

PBD, *trans trans*-1,4-polybutadiene

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	<i>trans</i> -1,4-polybutadiene	
Acronym	-	<i>trans</i> -PBD	
CAS number	-	9003-17-2	
HISTORY			
Person to discover	-	Carlson, E J; Horne, S E	Carlson, E J; Horne, S E, US Patent 3,657,209, Goodrich-Gulf Chemicals, Apr. 18, 1972.
Date	-	1972 (filed 1955)	
Details	-	all- <i>trans</i> polymerization	
SYNTHESIS			
Monomer(s) structure	-	H ₂ C=CHCH=CH ₂	
Monomer(s) CAS number(s)	-	106-99-0	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	54.09	
Method of synthesis	-	polymerization with application of Ziegler-Natta catalyst system; anionic polymerization	
Temperature of polymerization	°C	20	
Catalyst	-	TiCl ₄ +triisobutyl aluminum; iron bisiminopyridyl complexes; lithium catalyst	Gong, D; Jia, X; Wang, B; Wang, F; Zhang, C; Zhang, X; Jiang, L; Dong, W, Inorg. Chim. Acta, 373, 47-53, 2001; Rodriguez Garraza, A L; Sorichetti, P; Marzocca, A J; Matteo, C L; Monti, G A, Polym. Test., in press, 2011.
Yield	%	over 90% <i>trans</i> ; up to 99% <i>trans</i> ; mixture of isomers	
Number average molecular weight, M _n	dalton, g/mol, amu	68,000-290,000	
Mass average molecular weight, M _w	dalton, g/mol, amu	250,000-580,00	
Polydispersity, M _w /M _n	-	1.07-3.7	
Molar volume at 298K	cm ³ mol ⁻¹	calc.=59.8; exp.=60.7	
Van der Waals volume	cm ³ mol ⁻¹	54.1	
STRUCTURE			
Crystallinity	%	11-55.8; amorphous (less than 65 <i>trans</i>)	Benvenuta-Tapia, J J; Tenorio-Lopez, J A; Herrera-Najera, R; Rios-Guerrero, L, Polym. Eng. Sci., 49, 1-10, 2009; Yang, X; Cai, J; Kong, X; Dong, W; Li, G; Ling, W; Zhou, E, Eur. Polym. J., 37, 763-69, 2001.
Cell type (lattice)	-	monoclinic; hexagonal	Yang, X; Cai, J; Kong, X; Dong, W; Li, G; Ling, W; Zhou, E, Eur. Polym. J., 37, 763-69, 2001.
Cell dimensions	nm	a:b:c=0.863:0.911:0.483; a:b:c=0.495:0.495:0.466	Yang, X; Cai, J; Kong, X; Dong, W; Li, G; Ling, W; Zhou, E, Eur. Polym. J., 37, 763-69, 2001.
Unit cell angles	degree	β=114; γ=120	Yang, X; Cai, J; Kong, X; Dong, W; Li, G; Ling, W; Zhou, E, Eur. Polym. J., 37, 763-69, 2001.
Number of chains per unit cell	-	4	

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Trans content	%	40-80 (elastomer); >90 (thermoplastic resin)	Benvenuta-Tapia, J J; Tenorio-Lopez, J A; Herrera-Najera, R; Rios-Guerrero, L, Polym. Eng. Sci., 49, 1-10, 2009.
Dielectric moment	Debye	0 (<i>trans</i>)	
Chain conformation	-	1/0	
Entanglement molecular weight	dalton, g/mol, amu	calc.=1,581	
Lamellae thickness	nm	4-16	Yang, X; Cai, J; Kong, X; Dong, W; Li, G; Ling, W; Zhou, E, Eur. Polym. J., 37, 763-69, 2001.
PHYSICAL PROPERTIES			
Density at 20°C	g cm ⁻³	0.91; 1.04 (crystalline)	
Color	-	white to light yellow	
Refractive index, 20°C	-	calc.=1.502-1.5188; exp.=1.516-1.605	
Melting temperature, DSC	°C	80-145	
Thermal conductivity, melt	W m ⁻¹ K ⁻¹	calc.=0.1788; exp.=0.22	
Glass transition temperature	°C	calc.=-72 to -103.0; ; -102 (<i>cis</i>) and -72 to -87 (<i>trans</i>)	Di Lorenzo, M L, Polymer, 50, 578-84, 2009.
Heat of fusion	kJ mol ⁻¹	4.18	
Maximum service temperature	°C	-101 to 93	
Enthalpy of melting	J g ⁻¹	19.4-34.6	Yang, X; Cai, J; Kong, X; Dong, W; Li, G; Ling, W; Zhou, E, Eur. Polym. J., 37, 763-69, 2001.
Hildebrand solubility parameter	MPa ^{0.5}	calc.=14.65-17.15; exp.=17.09-17.6	
Surface tension	mN m ⁻¹	calc.=33.5-39.8; exp.=32.0	
Dielectric constant at 100 Hz/1 MHz	-	/2.8	
Dielectric loss factor at 1 kHz	-	0.002	
Diffusion coefficient of nitrogen	cm ² s ⁻¹ x10 ⁶	0.5	
Diffusion coefficient of oxygen	cm ² s ⁻¹ x10 ⁶	0.7	
Contact angle of water, 20°C	degree	96	
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	250-400 (draw ratio - 10-20)	
Elongation	%	400	
Young's modulus	MPa	15,000-20,000 (draw ratio - 10-20)	
Poisson's ratio	-	calc.=0.432	
Intrinsic viscosity, 25°C	dl g ⁻¹	2.1	
Mooney viscosity	-	50-68	
CHEMICAL RESISTANCE			
Acid dilute/concentrated	-	good/poor	
Alcohols	-	good	
Alkalis	-	good/poor	
Aliphatic hydrocarbons	-	poor	

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PARAMETER	UNIT	VALUE	REFERENCES
Aromatic hydrocarbons	-	poor	
Esters	-	poor	
Ketones	-	poor	
Theta solvent, Theta-temp.=212, 240, 146°C	-	diethyl ketone, ethyl propyl ketone, propylene oxide	
Good solvent	-	higher ketones, higher aliphatic esters, hydrocarbons, THF	
Non-solvent	-	alcohol, dilute acids, dilute alkalies, nitromethane, propanitrile, water	
FLAMMABILITY			
Ignition temperature	°C	200	
Autoignition temperature	°C	350	
BIODEGRADATION			
Typical biodegradants	-	horseradish peroxidase	Enoki, M; Kaita, S; Wakatsuki, Y; Doi, Y; Iwata, T, Polym. Deg. Stab., 84, 321-26, 2004.
TOXICITY			
NFPA: Health, Flammability, Reactivity rating	-	1/1/0	
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
PROCESSING			
Applications	-	golf ball covers	
ANALYSIS			
FTIR (wavenumber-assignment)	cm ⁻¹ /-	725 (<i>cis</i> -1,4), 910 (vinyl-1,2), and 965 (<i>trans</i> -1,4)	Pires, N M T; Coutinho, F M B; Costa, M A S, Eur. Polym. J, 40, 2599-2603, 2004.
Raman (wavenumber-assignment)	cm ⁻¹ /-	C=C – 1666	Pathak, A; Saxena, V; Tandon, P; Gupta, V D, Polymer, 5154-60, 2006.
NMR (chemical shifts)	ppm	H NMR: =CH- – 5.6; =CH ₂ – 4.9; CH ₃ – 0.85; C NMR: CH= – 142.7; CH ₂ = – 114.5	Hung, N Q; Sanglar, C; Grenier-Loustalot, M F; Huoung, P V; Cuong, H N, Polym. Deg. Stab., 96, 1255-60, 2011.