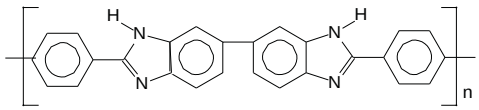
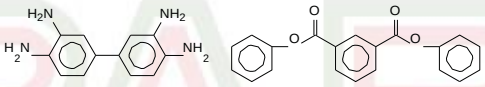
PBI polybenzimidazole

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	polybenzimidazole	
CAS name	-	poly[(1,5-dihydrobenzo[1,2-d:4,5-d']diimidazole-2,6-diyl)-1,3-phenylene] (27233-57-4); poly[(1,5-dihydrobenzo[1,2-d:4,5-d']diimidazole-2,6-diyl)-1,4-phenylene] (32075-68-6); poly(1H-benzimidazole-2,5-diyl) (32109-42-5); poly(1H-benzimidazole-2,5-diylsulfonyl-1H-benzimidazole-5,2-diyl-1,4-phenyleneoxy-1,4-phenylene) (928655-57-6); poly[(1,5-dihydrobenzo[1,2-d:4,5-d']diimidazole-2,6-diyl)-1,2-phenylene] (1073316-19-4)	
Acronym	-	PBI	
CAS number	-	27233-57-4; 32075-68-6; 32109-42-5; 928655-57-6; 1073316-19-4	
Formula			
HISTORY			
Person to discover	-	Marvel C S; Vogel, H A	Marvel C S; Vogel, H A, US Patent 3,174,947, University of Illinois, Mar. 23, 1965.
Date	-	1965 (filed in 1962)	
Details	-	synthesis	
SYNTHESIS			
Monomer(s) structure	-		
Monomer(s) CAS number(s)	-	91-95-2; 744-45-6	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	214.27; 318.32	
Monomer ratio	-	1:1.49	
Method of synthesis	-	condensation of 3,3'4,4'-tetraaminobiphenyl and diphenyl isophthalate in suitable solvent	
Temperature of polymerization	°C	100-290	Marsano, E; Azzurri, F; Corsini, P, Macromol. Symp., 234, 33-41, 2006.
Time of polymerization	h	1-2.5	Marsano, E; Azzurri, F; Corsini, P, Macromol. Symp., 234, 33-41, 2006.
Yield	%	93-100	
Number average molecular weight, M_n	dalton, g/mol, amu	2,500-32,700	
Mass average molecular weight, M_w	dalton, g/mol, amu	19,600-55,900	Ohishi, T; Sugi, R; Yokoyama, A; Yokozawa, T, J. Polym. Sci. a, 44, 4990-5003, 2006.
Polydispersity, M_w/M_n	-	1.08-5.4	
STRUCTURE			
Cell type (lattice)	-	monoclinic; triclinic	

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PARAMETER	UNIT	VALUE	REFERENCES
Cell dimensions	nm	a:b:c=0.9921:1.868:1.422 (monoclinic); a:b:c=1.070:1.199:1.371 (triclinic)	Tanatani, A; Yokoyama, A; Azumaya, I; Takakura, Y; Mitsui, C; Shiro, M; Uchiyama, M; Muranaka, A; Kobayashi, N; Yokozawa, T, JACS, 127, 8553-61, 2005.
Unit cell angles	degree	α:β:γ=101.4; α:β:γ=87.72:87.36:85.13	Tanatani, A; Yokoyama, A; Azumaya, I; Takakura, Y; Mitsui, C; Shiro, M; Uchiyama, M; Muranaka, A; Kobayashi, N; Yokozawa, T, JACS, 127, 8553-61, 2005.
Crystallite size	nm	9.5-12.4	
COMMERCIAL POLYMERS			
Some manufacturers	-	PBI Performance Products	
Trade names	-	Celazole	
PHYSICAL PROPERTIES			
Density at 20°C	g cm^{-3}	1.30-1.43	
Color	-	black	
Odor	-	odorless	
Melting temperature, DSC	°C	300	
Thermal expansion coefficient, 23-80°C	10^{-4} $°C^{-1}$	0.23-0.25	
Thermal conductivity, melt	W m^{-1} K^{-1}	0.038 (fiber)	
Glass transition temperature	°C	420-510; 399 (amorphous)	MacKnight, W J; Kantor, S W; Zhu, H, Antec, 1594-98, 1996.
Specific heat capacity	J K^{-1} kg^{-1}	1,300	
Maximum service temperature	°C	-196 to 500; 760 (short burst)	Bhowmik, S; Benedictus, R; Poulis, H, Polymers in Defence and Aerospace 2007, Rapra, 2007, paper 8.
Long term service temperature	°C	260-315	
Heat deflection temperature at 1.8 MPa	°C	435	
Dielectric constant at 100 Hz/1 MHz	-	5.4/3.2	
Relative permittivity at 100 Hz	-	3.3	
Relative permittivity at 1 MHz	-	3.2	
Dissipation factor at 100 Hz	E-4	10	
Dissipation factor at 1 MHz	E-4	30	
Volume resistivity	ohm-m	1E11	
Surface resistivity	ohm	1E10-2E15	
Electric strength K20/P50, d=0.60.8 mm	kV mm^{-1}	21-23	
Arc resistance	s	185	
Coefficient of friction	-	0.19-0.27	
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	94-160	
Tensile modulus	MPa	5,900	
Tensile stress at yield	MPa	74.4	Ngamsantivongsa, P; Lin, H-L; Yu, T L, , J. Membrane Sci., 491, 10-21, 2015.

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PARAMETER	UNIT	VALUE	REFERENCES
Elongation	%	3-8; 9-27 (fiber)	
Flexural strength	MPa	220	
Flexural modulus	MPa	6,500	
Elastic modulus	MPa	5,800	
Compressive strength	MPa	344-400	
Young's modulus	MPa	2,300	Ngamsantivongsa, P; Lin, H-L; Yu, T L, , J. Membrane Sci., 491, 10-21, 2015.
Charpy impact strength, notched, 23°C	kJ m^{-2}	3.5	
Izod impact strength, unnotched, 23°C	J m^{-1}	590	
Izod impact strength, notched, 23°C	J m^{-1}	30	
Poisson's ratio	-	0.34	
Shore D hardness	-	94	
Rockwell hardness	-	M125	
Ball indention hardness at 358 N/30 S (ISO 2039-1)	MPa	375	
Shrinkage	%	1	
Intrinsic viscosity, 25°C	dl g^{-1}	0.39-0.51	
Water absorption, 24h at 23°C	%	0.4-0.5; 5-15 (saturation)	
CHEMICAL RESISTANCE			
Acid dilute/concentrated	-	poor	
Alcohols	-	good	
Alkalis	-	poor	
Aliphatic hydrocarbons	-	good	
Aromatic hydrocarbons	-	good	
Esters	-	good	
Greases & oils	-	good	
Halogenated hydrocarbons	-	good/poor	
Ketones	-	good	
Good solvent	-	96% H_2SO_4, N,N-dimethylacetimide	
FLAMMABILITY			
Ignition temperature	°C	>540	
Autoignition temperature	°C	>540	
Limiting oxygen index	% O_2	41-58	
Char at 500°C	%	67.5	Lyon, R E; Walters, R N, J. Anal. Appl. Pyrolysis, 71, 27-46, 2004.
Heat of combustion	J g^{-1}	31,650	Walters, R N; Hacket, S M; Lyon, R E, Fire Mater., 24, 5, 245-52, 2000.
UL 94 rating	-	V-0	

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PARAMETER	UNIT	VALUE	REFERENCES
WEATHER STABILITY			
Spectral sensitivity	nm	260-300	Tanatani, A; Yokoyama, A; Azumaya, I; Takakura, Y; Mitsui, C; Shiro, M; Uchiyama, M; Muranaka, A; Kobayashi, N; Yokozawa, T, JACS, 127, 8553-61, 2005.
TOXICITY			
HMIS: Health, Flammability, Reactivity rating	-	0/1/0	
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
PROCESSING			
Typical processing methods	-	compression molding, melt spinning	
Additives used in final products	-	graphene oxide	
Applications	-	ball valve seats, clamp rings, electrical connectors, fiber, fuel cell membranes, insulator bushings, protective apparel (e.g., firefighter coats and suits)	
Outstanding properties	-	temperature stability (204°C) and chemical resistance, high heat deflection (427°C), with continuous service capability (399°C) in inert environment	
BLENDS			
Suitable polymers	-	aramid, PAES, PEI, PES, PI, PVF	Zhu, W-P; Sun, S-P; Gao, J; Fu, F-J; Chung, T-S, J. Membrane Sci.,456, 117-27, 2014.
ANALYSIS			
FTIR (wavenumber-assignment)	cm^{-1}/-	N-H – 3283; C=O – 1653	
x-ray diffraction peaks	degree	17.84, 18.76, 20.44-20.47, 22.76-23.67, 25.29, 28.06	Kobashi, K; Kobayashi, K; Yasuda, H; Arimachi, K; Uchida, T; Wakabayashi, K; Yamazaki, S; Kimura, K, Macromolecules, 42, 6128-35, 2009.