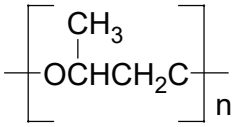
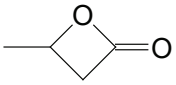
PHB poly(3-hydroxybutyrate)

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	poly(3-hydroxybutyrate)	
CAS name	-	butanoic acid, 3-hydroxy-, homopolymer (26063-00-3); poly[oxy(1-methyl-3-oxo-1,3-propanediyl)] (26744-04-7); poly[oxy[(1R)-1-methyl-3-oxo-1,3-propanediyl]] (31759-58-7)	
Acronym	-	PHB	
CAS number	-	26063-00-3; 26744-04-7; 31759-58-7	
Linear formula			
HISTORY			
Person to discover	-	Maurice Lemoigne	
Date	-	1925	
Details	-	isolated and characterized	
SYNTHESIS			
Monomer(s) structure	-		
Monomer(s) CAS number(s)	-	3068-88-0	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	86.09	
Monomer(s) expected purity(ies)	%	98 (glycerol)	Posada, J A; Naranjo, J M; Lopez, J A; Higuita, J C; Cardona, C A, Process Biochem., 46, 310-17, 2011.
Method of synthesis	-	produced by biosynthesis by bacteria and plants in response to physiological stress; also *Haloarcula sp.* can be used to produce PHB from petrochemical wastewater; economical high scale production from glycerol is feasible	Taran, M, J. Hazardous Mater., 188, 26-28, 2011; Posada, J A; Naranjo, J M; Lopez, J A; Higuita, J C; Cardona, C A, Process Biochem., 46, 310-17, 2011.
Temperature of polymerization	°C	139 (sterilization); 35 (fermentation)	Posada, J A; Naranjo, J M; Lopez, J A; Higuita, J C; Cardona, C A, Process Biochem., 46, 310-17, 2011.
Time of polymerization	h	21-22.5	
Pressure of polymerization	Pa	atmospheric	
Number average molecular weight, M_n	dalton, g/mol, amu	22,000-768,000	
Mass average molecular weight, M_w	dalton, g/mol, amu	12,000 (*Eubacteria, Archaebacteria*, and *Eukaryotes*); 200,000-3,000,000 (microbial cell cytoplasm); ultra high molecular weight >3,000,000 (*Escherichia coli*)	Bastioli, C, Handbook of Biodegradable Polymers, Rapra, 2005.
Polydispersity, M_w/M_n	-	1.95-3.7	Oliveira, F C; Dias, M L; Castilho, L R; Freire, D M G, Biosource Technol., 98, 633-38, 2007.
Polymerization degree (number of monomer units)	-	120-200 (low molecular weight)	Bastioli, C, Handbook of Biodegradable Polymers, Rapra, 2005.
STRUCTURE			
Crystallinity	%	30-80	
Cell type (lattice)	-	orthorhombic	Cornibert, J; Marchessault, R H, J. Mol. Biol. 71, 735, 1972.

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PARAMETER	UNIT	VALUE	REFERENCES
Cell dimensions	nm	a:b:c=0.576:1.320:0.596	
Unit cell angles	degree	90	
Rapid crystallization temperature	°C	90-110	
COMMERCIAL POLYMERS			
Some manufacturers	-	Mirel Plastics; PHB Industrial	
Trade names	-	Mirel; Biocycle	
PHYSICAL PROPERTIES			
Density at 20°C	g cm^{-3}	1.17-1.25; 1.177 (amorphous); 1.262 (crystalline)	
Color	-	white to yellow	
Odor	-	mild	
Melting temperature, DSC	°C	166-185	Bastioli, C, Handbook of Biodegradable Polymers, Rapra, 2005.
Storage temperature temperature	°C	25	
Glass transition temperature	°C	-4 to +2.4	
Maximum service temperature	°C	130	
Vicat temperature VST/B/50	°C	53-96	
Enthalpy of fusion	J g^{-1}	93.56; 66.9 (enthalphy of melting)	Suttiwijitpukdee, N; Sato, H; Zhang, J; Hashimoto, T; Ozaki, Y, Polymer, 52, 461-71, 2011.
Hildebrand solubility parameter	$MPa^{0.5}$	19.2	
Dielectric constant at 100 Hz/1 MHz	-	-/3	
Volume resistivity	ohm-m	1E14	
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	40-62	Bastioli, C, Handbook of Biodegradable Polymers, Rapra, 2005.
Tensile creep modulus, 1000 h, elongation 0.5 max	MPa	10-27	
Elongation	%	5-58	Bastioli, C, Handbook of Biodegradable Polymers, Rapra, 2005.
Flexural modulus	MPa	1,000-2,000	
Young's modulus	MPa	3,500	
Melt index, 230°C/3.8 kg	g/10 min	5-100	
CHEMICAL RESISTANCE			
Acid dilute/concentrated	-	non-resistant	
Alcohols	-	resistant	
Esters	-	non-resistant	
Halogenated hydrocarbons	-	non-resistant	
Good solvent	-	chloroform, dichloroacetic acid, 1,2-dichloroethane, DMF, ethylacetoacetate, glacial acetic acid, trichloroethyelene	
Non-solvent	-	acetone, n-butanol, carbon tetrachloride, ethanol, ethyl acetate, methanol	

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PARAMETER	UNIT	VALUE	REFERENCES
WEATHER STABILITY			
Depth of UV penetration	μm	>100	Sadi, R K; Fechine, G J M; Demarquette, N R, Polym. Deg. Stab., 95, 2318-27, 2010.
BIODEGRADATION			
Typical biodegradants	-	enzymes, animal tissue active components, basic environment; biodegradation is hindered by previous UV degradation	Artsis, M I; Bonartsev, A P; Iordanskii, A L; Bonartseva, G A; Zaikov, G E, Mol. Cryst. Liq. Crys, 523, 21-49, 2010; Sadi, R K; Fechine, G J M; Demarquette, N R, Polym. Deg. Stab., 95, 2318-27, 2010.
TOXICITY			
NFPA: Health, Flammability, Reactivity rating	-	0/1/0	
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
ENVIRONMENTAL IMPACT			
Cradle to grave non-renewable energy use	MJ/kg	67.0-113.7	Harding, K G; Dennis, J S; von Blottnitz, H; Harrison, S T L, J. Biotechnol., 130, 57-66, 2007.
PROCESSING			
Typical processing methods	-	film, injection molding	
Processing temperature	°C	160 (injection)	
Applications	-	biodegradable plastics, medical (surgical film manufactured by Tepha, surgical mesh, sutures), pharmaceutical (controlled drug release)	
Outstanding properties	-	biodegradable, sustainable	
BLENDS			
Suitable polymers	-	C, CA, cellulose ester, PCL, PEG, PEO, PLA, PVAc, PVF	
ANALYSIS			
FTIR (wavenumber-assignment)	cm^{-1}/-	C-O stretching – 1053, 1130, 1181; C-C-O stretching – 1276; CH_3 symmetric deformation – 1378; C=O (free, amorphous) – 1747; C=O (intra, crystal) – 1723	Suttiwijitpukdee, N; Sato, H; Zhang, J; Hashimoto, T; Ozaki, Y, Polymer, 52, 461-71, 2011.
Raman (wavenumber-assignment)	cm^{-1}/-	C=O – 1740, 1725; helical structure bands – 3009, 2998, 1725, 1402, 1220; disordered domain bands – 2990, 2938, 2881, 1740, 1453; and much more in ref.	Izumi, C M S; Temperini, M L A, Vibrational Spectroscopy, 54, 127-32, 2010.
NMR (chemical shifts)	ppm	H NMR: methyl – 1.268; methylene – 2.430-2.620; methylidene – 5.232	Zhang, X; Wei, C; He, Q; Ren, Y, J. Env. Sci., 22, 8, 1267-72, 2010.
x-ray diffraction peaks	degree	13.4, 16.1, 16.7, 19.9, 21.7, 22.5, 30.3	Suttiwijitpukdee, N; Sato, H; Zhang, J; Hashimoto, T; Ozaki, Y, Polymer, 52, 461-71, 2011.