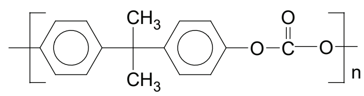
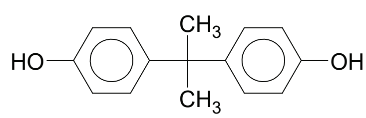
PC polycarbonate

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	polycarbonate	
IUPAC name	-	poly(oxycarbonyloxy-1,4-phenylene(dimethylmethylene)-1,4-phenylene]	
ACS name	-	carbonic acid, polymer with 4,4'-(1-methylethylidene) bis[phenol]; polycarbonates	
Acronym	-	PC	
CAS number	-	25037-45-0; 25766-59-0	
RTECS number	-	TR1580150	
Formula			
HISTORY			
Person to discover	-	Hermann Schnell	
Date	-	1953; 1958	
Details	-	Bayer chemist synthesized polycarbonate in the first attempt; the experiment was based on analysis of previous research and selection of right building blocks; in order to succeed with implementation, he had to overcome scepticism of his peers that such reaction and outcome are possible; polymer was patented immediately but production begun in 1958	
SYNTHESIS			
Monomer(s) structure	-	 CCl_2O	
Monomer(s) CAS number(s)	-	80-05-7; 75-44-5	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	228.29; 98.92	
Monomer(s) expected purity(ies)	%	98; 99	
Method of synthesis	-	Bisphenol A is treated with NaOH, which is then reacted with phosgene. It can also be manufactured by transesterification of bisphenol A with diphenyl carbonate.	
Temperature of polymerization	°C	30-40 (polycondesation); 160-240 (transesterification)	Couper, J R; Penney, W R; Fair, J R; Walas, S M, Chemical Equipment, 2nd Ed., Elsevier, 2010, pp. 581-640; Kim, J; Kim, Y J; Kim, J-D; Ahmed, T S; Dong, L B; Roberts, G W; Oh, S-G, Polymer, 2520-26, 2010.
Time of polymerization	h	0.25-4 (polycondesation)	
Pressure of polymerization	Pa	atmospheric	
Catalyst	-	benzyltriethylammonium chloride (polycondesation); LiOH (transesterification)	Couper, J R; Penney, W R; Fair, J R; Walas, S M, Chemical Equipment, 2nd Ed., Elsevier, 2010, pp. 581-640; Kim, J; Kim, Y J; Kim, J-D; Ahmed, T S; Dong, L B; Roberts, G W; Oh, S-G, Polymer, 2520-26, 2010.
Number average molecular weight, M_n	dalton, g/mol, amu	17,500-41,300	
Mass average molecular weight, M_w	dalton, g/mol, amu	19,000-56,000	

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PARAMETER	UNIT	VALUE	REFERENCES
Polydispersity, M_w/M_n	-	1.3-3.2	
Molar volume at 298K	cm^3 mol^{-1}	calc.=213.8; exp.=211.9	
Van der Waals volume	cm^3 mol^{-1}	calc.=136.21; exp.=138.36	
Molecular cross-sectional area, calculated	cm^2 x 10^{-16}	19.8	
Radius of gyration	nm	13	Fornes, T D; Baur, J W; Sabba, Y; Thomas, E L, Polymer, 47, 1704-14, 2006.
STRUCTURE			
Crystallinity	%	typically amorphous because of its rigid backbone; 20-42	Farmer, R, A Study of Crystallization in Bisphenol A Polycarbonate. Dissertation, Virginia Polytgechnic Institute, 2001; Kim, J; Kim, Y J; Kim, J-D; Ahmed, T S; Dong, L B; Roberts, G W; Oh, S-G, Polymer, 2520-26, 2010.
Entanglement molecular weight	dalton, g/mol, amu	calc.=1,734-2,495; exp.=2,495-4,800	
Lamellae thickness	nm	3.18-5.39	Farmer, R, A Study of Crystallization in Bisphenol A Polycarbonate. Dissertation, Virginia Polytgechnic Institute, 2001.
COMMERCIAL POLYMERS			
Some manufacturers	-	Bayer; Sabic	
Trade names	-	Makrolon; Lexan	
PHYSICAL PROPERTIES			
Density at 20°C	g cm^{-3}	1.19-1.22; 1.04 (melt); 1.25-1.52 (10-40% glass fiber)	
Bulk density at 20°C	g cm^{-3}	0.66 (pellets)	
Refractive index, 20°C	-	calc.=1.5773-1.587; exp.=1.586-1.587	
Birefringence	-	-0.001 (surface) to 0.001 (bulk)	Lin, T H; Isayev, A I, Antec, 1664-68, 2006.
Transmittance	%	82-91	
Haze	%	<0.8 to 3	
Melting temperature, DSC	°C	255-267	
Storage temperature (max)	°C	93	
Decomposition onset temperature	°C	420	
Thermal expansion coefficient, -40 to 95°C	$°C^{-1}$	6.0-7.5E-5; 1.6-6.5E-5 (10-40% glass fiber)	
Thermal conductivity, melt	W m^{-1} K^{-1}	0.19-0.24; 0.2-0.22 (10-40% glass fiber)	
Glass transition temperature	°C	calc.=134-158; exp.=137-154	
Specific heat capacity	J K^{-1} kg^{-1}	1,200; 1,040-1,210 (10-40% glass fiber)	
Heat of fusion	kJ kg^{-1}	100-115 (crystal); 22.95-23.11 (heat to melt)	DeLassus, P T; Landes, B G; Harris, L M, Antec, 1636-39, 1997.
Maximum service temperature	°C	-40 to 130	

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PARAMETER	UNIT	VALUE	REFERENCES
Temperature index (50% tensile strength loss after 20,000 h/5000 h)	°C	120	
Heat deflection temperature at 0.45 MPa	°C	133-166; 141-154 (10-40% glass fiber)	
Heat deflection temperature at 1.8 MPa	°C	119-156; 135-146 (10-40% glass fiber)	
Vicat temperature VST/A/50	°C	138-150; 144-149 (10-35% glass fiber)	
Vicat temperature VST/B/50	°C	144-170; 154 (10-40% glass fiber)	
Hansen solubility parameters, δ_D, δ_P, δ_H	$MPa^{0.5}$	19.6, 8.8, 5.7	
Interaction radius		10.2	
Hildebrand solubility parameter	$MPa^{0.5}$	22.2	
Surface tension	mN m^{-1}	calc.=33.0-37.9; exp.=28.4-42.9	Liao, C-C; Wang, C-C; Shih, K-C; Chen, C-Y, Eur. Polym. J., 47, 911-24, 2011.
Dielectric constant at 100 Hz/1 MHz	-	3.2/2.9	
Relative permittivity at 100 Hz	-	2.9-3.2; 3.1-3.6 (10-40% glass fiber)	
Relative permittivity at 1 MHz	-	2.8-3.1; 3.0-3.6 (10-40% glass fiber)	
Dissipation factor at 100 Hz	E-4	5-310; 8-13 (10-40% glass fiber)	
Dissipation factor at 1 MHz	E-4	90-120; 67-90 (10-40% glass fiber)	
Volume resistivity	ohm-m	1E12 to 1E15	
Surface resistivity	ohm	1E15 to 1E17	
Electric strength K20/P50, d=0.60.8 mm	kV mm^{-1}	15-67; 18-36 (10-40% glass fiber)	
Comparative tracking index, CTI, test liquid A	-	200-250; 175 (10-35% glass fiber)	
Comparative tracking index, CTIM, test liquid B	-	125M	
Coefficient of friction	ASTM D1894	0.21 (chrome steel); 0.41-0.54 (aluminum)	Maldonado, J E, Antec, 3431-35, 1998.
Permeability to nitrogen, 25°C	cm^3 m^{-2} 24 h^{-1} bar^{-1}	130 (100 μm film), 510 (25.4 μm film)	
Permeability to oxygen, 25°C	cm^3 m^{-2} 24 h^{-1} bar^{-1}	700 (100 μm film), 2,760 (25.4 μm film)	
Permeability to water vapor, 25°C	g m^{-2} 24 h^{-1} bar^{-1}	15	
Contact angle of water, 20°C	degree	81.3-84.0	
Surface free energy	mJ m^{-2}	42.3	
Speed of sound	m s^{-1}	38	
Acoustic impedance		2.69-2.77	
Attenuation	dB cm^{-1}, 5 MHz	22.1-24.9	
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	55-88; 45-158 (10-40% glass fiber)	Chang, M C O; Garrett, P D, Antec, 2588-93, 1996.
Tensile modulus	MPa	2,200-3,100; 3,800-9,400 (10-35% glass fiber)	

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PARAMETER	UNIT	VALUE	REFERENCES
Tensile stress at yield	MPa	57-74	Chang, M C O; Garrett, P D, Antec, 2588-93, 1996.
Tensile creep modulus, 1000 h, elongation 0.5 max	MPa	1,700-1,900; 2,900-8,500 (10-35% glass fiber)	
Elongation	%	66-140; 1.8-15 (10-40% glass fiber)	Chang, M C O; Garrett, P D, Antec, 2588-93, 1996.
Tensile yield strain	%	5.7-7; 8 (10-40% glass fiber)	
Flexural strength	MPa	94-120; 103-186 (10-40% glass fiber)	
Flexural modulus	MPa	2,220-2,600; 3,440-9,600 (10-40% glass fiber)	
Elastic modulus	MPa	1,600	
Compressive strength	MPa	70	
Young's modulus	MPa	2,390-2,600	Chang, M C O; Garrett, P D, Antec, 2588-93, 1996.
Charpy impact strength, unnotched, 23°C	kJ m^{-2}	no break; 40-150 (10-35% glass fiber)	
Charpy impact strength, unnotched, -30°C	kJ m^{-2}	no break	
Charpy impact strength, notched, 23°C	kJ m^{-2}	11-80; 8-12 (10-35% glass fiber)	
Charpy impact strength, notched, -30°C	kJ m^{-2}	9-14	
Izod impact strength, unnotched, 23°C	J m^{-1}	12-90 to NB; 1280-2140 (10-40% glass fiber)	
Izod impact strength, notched, 23°C	J m^{-1}	12-736; 8-133 (10-40% glass fiber)	
Izod impact strength, notched, -30°C	J m^{-1}	55-618	
Shear modulus	MPa	805	Ozcelik, B; Sonat, I, Mater. Design, 30, 367-75, 2009.
Abrasion resistance (ASTM D1044)	mg/1000 cycles	11 (10-40% glass fiber)	
Poisson's ratio	-	calc.=0.424; exp.=0.401-0.420	Lin, T H; Isayev, A I, Antec, 1664-68, 2006.
Rockwell hardness	-	L89; M85, R124 (10-40% glass fiber)	
Ball indention hardness at 358 N/30 S (ISO 2039-1)	MPa	116	
Shrinkage	%	0.4-0.9; 0.2-0.55 (10-35% glass fiber)	
Melt volume flow rate (ISO 1133, procedure B), 300°C/1.2 kg	cm^3/10 min	1.25-36	
Pressure coefficient of melt viscosity, b	G Pa^{-1}	26.6	Aho, J; Syrjala, S, J. Appl. Polym. Sci., 117, 1076–84, 2010.
Melt index, 300°C/1.2 kg	g/10 min	6-80	
Water absorption, equilibrium in water at 23°C	%	0.12-0.40; 0.23 (10-40% glass fiber)	
Moisture absorption, equilibrium 23°C/50% RH	%	0.09-0.3	
CHEMICAL RESISTANCE			
Acid dilute/concentrated	-	good/poor	
Alcohols	-	good	
Alkalis	-	good-poor	
Aliphatic hydrocarbons	-	good	

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PARAMETER	UNIT	VALUE	REFERENCES
Aromatic hydrocarbons	-	poor	
Esters	-	poor	
Greases & oils	-	good-poor	
Halogenated hydrocarbons	-	poor	
Ketones	-	poor	
Θ solvent, Θ-temp.=170°C	-	n-butyl benzyl ether	
Good solvent	-	acetophenone (hot), aniline (hot), benzene (hot), chloroform, cresol, 1,2-dichloroethane, methylene chloride	
Non-solvent	-	amyl alcohol, ethylene glycol, heptane, isopropyl alcohol	
Chemicals causing environmental stress cracking	list	acetone, benzyl alcohol, carbon tetrachloride, cyclohexanone, nitrobenzene	Wang, H T; Pan, Q G; Du, Q C; Li, Y Q, Polym. Test., 22, 125-28, 2003.
Effect of EtOH sterilization (tensile strength retention)	%	98-100	Navarrete, L; Hermanson, N, Antec, 2807-18, 1996.
FLAMMABILITY			
Ignition temperature	°C	480	
Autoignition temperature	°C	550	
Limiting oxygen index	% O_2	25-30; 30-43 (flame retardant grades)	
Minimum ignition energy	J	0.025	
Heat release	kW m^{-2}	479-548; 124-385 (with fire retardant)	Yu, B; Liu, M; Lu, L; Dong, X; Gao, W; Tang, K, Fire Mater., 34, 251-61, 2010.
NBS smoke chamber	Ds	190	Padey, D; Walling, J; Wood A, Polymers in Defence and Aerospace 2007, Rapra, 2007, paper 15.
Burning rate (Flame spread rate)	mm min^{-1}	passed	
Char at 500°C	%	21.7	Lyon, R E; Walters, R N, J. Anal. Appl. Pyrolysis, 71, 27-46, 2004.
Heat of combustion	J g^{-1}	31,060-31,530	Walters, R N; Hacket, S M; Lyon, R E, Fire Mater., 24, 5, 245-52, 2000.
Volatile products of combustion	-	carbon monoxide, carbon dioxide, bisphenol A, diphenyl carbonate, phenol and phenol derivatives. Traces of aliphatic and aromatic hydrocarbons, aldehydes and acids.	
UL 94 rating	-	HB to V-2; V-0 (some flame retardant grades); HB to V-0 (10-35% glass fiber)	
WEATHER STABILITY			
Spectral sensitivity	nm	<275 (completely absorbed); 260-300 (photo-Fries rearrangement); 280-305; 330-360	
Activation wavelengths	nm	290-320; 310 (chain scission), 330-360	
Important initiators and accelerators	-	4-hydroxystilbene; products of thermal degradation; bisphenol A, stilbene-like structures, water, bis(3-hydroxyphenyl)ether structures in main chain, some inorganic pigments	
Products of degradation	-	photo-Fries rearrangement; chain scissions, crosslinks, free radicals, hydroxyl groups, ethers, unsaturations (photolysis); chain scissions, hydroperoxides, free radicals, hydroxyl groups, carbonyl groups (photooxidation)	

PARAMETER	UNIT	VALUE	REFERENCES
Stabilizers	-	UVA: 2-hydroxy-4-octyloxybenzophenone; 2,2',4,4'-tetrahydroxybenzophenone; 2-(2H-benzotriazol-2-yl)-p-cresol; 2-benzotriazol-2-yl-4,6-di-tert-butylphenol; 2-(2H-benzotriazole-2-yl)-4,6-di-tert-pentylphenol; 2-(2H-benzotriazole-2-yl)-4-(1,1,3,3-tetraethylbutyl)phenol; 2-(2H-benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl) phenol; 2,2'-methylenebis(6-(2H-benzotriazol-2-yl)-4-1,1,3,3-tetramethylbutyl)phenol; 2-(2H-benzotriazol-2-yl)-6-dodecyl-4-methylphenol, branched & linear; 2-(2'-hydroxy-5'-methacryloxyethylphenyl)-2H-benzotriazole; 2-(2H-benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl) phenol; 2-(3-sec-butyl-5-tert-butyl-2-hydroxyphenyl) benzotriazole; reaction product of methyl 3(3-(2H-benzotriazole-2-yl)-5-t-butyl-4-hydroxyphenyl propionate/PEG 300; 2-(4,6-diphenyl-1,3,5-triazin-2-yl)-5-hexyloxy-phenol; 2-[4,6-bis(2,4-dimethylphenyl)-1,3,5-triazin-2-yl]-5-(octyloxy) phenol; 1,3-bis-[(2'-cyano-3',3'-diphenylacryloyl)oxy]-2,2-bis-{[(2'-cyano-3',3'-diphenylacryloyl)oxy]methyl}-propane; propanedioic acid, [(4-methoxyphenyl)-methylene]-dimethyl ester; 2,2'-(1,4-phenylene)bis[4H-3,1-benzoxazin-4-one]; Screener: zinc oxide; Phenolic antioxidant: 2-(1,1-dimethylethyl)-6-[[3-(1,1-dimethylethyl)-2-hydroxy-5-methylphenyl] methyl-4-methylphenyl acrylate; Phosphite: tris (2,4-di-tert-butylphenyl) phosphite; isodecyl diphenyl phosphite; di(p-butoxyphenyl) cyclohexylphosphine oxide; Optical brightener: 2,2'-(2,5-thiophenediyl)bis(5-tert-butylbenzoxazole); 2,2'-(1,2-ethylenediyl-di-4,1-phenylene)bisbenzoxazole; Plasticizer: dicyclohexyl phthalate (reduces yellowing on exposure to gamma radiation	
Results of exposure	-	yellowness index: 45 after 60 month exposure in florida without stabilization nad 22 after 60 month exposure in Florida with stabilization; 13 and 26 after 120 month exposure in Engerfeld, Germany with and without stabilization, respectively	
Low earth orbit erosion yield	cm^3 $atom^{-1}$ x 10^{-24}	4.29	Waters, D L; Banks, B A; De Groh, K K; Miller, S K R; Thorson, S D, High Performance Polym., 20, 512-22, 2008.
BIODEGRADATION			
Colonized products	-	compact disks, medical devices	
Typical biodegradants	-	microorganisms producing esterase are capable of damage; marine environment	Artham, T; Doble, M, J. Polym. Environ., 17, 170-80, 2009.
Stabilizers	-	silver-based biocides	
TOXICITY			
NFPA: Health, Flammability, Reactivity rating	-	0/1/0	
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
OSHA	mg m^{-3}	5 (respirable), 15 (total)	
Oral rat, LD_{50}	mg kg^{-1}	>10,000	
Skin rabbit, LD_{50}	mg kg^{-1}	>2,000	
ENVIRONMENTAL IMPACT			
Aquatic toxicity, *Daphnia magna*, LC_{50}, 48 h	mg l^{-1}	5,000	Lither, D; Damberg, J; Dave, G; Larsson, A, Chemosphere, 74, $1198^{-1}200$, 2009.
Cradle to grave non-renewable energy use	MJ/kg	111	

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PARAMETER	UNIT	VALUE	REFERENCES
Cradle to pellet greenhouse gasses	kg CO_2 kg^{-1} resin	7.8	
PROCESSING			
Typical processing methods	-	blow molding, calendering, electrospinning, extrusion, gas-assisted injection molding, injection molding, solution casting, thermoforming	
Preprocess drying: temperature/ time/residual moisture	°C/h/%	120-135/2-12/0.02	
Processing temperature	°C	280-355; 310-340 (10-40% glass fiber)	
Processing pressure	MPa	0.3-0.7 (back pressure)	
Additives used in final products	-	Fillers: boric oxide, glass beads, carbon black and graphite fibers for EMI shielding, glass fiber, graphite, molybdenum sulfide, nanosilica, nickel-coated graphite fibers, PTFE, single-walled carbon nanotubes, steel fibers, titanium dioxide, wollastonite; Plasticizers: dibutyl phthalate, dioctyl phthalate, dicyclohexyl phthalate, mineral oil, pentaerythritol tetraborate, trimellitic acid tridecyloctyl ester, tritolyl phosphate, tetra-ethylene glycol dimethyl ether, tri-(2-ethylhexyl) phosphate; Antistatics: carbon black, carbon nanotubes, copper oxide, glycerol mono-iso-stearate, indium tin oxide, nickel-coated carbon fiber, polyetheresteramide, polyoxyethylene fatty acid ester; Antiblocking: amorphous silica, calcium carbonate, dimethylsiloxane grafting, siloxane particles; Release: glycerol monostearate, pentaerythritol tetrastearate, siloxane, zinc stearate; impact modifier; UV stabilizers; release agents	
Applications	-	bearings, blood collector containers, camera components, computer printers, copying machines, corrective eyeglasses, dental applications, data storage (CD, DVD, etc.), dinner-ware, drinking cups, disposable syringes, head lamp covers and housings, gears, glazing, goggles, golf tees, guide pins, helmets, instrument panels, laminated walls, lenses, medical tubing, microfibers, needles syringes, optical lenses, pace-maker components, projection screens, rollers, roofing, safety glasses, skylights, speedometer needles, solar modules, tool boxes, toys, water bottles, windows, windscreens	
BLENDS			
Suitable polymers	-	ABS, PBT, PET, PHEMA, PLA, PVDF	
ANALYSIS			
FTIR (wavenumber-assignment)	cm^{-1}/-	C-H – 3047, 2877; C-O-C – 989; C=O – 1778	Abdel-Salam, M H; Nouh, S A; Radwan, Y E; Fouad, S S, Mater. Chem. Phys., 127, 305-9, 2011.
Raman (wavenumber-assign-ment)	cm^{-1}/-	C=O – 1769, 1597, 712; CH_3 – 1453	Hoeller, T L, Antec, 3124-30, 2007.