	4	40	77	111	RT
N	17	4	6	2	4
a Å	3.4669	3.4677	3.4671	3.4677	3.4707
c Å	11.2324	11.2334	11.2366	11.2386	11.2553

95.5 Low temperature evaluation

Length change values derived from the above averaged lattice parameter measurements of Marples 1988 at 4 K and 77 K for the *a* axis and 4 K and 111 K for the *c* axis were combined with the selected thermal expansion coefficients of Seleznev et al. 1977:

$\alpha_a = 6.5 \times 10^{-6}\ K^{-1}$ and $\alpha_c = 8.8 \times 10^{-6}\ K^{-1}$ and the criterion at 293.15 K that both $\varepsilon = 0$ and $d\alpha/dT = 0$.

$$\ln (L_a) = -4.49285 \times 10^{-7} T + 1.44547 \times 10^{-8} T^2 + 1.51207 \times 10^{-11} T^3 - 5.38236 \times 10^{-14} T^4 - 1.09392 \times 10^{-3} \quad (95g)$$

$$\ln (L_c) = 3.16825 \times 10^{-6} T + 2.06263 \times 10^{-8} T^2 - 2.82810 \times 10^{-11} T^3 + 8.23356 \times 10^{-15} T^4 - 2.04967 \times 10^{-3} \quad (95h)$$

Because the derived thermal expansion coefficients from these polynomial equations do not pass through zero at 0 K then values below 30 K for the *a* axis and 40 K for the *c* axis where adjusted in order to meet this criterion. Because of the procedure used in the evaluation the values must be considered to be tentative.

Table 95b. Crystallographic properties of alpha americium

T K	α_a x 10^6 K^{-1}	α_c x 10^6 K^{-1}	α_{avr} x 10^6 K	100 $\varepsilon_T a$	100 $\varepsilon_T c$	100 ε_T avr
0	0	0	0	- 0.110	- 0.200	- 0.140
10	0.1	1.0	0.4	- 0.110	- 0.199	- 0.140
20	0.2	3.1	1.2	- 0.110	- 0.197	- 0.139
30	0.5	4.2	1.7	- 0.109	- 0.193	- 0.137
40	0.8	4.7	2.1	- 0.109	- 0.189	- 0.135
50	1.1	5.0	2.4	- 0.108	- 0.184	- 0.133
60	1.4	5.3	2.7	- 0.107	- 0.179	- 0.131
70	1.7	5.7	3.0	- 0.105	- 0.173	- 0.128
80	2.0	5.9	3.3	- 0.103	- 0.168	- 0.125
90	2.4	6.2	3.6	- 0.101	- 0.162	- 0.121
100	2.7	6.5	3.9	- 0.098	- 0.155	- 0.117
110	3.0	6.7	4.2	- 0.096	- 0.149	- 0.133
120	3.3	7.0	4.5	- 0.092	- 0.142	- 0.109
130	3.6	7.2	4.8	- 0.089	- 0.135	- 0.104
140	3.9	7.4	5.1	- 0.085	- 0.128	- 0.099
150	4.2	7.6	5.3	- 0.081	- 0.120	- 0.094
160	4.5	7.7	5.6	- 0.077	- 0.112	- 0.089
170	4.7	7.9	5.8	- 0.072	- 0.105	- 0.083
180	5.0	8.0	6.0	- 0.067	- 0.097	- 0.077
190	5.2	8.2	6.2	- 0.062	- 0.089	- 0.071
200	5.4	8.3	6.4	- 0.057	- 0.080	- 0.065
210	5.6	8.4	6.6	- 0.052	- 0.072	- 0.058
220	5.8	8.5	6.7	- 0.046	- 0.064	- 0.052
230	6.0	8.6	6.8	- 0.040	- 0.058	- 0.045
240	6.1	8.6	7.0	- 0.034	- 0.046	- 0.038
250	6.2	8.7	7.1	- 0.028	- 0.038	- 0.031
260	6.3	8.7	7.2	- 0.021	- 0.029	- 0.024
270	6.4	8.8	7.2	- 0.015	- 0.020	- 0.017
280	6.5	8.8	7.3	- 0.009	- 0.011	- 0.010
290	6.5	8.8	7.3	- 0.002	- 0.003	- 0.023
293.15	6.5	8.8	7.3	0	0	0
300	6.5	8.8	7.3	0.004	0.006	0.005
350	6.5	8.8	7.3	0.037	0.050	0.041
400	6.5	8.8	7.3	0.069	0.094	0.078
450	6.5	8.8	7.3	0.102	0.138	0.114
500	6.5	8.8	7.3	0.134	0.182	0.150
550	6.5	8.8	7.3	0.167	0.226	0.187
600	6.5	8.8	7.3	0.199	0.270	0.223
650	6.5	8.8	7.2	0.232	0.314	0.259
700	6.5	8.8	7.2	0.264	0.358	0.296
750	6.5	8.8	7.2	0.297	0.402	0.332
800	6.5	8.8	7.2	0.329	0.446	0.368
850	6.5	8.8	7.2	0.362	0.490	0.405
900	6.5	8.8	7.2	0.394	0.534	0.441
950	6.5	8.7	7.2	0.427	0.578	0.477
1000	6.5	8.7	7.2	0.459	0.622	0.514
1042	6.5	8.7	7.2	0.487	0.659	0.544

Table 95c. Crystallographic properties of alpha americium

T K	*a* nm	*c* nm	*c*/2*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$ ^{241}Am	Density $kg\ m^{-3}$ ^{243}Am
0	0.3467	1.1223	1.6184	0.3447	17.59	13700	13820
10	0.3467	1.1223	1.6184	0.3447	17.59	13700	13820
20	0.3467	1.1223	1.6184	0.3447	17.59	13700	13820
30	0.3467	1.1223	1.6185	0.3447	17.59	13700	13820
40	0.3467	1.1224	1.6186	0.3447	17.59	13700	13820
50	0.3467	1.1224	1.6186	0.3447	17.59	13700	13810
60	0.3467	1.1225	1.6187	0.3447	17.60	13700	13810
70	0.3467	1.1225	1.6188	0.3447	17.60	13700	13810
80	0.3467	1.1226	1.6188	0.3447	17.60	13700	13810
90	0.3467	1.1227	1.6189	0.3448	17.60	13700	13810
100	0.3468	1.1228	1.6190	0.3448	17.60	13690	13810
110	0.3468	1.1228	1.6190	0.3448	17.60	13690	13810
120	0.3468	1.1229	1.6191	0.3448	17.61	13690	13800
130	0.3468	1.1230	1.6191	0.3448	17.61	13690	13800
140	0.3468	1.1231	1.6192	0.3448	17.61	13690	13800
150	0.3468	1.1231	1.6192	0.3449	17.61	13680	13800
160	0.3468	1.1232	1.6193	0.3449	17.62	13680	13800
170	0.3468	1.1233	1.6194	0.3449	17.62	13680	13790
180	0.3469	1.1234	1.6194	0.3449	17.62	13680	13790
190	0.3469	1.1235	1.6194	0.3450	17.63	13680	13790
200	0.3469	1.1236	1.6195	0.3450	17.63	13670	13790
210	0.3469	1.1237	1.6195	0.3450	17.63	13670	13780
220	0.3469	1.1238	1.6196	0.3450	17.64	13670	13780
230	0.3470	1.1239	1.6196	0.3451	17.64	13660	13780
240	0.3470	1.1240	1.6197	0.3451	17.64	13660	13780
250	0.3470	1.1241	1.6197	0.3451	17.65	13660	13770
260	0.3470	1.1242	1.6198	0.3451	17.65	13660	13770
270	0.3470	1.1243	1.6198	0.3452	17.65	13650	13770
280	0.3471	1.1244	1.6198	0.3452	17.66	13650	13760
290	0.3471	1.1245	1.6199	0.3452	17.66	13650	13760
293.15	0.3471	1.1245	1.6199	0.3452	17.66	13650	13760
300	0.3471	1.1246	1.6199	0.3453	17.67	13640	13760
350	0.3472	1.1251	1.6201	0.3454	17.69	13630	13740
400	0.3473	1.1256	1.6203	0.3455	17.71	13620	13730
450	0.3475	1.1261	1.6205	0.3457	17.72	13600	13710
500	0.3476	1.1265	1.6206	0.3458	17.74	13580	13700
550	0.3477	1.1270	1.6208	0.3460	17.76	13570	13680
600	0.3478	1.1275	1.6210	0.3461	17.78	13560	13670
650	0.3479	1.1280	1.6212	0.3462	17.80	13540	13650
700	0.3480	1.1285	1.6214	0.3464	17.82	13530	13640
750	0.3481	1.1290	1.6215	0.3465	17.84	13510	13620
800	0.3482	1.1295	1.6217	0.3466	17.86	13500	13610
850	0.3484	1.1300	1.6219	0.3468	17.88	13480	13590
900	0.3485	1.1305	1.6221	0.3469	17.90	13470	13580
950	0.3486	1.1310	1.6223	0.3471	17.92	13450	13560
1000	0.3487	1.1315	1.6225	0.3472	17.94	13440	13550
1042	0.3488	1.1319	1.6227	0.3473	17.95	13430	13540

$$d1 = [\ a^{\,2}/3 + c^{\,2}/16\ ]^{\,½} \qquad d2 = a$$

Table 95d. Crystallographic properties of beta americium

T K	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$ ^{241}Am	Density $kg\ m^{-3}$ ^{243}Am
1042	0.381	0.4914	0.3475	17.87	13490	13600
1050	0.387	0.4914	0.3475	17.87	13490	13600
1100	0.423	0.4916	0.3476	17.89	13470	13590
1150	0.460	0.4918	0..3478	17.91	13460	13570
1200	0.497	0.4920	0.3479	17.93	13450	13560
1250	0.534	0.4922	0.3480	17.95	13430	13540
1300	0.571	0.4923	0.3481	17.97	13420	13530
1350	0.608	0.4925	0.3483	17.99	13400	13510

$$d = a/\sqrt{2}$$

Table 95e. Estimated crystallographic properties of gamma americium

T K	100 ε_T	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$ ^{241}Am	Density $kg\ m^{-3}$ ^{243}Am
1350	0.839	0.3918	0.3393	18.11	13310	13420
1360	0.857	0.3919	0.3394	18.12	13300	13410
1380	0.893	0.3920	0.3395	18.14	13290	13400
1400	0.930	0.3922	0.3396	18.16	13270	13380
1420	0.966	0.3923	0.3398	18.18	13260	13370
1440	1.002	0.3925	0.3399	18.20	13250	13360
1449	1.019	0.3925	0.3399	18.21	13240	13350

$$d = \sqrt{3}a/2$$

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96 CURIUM Cm

Atomic mass ^{247}Cm: 247.070353 (4) (Wang et al. 2017)
Atomic mass ^{248}Cm: 248.0723491 (25) (Wang et al. 2017)

^{247}Cm is the longest living isotope with a half life of 1.56 x 10^7 y (Audi et al. 2017) but most experiments have been carried out on ^{244}Cm (half life 18.10 y) and ^{248}Cm (half life 3.48 x 10^5 y) so density values have also been calculated for the latter isotope.

Allotropy: Alpha: Double hexagonal close-packed (hP4)
Beta: Face-centered cubic (cF4)

Konings 2001 selected 1619 (50) K for the melting point while Oetting et al. 1976 estimated 1550 K for the alpha – beta transformation temperature.

96.1 Alpha Phase: Double hexagonal close-packed (hP4): 0 K to 1550 K

Table 96a. The lattice parameters of alpha curium at room temperature

References	*a* nm	*c* nm	Note
Cunningham and Wallmann 1964	0.3496	1.1332	
Baybarz and Adair 1972	0.3492	1.1339	
Fuger et al. 1975	0.3498	1.1339	
Kanellakopulos et al. 1976	0.3494	1.1335	
Stevenson and Peterson 1979	0.3500	1.134	
Huray et al. 1980	0.3502	1.1381	a
Haire et al. 1985	0.3502	1.132	
Seleznev et al. 1989	0.3486	1.1300	
Selected	0.3496 (5)	1.1330 (15)	

Note for Table 96a

a. *c* axis value not included in the average

At room temperature: Density: ^{247}Cm 13684 (43) kg m^{-3} ^{248}Cm 13740 (43) kg m^{-3}
Molar volume: 18.055 (57) cm^3 mol^{-1}.

Seleznev et al. 1989 obtained mean thermal expansion coefficients between 90 and 300 K at α_a = 8.7 (1.7) x 10^{-6} K^{-1} and α_c = 12.8 (7) x 10^{-6} K^{-1} but this is considered to be insufficient information to produce a table of low temperature thermal expansion data.

96.2 Beta Phase: Face-centered cubic (cF4): 1550 K to 1619 K

From high temperature quench experiments Baybarz and Adair 1972 obtained a lattice parameter of 0.5039 (2) nm while Baybarz et al. 1976 obtained 0.5038 (2) nm but both values are very similar to that of 0.5041 nm obtained by Charvillat et al. 1976 for CmN. From pressure quench experiments Haire et al. 1986 obtained a much lower value of

0.493 (1) nm which has now been confirmed by temperature quench experiments by Seleznev et al. 1989 who obtained 0.4933 (4) nm. The derived molar volume of 18.073 (44) $cm^3\ mol^{-1}$ derived from the latter overlaps that of the alpha phase but is expected to be lower in order to explain the presence of the face-centered cubic phase at room temperature and high pressure with the pressure transition determined by Benedict et al. 1985 to be 23 GPa.. A lattice parameter value of less than 0.493_1 nm at room temperature and pressure would be required to satisfy the requirement that the molar volume of the beta phase was less than that of the alpha phase.

Table 96b. Crystallographic properties of alpha curium

T K	*a* nm	*c* nm	*c*/2*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density kg m^{-3} ^{247}Cm	Density kg m^{-3} ^{248}Cm
RT	0.3496	1.1330	1.6204	0.3478	18.05	13680	13740

$$d1 = [\ a^2/3 + c^2/16\ ]^{½} \qquad d2 = a$$

Table 96c. Crystallographic properties of beta curium

T K	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density kg m^{-3} ^{247}Cm	Density kg m^{-3} ^{248}Cm
RT	0.4933	0.3488	18.07	13670	13730

$$d = a/\sqrt{2}$$

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97 BERKELIUM Bk

Atomic mass ^{247}Bk: 247.070306 (6) (Wang et al. 2017)
Atomic mass ^{249}Bk: 249.0749832 (13) (Wang et al. 2017)

Although ^{247}Bk is the longest living isotope with a half life of 1380 y (Audi et al. 2017) all lattice parameter experiments have been carried out on ^{249}Bk with a half life of 327.2 d.

Allotropy: Alpha: Double hexagonal close-packed (hP4)
Beta: Face-centered cubic (cF4)

Ward et al. 1982, 1986 selected 1323 (50) K for the melting point based on a change of slope for the vapour pressure curve and estimated the alpha – beta transition temperature to be 1250 (50) K.

97.1 Alpha Phase: Double hexagonal close-packed (hP4): 0 K to 1250 K

Table 97a. The lattice parameters of alpha berkelium at room temperature

References	*a* nm	*c* nm
Peterson et al. 1971	0.3416	1.1070
Haire et al. 1984	0.3428	1.1076
Seleznev et al. 1989	0.3412	1.1061
Selected	0.3414 (2)	1.1065 (5)

The selected values are based on the close agreement between the measurements of Peterson et al. 1971 and Seleznev et al. 1989

At room temperature: Density: ^{247}Bk 14693 (18) kg m^{-3} ^{249}Bk 14813 (18) kg m^{-3}
Molar volume: 16.815 (21) cm^3 mol^{-1}.

Seleznev et al. 1989 obtained mean thermal expansion coefficients between 90 and 300 K at α_a = 10.8 (1.4) x 10^{-6} K^{-1} and α_c = 17.8 (1.2) x 10^{-6} K^{-1} but this is considered to be insufficient information to produce a satisfactory Table of low temperature thermal expansion data.

97.2 Beta Phase: Face-centered cubic (cF4): 1250 K to 1323 K

From high temperature quench experiments Peterson et al. 1971 obtained a lattice parameter of 0.4997 (4) nm which is very similar to that of 0.5010 (4) nm obtained by Stevenson and Peterson 1979 for BkN. From pressure quench experiments Haire et al. 1986 obtained a much lower value of 0.482 (1) nm. The derived molar volume of 16.86 (10) cm^3 mol^{-1} overlaps that of the alpha phase but is expected to be lower in order to explain the presence of the face-centered cubic phase at room temperature and high pressure with the transition pressure determined by Itié et al. 1985 to be 9.5 GPa. A

lattice parameter value of less than 0.481_6 nm at room temperature and pressure would be required to satisfy the requirement that the molar volume of the beta phase was less than that of the alpha phase.

Table 97b. Crystallographic properties of alpha berkelium

T K	*a* nm	*c* nm	*c*/2*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density kg m^{-3} ^{247}Bk	Density kg m^{-3} ^{249}Bk
RT	0.3414	1.1065	1.6205	0.3397	16.82	14690	14810

$$d1 = [\ a^{\,2}/3 + c^{\,2}/16\ ]^{\,½} \qquad d2 = a$$

Table 97c. Crystallographic properties of beta berkelium

T K	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density kg m^{-3} ^{247}Bk	Density kg m^{-3} ^{249}Bk
RT	0.482	0.341	16.86	14660	14770

$$d = a/\sqrt{2}$$

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98 CALIFORNIUM Cf

Atomic mass ^{249}Cf: 249.0748505 (13) (Wang et al. 2017)
Atomic mass ^{251}Cf: 251.079587 (4) (Wang et al. 2017)

Although ^{251}Cf is the longest living isotope with a half life of 900 y (Audi et al. 2017) all lattice parameter experiments have been carried out on ^{249}Cf half life of 351 y.

Allotropy: Alpha: Double hexagonal close-packed (hP4)
Beta: Face-centered cubic (cF4)

Haire and Baybarz 1974 obtained a melting point of 1173 (30) K while Ward et al. 1986 estimated the alpha – beta transition temperature to be 863 K.

98.1 Alpha Phase: Double hexagonal close-packed (hP4): 0 K to 863 K

Table 98a. The lattice parameters of alpha californium at room temperature

References	*a* nm	*c* nm
Haire and Asprey 1976	0.3384	1.1041
Fuger et al. 1984	0.3399	1.1041
Seleznev et al. 1989	0.3380	1.1026
Selected	0.3382 (2)	1.1033 (8)

The selected value is based on the close agreement between the measurements of Haire and Asprey 1976 and Seleznev et al. 1989

At room temperature: Density: ^{249}Cf 15138 (21) kg m^{-3} ^{251}Cf 15260 (21) kg m^{-3}
Molar volume: 16.454 (23) cm^3 mol^{-1}

98.2 Beta Phase: Face-centered cubic (cF4): 863 K to 1173

Because of the extremely small samples available, contamination could lead to ambiguous results. For example, Noé and Peterson 1976 suggested that above 998 K californium existed in an expanded face-centered cubic stucture with a lattice parameter of 0.575 (1) nm at room temperature and a collapsed face-centered cubic structure between 873 K and 998 K with a room temperature lattice parameter of 0.494 (1) nm. Using the same samples Burns and Peterson 1978 observed exactly the same behavior and obtained lattice parameters of 0.5750 nm and 0.4956 nm respectively. However, in order to retain the face-centered cubic structure at room temperature then the molar volume of the beta phase must definitely be lower than that of the alpha phase so the observation of the expanded lattice as the high temperature cannot be a true structure. By pressure quenching at room temperature Haire et al. 1986 obtained a much lower lattice parameter of 0.478 (1) nm which is selected. The derived molar volume from this value at 16.44 (10) should be lower than that obtained for the alpha phase to explain the presence of the face-centered cubic phase at room temperature and high pressure determined by Benedict et al. 1984 to be a transition pressure of 17 GPa. A lattice

parameter value of less than 0.478_1 nm at room temperature and pressure would be required to satisfy the requirement that the molar volume of the beta phase was less than that of the alpha phase.

Table 98b. Crystallographic properties of alpha californium

T K	*a* nm	*c* nm	*c*/2*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density kg m^{-3} ^{249}Cf	Density kg m^{-3} ^{251}Cf
RT	0.3382	1.1033	1.6311	0.3379	16.45	15140	15260

$$d1 = [\ a^{\,2}/3 + c^{\,2}/16\ ]^{\,½} \qquad d2 = a$$

Table 98c. Crystallographic properties of beta californium

T K	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density kg m^{-3} ^{249}Cf	Density kg m^{-3} ^{251}Cf
RT	0.478	0.338	16.44	15150	15270

$$d = a/\sqrt{2}$$

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99 EINSTEINIUM Es

Atomic mass ^{252}Es: 252.082980 (50) (Wang et al. 2017)
Atomic mass ^{253}Es: 253.0848213 (13) (Wang et al. 2017)

The half life of the longest living isotope, ^{252}Es, is 471.7 d (Audi et al. 2017) but measurements have actually been carried out using ^{253}Es of half life 20.47 d.

Allotropy: Alpha phase: Hexagonal close-packed (hP2)
Beta phase: Face-centered cubic (cF4)

Determination of the enthalpy of sublimation by Kleinschmidt et al. 1984 established that the metal was divalent and therefore unlikely to have the same structures as the trivalent metals americium to californium. Unfortunately, measurements have only been carried out on thin films and therefore it is uncertain if these are representative of the actual metal. Haire and Baybarz 1979 identified a face-centered cubic structure with a lattice parameter of 0.575 (1) nm and also determined the melting point to be 1133 (50) K. Haire 1986 identified a hexagonal close packed structure of lattice parameters *a* 0.398 nm and *c* 0.650 nm which transformed into the face-centered cubic structure above 573 K and therefore followed the same structure sequence as ytterbium. Therefore, the hexagonal close-packed structure is tentatively identified as the alpha phase and the face-centered cubic structure as the beta phase. However, the apparent large difference between the molar volumes of the two phases would perhaps indicate the highly tentative nature of the measurements.

Table 99a. Crystallographic properties of alpha einsteinium

T K	*a* nm	*c* nm	*c*/*a*	*d*1 nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$ ^{252}Es	Density $kg\ m^{-3}$ ^{253}Es
RT	0.398	0.650	1.633	0.398	26.85	9390	9430

$$d1 = [\ a^{\,2}/3 + c^{\,2}/4\ ]^{\,½} \qquad d2 = a$$

Table 99b. Crystallographic properties of beta einsteinium

T K	*a* nm	*d* nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$ ^{252}Es	Density $kg\ m^{-3}$ ^{253}Es
RT	0.575	0.407	28.62	8810	8840

$$d = a/\sqrt{2}$$

References for Einsteinium

Audi G., Kondev F.G., Wang M., Huang W.J. and Naimi S., 2017, Chinese Phys. C, **41**. p 030001 (138 pp)

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100 – 103 TRANS-EINSTEINIUM ACTINIDES Fm – Lr

The following are considered to be the principal isotopes of the elements fermium, mendelevium, nobelium and lawrencium where the half lives are selected by Audi et al. 2017 and the atomic masses by Wang et al. 2017.

Table 100-103a. Half lives and masses of the trans-einsteinium actinides

Atomic Number	Symbol	Principal Isotope	Half Life	Atomic Mass
100	Fm	257	100.5 d	257.095105 (5)
101	Md	258	51.5 d	258.098430 (5)
102	No	259	58 m	259.100998 (7)
103	Lr	262	4 h	262.10961 (22)

David 1986 has estimated the metallic radii, r, of these elements and the first three are divalent and assumed to have a face-centered cubic structure (cF4) so that $a = 2\sqrt{2}\, r$.

Table 100-103b. Estimated crystallographic properties of the divalent trans-einsteinium actinides

Symbol	r nm	a nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
Fm	0.200	0.566	27.25	9430
Md	0.1985	0.561	26.64	9690
No	0.197	0.557	26.05	9950

Silva et al. 1970 established that lawrencium was trivalent. David 1986 suggested that the structure could be cubic but based on the heavy trivalent lanthanides it is suggested the structure is more likely to be hexagonal close-packed (hP2). The estimated metallic radius of 0.166 nm as suggested by David 1986 leads to lattice parameters of $a = 0.332$ nm and $c = 0.542$ nm assuming the ideal c/a ratio of 1.633.

Table 100-103c. Estimated crystallographic properties of lawrencium

T K	a nm	c nm	c/a	$d1$ nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
RT	0.332	0.542	1.633	0.332	15.58	16820

$$d1 = [\ a^{\,2}/3 + c^{\,2}/4\ ]^{\,½} \qquad d2 = a$$

References for Trans-Einsteinium Actinides

Audi G., Kondev F.G., Wang M., Huang W.J. and Naimi S., 2017, Chinese Phys. C, **41** p 030001 (138 pp)

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APPENDIX A: REPRESENTATION OF LOW TEMPERATURE THERMAL EXPANSION DATA

Summary of Representative Equations

$$\alpha = C_p (A + B\,T + C/\,T) \quad \textbf{(A)}$$

$$\ln (L_T) = (H_T - H_0)\,(D + E\,T + F/\,T) + G \quad \textbf{(B)}$$

$$\alpha = D\,C_p + E\,[\,C_p\,T + (H_T - H_0)\,] + F\,[\,C_p/\,T - (H_T - H_0)/\,T^{2}] \quad \textbf{(C)}$$

where T is temperature, units K

α is the thermodynamic thermal expansion coefficient, units K^{-1}

C_p is specific heat, units J mol^{-1} K^{-1}

$H_T - H_0$ is absolute enthalpy, units J mol^{-1}

A, B, C, D, E, F and G are constants

Part 1. A Precision Relationship Between Thermal Expansion and Specific Heat

Based on the Grüneisen equation, Mel'nikova et al. 1987 proposed that the volume thermal expansion (β) of lithium and rubidium could be expressed by the relationship:

$$\beta = a\,C_p \quad \text{(D)}$$

where *a* is a constant. However, Mel'nikova and Mozgovoi 1989 found that this equation was inadequate for describing the volume thermal expansion of sodium and potassium and extended the equation to:

$$\beta = C_p\,(a + b\,T) \quad \text{(E)}$$

However, because thermodynamically $\beta = 3\alpha$ then Equation E can be considered as an equivalent linear thermodynamic thermal expansion equation and can be re-arranged into the linear equation:

$$\alpha / C_p = A1 + B1\,T \quad \text{(F)}$$

where A1 = *a*/3 and B1 = *b*/3. In order to test the validity of Equation F for other elements it was applied to the linear thermal expansion values of aluminum, copper and tungsten where the values for aluminum and copper are calculated from the equations as given by Kroeger and Swenson 1977, which form the basis of Tables 13h and 29e, while for tungsten the selected values are those given in Table 74c. The selected specific heat values are given below in Tables A, B and C respectively. It was found in all three cases that Equation F was valid down to about 150 K but below this temperature there where major deviations (δ) which could be expressed as a function of temperature as:

$$\delta f\,T = \alpha / C_p - A1 - B1\,T \quad \text{(G)}$$

It was found that the best correlation for δfT between 20 and 150 K was given be:

$$\delta f\, T = A2 + C2/\, T \qquad (H)$$

Therefore, initially Equation F can be used above 150 K while below 150 K:

$$\alpha / C_p = A1 + A2 + B1\, T + C2/\, T \qquad (I)$$

In order to combine Equations F and I the evaluation was carried out over the whole temperature range to give the compromise equation:

$$\alpha / C_p = A + B\, T + C/\, T \qquad (J)$$

which can be re-arranged as the selected equation:

$$\alpha = C_p\, (A + B\, T + C/\, T) \qquad \textbf{(A)}$$

The fits of the data to Equation A are given in Table D with standard deviations of $\pm$ 1.7 x 10^{-8} K^{-1} for aluminum, $\pm$ 8 x 10^{-9} K^{-1} for copper and $\pm$ 1.2 x 10^{-8} K^{-1} for tungsten, all of which are highly satisfactory. In the text Equation A was also applied to anisotropic materials by assuming that the axes could be individually assessed but utilizing the total specific heat for each axis.

Part 2. A Precision Relationship Between Length Change Values and Absolute Enthalpy

When only length change values are available at low temperature these can be fitted to the integration of Equation A:

$$\ln (L_T/L_0) = (H_T - H_0)\, (\, A + B\, T + C/\, T) - \int_0^T (H_T - H_0)\, (B - C/\, T^{\,2}) \qquad (K)$$

where $L_T = 1 + \varepsilon_T$ where $\varepsilon_T = (l_T - l_{293.15\ K})/\, l_{293.15\ K}$ and L_0 is the value of L_T at absolute zero. The B component of the of the integral can easily be resolved as $(H_T - H_0)^{\,2}\, B/2$ but it is suggested that the C component containing the two variable $H_T - H_0$ and $C/T^{\,2}$ leads to an infinite series of partial integrations and therefore length changes are best derived using three-point integration.

In order to study how the integration part of Equation K actually contributes to the overall accuracy, only the first part of Equation K was considered and re-evaluated below for the three metals aluminum, copper and tungsten using length change values given in Tables 13h, 29e and 74c respectively and absolute enthalpy values given in Tables A, B and C below respectively:

$$\ln (L_T/L_0) = (H_T - H_0)\, (\, D + E\, T + F/\, T) \qquad (L)$$

Fits of the data to Equation L are given in Table E where values of L_0 where calculated from ε_T values at 0 K already given in Tables 13h, 29e and 74c. In all three cases there is a high degree of correlation with the values of L_T being reproduced to the six significant figures to which they are quoted and therefore Equation L can be considered to be independent of the Equation A on which it is based. However, as given, Equation L is a special case in which values of L_0 are known but in most cases there is a reliance on limited length change values and therefore, L_0 is unknown but can be determined by re-arranging Equation L:

$$\ln (L_T) = (H_T - H_0)\, (\, D + E\, T + F/\, T) + G \qquad \textbf{(B)}$$

where G ≈ ln (L_0) and approaches the true value of ln (L_0) the closer measurements are made to absolute zero. Differentiation of Equations L and B lead to thermal expansion:

$$\alpha = D\,C_p + E\,[\,C_p\,T + (H_T - H_0)\,] + F\,[\,C_p/\,T - (H_T - H_0)/\,T^{\,2}] \qquad \textbf{(C)}$$

Equation B was also applied to anisotropic materials by assuming that the axes could be individually assessed but utilizing the total absolute enthalpy for each axis. Although Equations L, B and C show an exact relationship, if in the low temperature region thermal expansion measurements are available then Equation A is preferred in view of the increased sensitivity of C_p because it is directly available whereas values of $H_T - H_0$ have to be obtained by three point integration.

In Table A, values of C_p for aluminum are based on the selected values of Desai 1987 while values for copper in Table B are calculated from the equation of Martin 1987 and those for tungsten from a combination of specific heat values of Clusius and Franzosini 1959 and Triplett et al. 1973, and extrapolation above 261 K by including the mean specific heat values of Bronson et al. 1933 and the enthalpy values of Ditmars 1979. In all three cases the values of $H_T - H_0$ were obtained by three point integration.

Table A. Low temperature specific heat and enthalpy values for aluminum

T K	C_p	$H_T - H_0$	T K	C_p	$H_T - H_0$	T K	C_p	$H_T - H_0$
20	0.223	1.214	120	15.637	768.3	220	22.203	2723
30	0.837	6.026	130	16.697	930.1	230	22.530	2946
40	2.064	20.08	140	17.615	1102	240	22.828	3173
50	3.827	49.36	150	18.453	1282	250	23.101	3403
60	5.800	97.50	160	19.190	1470	260	23.358	3635
70	7.776	165.4	170	19.852	1665	270	23.600	3870
80	9.690	252.9	180	20.439	1827	280	23.832	4107
90	11.424	358.6	190	20.968	2074	290	24.052	4346
100	12.996	480.9	200	21.435	2286	293.15	24.119	4423
110	14.400	618.0	210	21.840	2502			

Table B. Low temperature specific heat and enthalpy values for copper

T K	C_p	$H_T - H_0$	T K	C_p	$H_T - H_0$	T K	C_p	$H_T - H_0$
20	0.460	2.239	120	18.246	1014	220	23.097	3135
30	1.684	12.17	130	19.106	1201	230	23.327	3367
40	3.724	38.69	140	19.836	1395	240	23.531	3602
50	6.171	88.01	150	20.463	1597	250	23.713	3838
60	8.636	162.1	160	21.006	1804	260	23.879	4076
70	10.900	260.0	170	21.477	2017	270	24.035	4316
80	12.881	379.2	180	21.887	2234	280	24.186	4557
90	14.578	516.7	190	22.244	2454	290	24.327	4799
100	16.016	669.9	200	22.559	2679	293.15	24.369	4876
110	17.228	836.3	210	22.842	2906			

Table C. Low temperature specific heat and enthalpy values for tungsten

T K	C_p	$H_T - H_0$	T K	C_p	$H_T - H_0$	T K	C_p	$H_T - H_0$
20	0.333	1.676	120	18.248	996.4	220	23.027	3115
30	1.348	9.311	130	19.083	1183	230	23.277	3347
40	3.296	31.82	140	19.872	1378	240	23.498	3581
50	5.822	77.18	150	20.539	1580	250	23.683	3817
60	8.380	148.3	160	20.999	1788	260	23.828	4054
70	10.740	244.1	170	21.463	2000	270	23.947	4293
80	12.788	362.0	180	21.867	2217	280	24.053	4533
90	14.567	498.9	190	22.167	2437	290	24.150	4774
100	16.033	652.1	200	22.462	2660	293.15	24.179	4850
110	17.255	818.7	210	22.752	2887			

Table D. Values of the constants in Equation A for 20 K to 293.15 K

Element	A	B	C
Aluminum	8.71140×10^{-7}	2.16954×10^{-10}	4.08915×10^{-6}
Copper	6.79694×10^{-7}	4.29112×10^{-11}	-2.77450×10^{-6}
Tungsten	1.91900×10^{-7}	-2.06100×10^{-11}	-1.10756×10^{-6}

Table E. Values of the constants in Equation B for 0 K to 293.15 K

Element	L_0	D	E	F
Aluminum	0.995860	8.96010×10^{-7}	9.90180×10^{-11}	3.79261×10^{-6}
Copper	0.996743	6.71302×10^{-7}	3.01085×10^{-11}	-3.25552×10^{-6}
Tungsten	0.999124	1.88713×10^{-7}	-1.25649×10^{-11}	-1.28932×10^{-6}

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APPENDIX B : A SUMMARY OF THE CRYSTALLOGRAPHIC PROPERTIES OF THE ELEMENTS

Part 1. Crystallographic Properties at 293.15 K (20ºC)

Structure abbreviations

bcc: body-centered cubic
bct: body-centered tetragonal
dhcp: double hexagonal close packed
fcc: face-centered cubic
hcp: hexagonal close-packed
hex: hexagonal
mono: monoclinic
ortho: orthorhombic
rhomb: rhombohedral

Atomic Number	Symbol	Structure	Pearson Symbol	Lattice Parameter nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$	Notes
1	H	gas					Part 2
2	He	gas					Part 3
3	Li	bcc	cI2	0.35093	13.013	533.4	
4	Be	hcp	hP2	*a* 0.22860 *c* 0.35842	4.844	1845	
5	B	rhomb	hR12	*a*h 0.49065 *c*h 1.25658 *a*r 0.50566 *α* 58.046°	4.382	2467	α Rhomb
		rhomb	hR107	*a*h 1.0933 *c*h 2.3825 *a*r 1.0145 *α* 65.212°	4.640	2330	β Rhomb
6	C	hex	hP4	*a* 0.24614 *c* 0.67094	5.300	2266	Graphite
		cubic	cF8	0.356707	3.4166	3515	Diamond **m**
7	N	gas					Part 2
8	O	gas					Part 2
9	F	gas					Part 2
10	Ne	gas					Part 2
11	Na	bcc	cI2	0.42874	23.730	968.8	
12	Mg	hcp	hP2	*a* 0.32091 *c* 0.52103	13.992	1737	
13	Al	fcc	cF4	0.40493	9.996	2699	
14	Si	cubic	cF8	0.5430986	12.058600	2329.085	
15	P	cubic	cI232	1.869	67.78	1828	White
		ortho	oS8	*a* 0.33137 *b* 1.0477 *c* 0.43755	45.74	2709	Black
		mono	mP84	*a* 0.921 *b* 0.915 *c* 2.260 *β* 106.1°	52.47	2361	Violet
16	S	ortho	oF128	*a*1.0460 *b* 1.2861 *c* 2.4481	123.96	2069	α Rhomb
		mono	mP48	*a* 1.0923 *b* 1.0851 *c* 1.0787 *β* 95.90_5°	127.65	2010	β Mono **m**

Atomic Number	Symbol	Structure	Pearson Symbol	Lattice Parameter nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$	Notes
17	Cl	gas					Part 2
18	Ar	gas					Part 2
19	K	bcc	cI2	0.53269	45.514	859.0	
20	Ca	fcc	cF4	0.5588	26.27	1526	
21	Sc	hcp	hP2	*a* 0.33089 *c* 0.52680	15.041	2989	
22	Ti	hcp	hP2	*a* 0.29505 *c* 0.46833	10.632	4502	
23	V	bcc	cI2	0.30272	8.353	6099	
24	Cr	bcc	cI2	0.22849	7.230	7192	
25	Mn	cubic cubic	cI58 cP20	0.89116 0.63146	7.348 7.582	7476 7246	Alpha Beta m
26	Fe	bcc	cI2	0.28665	7.092	7874	
27	Co	hcp fcc	hP2 cF4	*a* 0.25071 *c* 0.40700 0.35447	6.671 6.705	8834 8789	Alpha Beta m
28	Ni	fcc	cF4	0.35241	6.589	8907	
29	Cu	fcc	cF4	0.36150	7.112	8935	
30	Zn	hcp	hP2	*a* 0.26646 *c* 0.49455	9.156	7140	
31	Ga	ortho	oS8	*a* 0.45205 *b* 0.76625 *c* 0.45266	11.803	5907	
32	Ge	cubic	cF8	0.565774	13.633	5327	
33	As	rhomb	hR2	*a*h 0.37599 *c*h 1.05458 *a*r 0.41315 α 54.133°	12.959	5782	
34	Se	hex	hP3	*a* 0.43646 *c* 0.49577	16.418	4810	
35	Br	liquid					Part 2
36	Kr	gas					Part 2
37	Rb	bcc	cI2	0.5699	55.73	1534	
38	Sr	fcc	cF4	0.6086	33.94	2582	
39	Y	hcp	hP2	*a* 0.36483 *c* 0.57317	19.894	4469	
40	Zr	hcp	hP2	*a* 0.32322 *c* 0.51479	14.024	6505	
41	Nb	bcc	cI2	0.33005	10.826	8582	
42	Mo	bcc	cI2	0.31471	9.385	10223	
43	Tc	hcp	hP2	*a* 0.27412 *c* 0.43990	8.620	11359 11475	98Tc 99Tc
44	Ru	hcp	hP2	*a* 0.27058 *c* 0.42816	8.174	12364	
45	Rh	fcc	cF4	0.38034	8.283	12423	
46	Pd	fcc	cF4	0.38902	8.864	12007	
47	Ag	fcc	cF4	0.40860	10.270	10503	
48	Cd	hcp	hP2	*a* 0.29789 *c* 0.56166	12.997	8649	
49	In	bct	tI2	*a* 0.32516 *c* 0.49471	15.749	7290	
50	Sn	bct cubic	tI4 cF8	*a* 0.58513 *c* 0.31811 0.64896	16.285 20.574	7289 5770	Beta Alpha m
51	Sb	rhomb	hR2	*a*h 0.43084 *c*h 1.12736 *a*r 0.45066 α 57.112°	18.190	6694	
52	Te	hex	hP3	*a* 0.44559 *c* 0.59275	20.460	6237	
53	I	ortho	oS8	*a* 0.72579 *b* 0.47828 *c* 0.98238	51.341	4944	
54	Xe	gas					Part 2
55	Cs	bcc	cI2	0.6162	70.45	1886	
56	Ba	bcc	cI2	0.5025	38.21	3594	

Appendix B

Atomic Number	Symbol	Structure	Pearson Symbol	Lattice Parameter nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$	Notes
57	La	dhcp	hP4	*a* 0.37742 *c* 1.2171	22.605	6145	Alpha
		fcc	cF4	0.53060	22.490	6176	Beta m
58	Ce	fcc	cF4	0.51612	20.699	6769	Gamma
		dhcp	hP4	*a* 0.36811 *c* 1.1857	20.948	6689	Beta m
59	Pr	dhcp	hP4	*a* 0.36723 *c* 1.18328	20.806	6773	
60	Nd	dhcp	hP4	*a* 0.36583 *c* 1.17968	20.585	7007	
61	Pm	dhcp	hP4	*a* 0.36393 *c* 1.1739	20.272	7149 7247	145Pm 147Pm
62	Sm	rhomb	hR3	*a*h 0.36291 *c*h 2.6207 *a*r 0.89834 α 23.307°	20.001	7518	
63	Eu	bcc	cI2	0.45822	28.970	5246	
64	Gd	hcp	hP2	*a* 0..36337 *c* 0.57821	19.908	7899	
65	Tb	hcp	hP2	*a* 0..36056 *c* 0.56966	19.312	8229	
66	Dy	hcp	hP2	*a* 0..35916 *c* 0.56501	19.006	8550	
67	Ho	hcp	hP2	*a* 0..35780 *c* 0.56177	18.753	8795	
68	Er	hcp	hP2	*a* 0..35593 *c* 0.55849	18.450	9065	
69	Tm	hcp	hP2	*a* 0.35377 *c* 0.55539	18.126	9320	
70	Yb	fcc	cF4	0.54856	24.839	6967	
71	Lu	hcp	hP2	*a* 0.35053 *c* 0.55493	17.780	9840	
72	Hf	hcp	hP2	*a* 0.39142 *c* 0.50512	13.439	13281	
73	Ta	bcc	cI2	0.33029	16.849	16678	
74	W	bcc	cI2	0.31652	9.548	19254	
75	Re	hcp	hP2	*a* 0.27610 *c* 0.44584	8.863	21010	
76	Os	hcp	hP2	*a* 0.27342 *c* 0.43199	8.421	22589	
77	Ir	fcc	cF4	0.38392	8.519	22562	
78	Pt	fcc	cF4	0.39236	9.094	21452	
79	Au	fcc	cF4	0.40786	10.215	19283	
80	Hg	liquid					Part 2
81	Tl	hcp	hP2	*a* 0.34566 *c* 0.55252	17.215	11873	
82	Pb	fcc	cF4	0.49499	18.259	11348	
83	Bi	rhomb	hR2	*a*h 0.45462 *c*h 1.18617 *a*r 0.47458 α 57.236°	21.310	9807	
84	Po	cubic	cP1	0.3359	22.82	9157 9200	209Po 210Po
85	At	fcc	cF4	0.539	23.6	8910 8950	210At 211At
86	Rn	gas					Part 2
87	Fr	bcc	cI2	0.6704	90.72	2458	223Fr
88	Ra	bcc	cI2	0.5148	41.08	5502	226Ra
89	Ac	fcc	cF4	0.5315	22.60	10040	227Ac
90	Th	fcc	cF4	0.50845	19.790	11725	
91	Pa	bct	tI2	*a* 0.3921 *c* 0.3235	14.98	15430	
92	U	ortho	oS4	*a* 0.28535 *b* 0.58697 *c* 0.49552	12.495	19050	
93	Np	ortho	oP8	*a* 0.4723 *b* 0.4887 *c* 0.6663	11.58	20480	237Np
94	Pu	mono	mP16	*a* 0.6183 *b* 0.4822 *c* 0.4375 *β* 101.79°	12.04	20260 19850	244Pu 239Pu

Atomic Number	Symbol	Structure	Pearson Symbol	Lattice Parameter nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$	Notes
95	Am	dhcp	hP4	*a* 0.3471 *c* 1.1245	17.66	13760 13650	243Am 241Am
96	Cm	dhcp	hP4	*a* 0.3496 *c* 1.1330	18.06	13680 13740	247Cm 248Cm
97	Bk	dhcp	hP4	*a* 0.3414 *c* 1.1065	16.82	14690 14810	247Bk 249Bk
98	Cf	dhcp	hP4	*a* 0.3382 *c* 1.1033	16.45	15260 15140	251Cf 249Cf
99	Es	hcp	hP2	*a* 0.398 *c* 0.650	26.85	9390 9430	252Es 253Es
100	Fm	fcc	cF4	0.566	27.25	9430	257Fm
101	Md	fcc	cF4	0.561	26.64	9690	258Md
102	No	fcc	cF4	0.557	26.05	9950	259No
103	Lr	hcp	hP2	***a*** 0.332 ***c*** 0.542	15.58	16820	262Lr

Note: m equals metastable at 293.15 K

Part 2. A Summary of the Crystallographic Properties at Their Melting Points for Elements which are Gaseous or Liquid at 293.15 K (20°C) (Except Helium)

Atomic Number	Symbol	Triple Point K	Structure	Pearson Symbol	Lattice Parameters nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
1	n-H_2	13.95	hcp	hP4	*a* 0.3789_7 *c* 0.6183_1	23.16	87.06
1	n-D_2	18.72	hcp	hP4	*a* 0.3636_2 *c* 0.5925_2	20.43	197.1
7	N_2	63.15	hcp	hP4	*a* 0.4115_8 *c* 0.6734_3	29.75	941.7
8	O_2	54.36	cubic	cP16	0.6782_8	23.49	1362
8	O_3	80.6	ortho	oP24	*a* 0.8035_3 *b* 0.6658_9 *c* 0.6949_3	27.99	1715
9	F_2	53.48	cubic	cP16	*0.6568*	*21.33*	*1781*
10	Ne	24.56	fcc	cF4	0.45377	14.067	1435
17	Cl_2	172.17	ortho	oS8	*a* 0.6308_0 *b* 0.4558_3 *c* 0.8154_9	35.30	2009
18	Ar	83.81	fcc	cF4	0.54691	24.629	1622
35	Br_2	265.90	ortho	oS8	*a* 0.6743_0 *b* 0.4668_5 *c* 0.8700_2	41.23	3876
36	Kr	115.78	fcc	cF4	0.58357	29.920	2801
54	Xe	161.41	fcc	cF4	0.63484	38.520	3408
80	Hg	234.32	rhomb	hR1	a_h 0.3476_4 c_h 0.6732_0 a_r 0.3010_6 α $70.52_9°$	14.143	14183
86	^{222}Rn	207.7	fcc	cF4	0.7008	51.82	4285

Part 3. A Summary of the Crystallographic Properties of the Helium Isotopes at the Minimums in Their Melting Curves

Helium cannot be obtained as a solid at atmospheric pressure. The following represent estimated crystallographic values at the minimum in the melting curves at 0.31524 K and 29.3113 bar for He^3 and 0.775 K and 25.316 bar for He^4.

For He4 the lattice parameters are calculated from the molar volume by assuming that the *c/a* ratio is ideal at $(8/3)^{½}$ or 1.6330.

Isotope	Structure	Pearson Symbol	Lattice Parameters nm	Molar Volume $cm^3\ mol^{-1}$	Density $kg\ m^{-3}$
He^3	bcc	cI2	0.4359	24.939	120.9
He^4	hcp	hP2	*a* 0.3666 *c* 0.5987	20.983	190.8

ELEMENT INDEX

Element Name	Symbol	Page	Element Name	Symbol	Page	Element Name	Symbol	Page
Actinium	Ac	611	Hafnium	Hf	518	Promethium	Pm	450
Aluminum	Al	124	Helium	He	15	Protactinium	Pa	618
Americium	Am	655	Holmium	Ho	489	Radium	Ra	610
Antimony	Sb	392	Hydrogen	H	1	Radon	Rn	606
Argon	Ar	167	Indium	In	378	Rhenium	Re	543
Arsenic	As	277	Iodine	I	403	Rhodium	Rh	350
Astatine	At	604	Iridium	Ir	555	Rubidium	Rb	298
Barium	Ba	420	Iron	Fe	217	Ruthenium	Ru	342
Berkelium	Bk	666	Krypton	Kr	295	Samarium	Sm	453
Beryllium	Be	37	Lanthanum	La	424	Scandium	Sc	178
Bismuth	Bi	594	Lawrencium	Lr	673	Selenium	Se	282
Boron	B	44	Lead	Pb	588	Silicon	Si	133
Bromine	Br	289	Lithium	Li	29	Silver	Ag	362
Cadmium	Cd	371	Lutetium	Lu	513	Sodium	Na	112
Calcium	Ca	174	Magnesium	Mg	118	Strontium	Sr	301
Californium	Cf	668	Manganese	Mn	208	Sulfur	S	148
Carbon	C	56	Mendelevium	Md	673	Tantalum	Ta	524
Cerium	Ce	430	Mercury	Hg	576	Technetium	Tc	338
Cesium	Cs	416	Molybdenum	Mo	328	Tellurium	Te	398
Chlorine	Cl	162	Neodymium	Nd	444	Terbium	Tb	474
Chromium	Cr	199	Neon	Ne	107	Thallium	Tl	582
Cobalt	Co	229	Neptunium	Np	634	Thorium	Th	612
Copper	Cu	247	Nickel	Ni	238	Thulium	Tm	502
Curium	Cm	663	Niobium	Nb	320	Tin	Sn	384
Dysprosium	Dy	481	Nitrogen	N	80	Titanium	Ti	184
Einsteinium	Es	671	Nobelium	No	673	Tungsten	W	533
Erbium	Er	495	Osmium	Os	549	Uranium	U	622
Europium	Eu	460	Oxygen	O	89	Vanadium	V	191
Fermium	Fm	673	Palladium	Pd	355	Xenon	Xe	411
Fluorine	F	103	Phosphorus	P	142	Ytterbium	Yb	508
Francium	Fr	608	Platinum	Pt	561	Yttrium	Y	305
Gadolinium	Gd	465	Plutonium	Pu	640	Zinc	Zn	258
Gallium	Ga	264	Polonium	Po	602	Zirconium	Zr	313
Germanium	Ge	270	Potassium	K	170			
Gold	Au	569	Praseodymium	Pr	437			