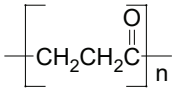
PK polyketone

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	polyketone	
CAS name	-	1-propene, polymer with carbon monoxide and ethene	
Acronym	-	PK	
CAS number	-	88995-51-1	
Linear formula			
HISTORY			
Person to discover	-	Brubaker, M M 1950. Van Broekhoven, J A M; Drent, E; Klei, E; Nozaki, K	Brubaker, M M, US Patent 2,495,286, DuPont, Jan. 24, 1950. Van Broekhoven, J A M; Drent, E; Klei, E; Nozaki, K, US Patent 4,880,903, Shell, Nov. 14, 1989.
Date	-	1950; 1989	
Details	-	monomers are polymerized in the presence of benzoyl peroxide; currently used technology has been patented by Shell in 1989	
SYNTHESIS			
Monomer(s) structure	-	CH_2=CH_2; CO	
Monomer(s) CAS number(s)	-	74-85-1; 630-08-0	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	28.05; 28.01	
Monomer ratio	-	1; some in addition have 6 mol% propylene (e.g, Carilon P1000)	Zuiderduin, W C J; Huetink, J; Gaymans, R J, J. Appl. Polym. Sci., 91, 2558-75, 2004.
Method of synthesis	-	polyketone can be made with a palladium(II) catalyst from ethylene and carbon monoxide (e.g., Carilon)	
Temperature of polymerization	°C	85	
Time of polymerization	h	5	
Pressure of polymerization	MPa	5.5	
Catalyst	-	palladium(ii) acetate+	
Yield	%	29.7-70 (oligomer)	Mul, W P; Dirkzwager, H; Broekhuis, A A; Heeres, H J; van der Linden, A J; Orpen, A G, Inorganica Chim. Acta, 327, 147-59, 2002.
Number average molecular weight, M_n	dalton, g/mol, amu	40,000-250,000; 1,500-5,000 (Carilite oligomer)	Mul, W P; Dirkzwager, H; Broekhuis, A A; Heeres, H J; van der Linden, A J; Orpen, A G, Inorganica Chim. Acta, 327, 147-59, 2002.
Mass average molecular weight, M_w	dalton, g/mol, amu	100,000-296,000	Zuiderduin, W C J; Homminga, D S; Huetink, H J; Gaymans, R J, Polymer, 44, 6361-70, 2003.
STRUCTURE			
Crystallinity	%	30-58; 30-40 (bulk-crystallized)	
Cell type (lattice)	-	orthorhombic	

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Cell dimensions	nm	a:b:c= 0.691:0.512:0.76 (α); a:b:c=0.797:0.476:0.757 (β)	Chatani, Y; Takizawa, T; Murahashi, S; Sakata, Y; Nishimura, Y, J. Polym. Sci., 55, 162, 811-19, 1961; Waddon, A J; Karttunen, N R; Lesser, A J, Macromolecules, 32, 423-28, 1999.
Unit cell angles	degree	26 (for angle between molecular plane and bc plane in α-form); 40 (in β-form)	Ohsawa, O; Lee, K-H; Kim, B-S; Lee, S; Kim, I-S, Polymer, 2007-12, 2010.
Number of chains per unit cell	-	4	
Polymorphs	-	α, β	
Chain conformation	-	planar zigzag	
Entanglement molecular weight	dalton, g/mol, amu	1,700	Zuiderduin, W C J; Homminga, D S; Huetink, H J; Gaymans, R J, Polymer, 44, 6361-70, 2003.
Lamellae thickness	nm	3.48-5.7	Blundell, D J; Liggat, J J; Flory, A, Polymer, 33, 12, 2475-82, 1992.
Avrami constants, k/n	-	n=2.02-2.85	Holt, G A; Spruiell, J E, Antec, 1780-88, 1996.
COMMERCIAL POLYMERS			
Some manufacturers	-	Shell	
Trade names	-	Carilon	
PHYSICAL PROPERTIES			
Density at 20°C	g cm^{-3}	1.24; 1.383 (crystalline)	Ohsawa, O; Lee, K-H; Kim, B-S; Lee, S; Kim, I-S, Polymer, 2007-12, 2010.
Melting temperature, DSC	°C	220-260 (replacement of some ethylene by propylene lowers MP)	
Thermal expansion coefficient, 23-80°C	10^{-4} $°C^{-1}$	1.1	
Thermal conductivity, melt	W m^{-1} K^{-1}	0.27	
Glass transition temperature	°C	13-15	
Specific heat capacity	J K^{-1} kg^{-1}	1,800	
Heat of fusion	J g^{-1}	62.6-73 (melt quenched material); 90.9-97.1 (solution crystallized)	Waddon, A J; Karttunen, N R; Lesser, A J, Macromolecules, 32, 423-28, 1999.
Temperature index (50% tensile strength loss after 20,000 h/5000 h)	°C	90	
Heat deflection temperature at 0.45 MPa	°C	210	
Heat deflection temperature at 1.8 MPa	°C	105	
Vicat temperature VST/A/50	°C	215	
Vicat temperature VST/B/50	°C	205	
Dielectric constant at 1000 Hz/1 MHz	-	5.7/5.2	
Dissipation factor at 1000 Hz	E-4	120	
Dissipation factor at 1 MHz	E-4	400	
Volume resistivity	ohm-m	1E11	
Surface resistivity	ohm	1E14	

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PARAMETER	UNIT	VALUE	REFERENCES
Arc resistance	s	60-120	
Coefficient of friction	-	0.07 (static); 0.49 (dynamic)	Kelley, J W, Antec, 3028-34, 1998.
Permeability to nitrogen, 25°C	cm^3 cm cm^{-3} min^{-1} atm^{-1} x 10^9	1.23	De Nobile, M A; Mensitieri, G; Sommazzi, A, Polymer, 36, 26, 4943-50, 1995.
Permeability to oxygen, 25°C	cm^3 cm cm^{-3} min^{-1} atm^{-1} x 10^9	6.43	De Nobile, M A; Mensitieri, G; Sommazzi, A, Polymer, 36, 26, 4943-50, 1995.
Diffusion coefficient of nitrogen	cm^2 s^{-1} $x10^9$	2.28	De Nobile, M A; Mensitieri, G; Sommazzi, A, Polymer, 36, 26, 4943-50, 1995.
Diffusion coefficient of oxygen	cm^2 s^{-1} $x10^9$	5.6-7.73	Backman, A; Lange, J; Hedenqvist, M S, J. Polym. Sci. B, 42, 947-55, 2004; De Nobile, M A; Mensitieri, G; Sommazzi, A, Polymer, 36, 26, 4943-50, 1995.
Diffusion coefficient of water vapor	cm^2 s^{-1} $x10^9$	29.3	De Nobile, M A; Mensitieri, G; Sommazzi, A, Polymer, 36, 26, 4943-50, 1995.
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	55-63	
Tensile modulus	MPa	1,600-2,300	
Tensile stress at yield	MPa	55-70	
Elongation	%	300-350	
Tensile yield strain	%	17-25	
Flexural strength	MPa	55	
Flexural modulus	MPa	1,600	
Young's modulus	MPa	1,500	
Charpy impact strength, unnotched, 23°C	kJ m^{-2}	NB	
Charpy impact strength, unnotched, -30°C	kJ m^{-2}	NB	
Charpy impact strength, notched, 23°C	kJ m^{-2}	1.8-20	
Charpy impact strength, notched, -30°C	kJ m^{-2}	0.4	
Izod impact strength, unnotched, 23°C	J m^{-1}	NB	
Izod impact strength, notched, 23°C	J m^{-1}	2.4-2.7	
Izod impact strength, notched, -40°C	J m^{-1}	0.5	
Abrasion resistance (ASTM D1044)	mg/1000 cycles	12	
Shore D hardness	-	75	
Rockwell hardness	-	R105	
Shrinkage	%	2-2.1	

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Intrinsic viscosity, 25°C	dl g^{-1}	1.21-2.84	Zuiderduin, W C J; Homminga, D S; Huetink, H J; Gaymans, R J, Polymer, 44, 6361-70, 2003.
Melt index, 240°C/2.16 kg	g/10 min	2.7-80	
Water absorption, equilibrium in water at 23°C	%	2.1	
Moisture absorption, equilibrium 23°C/50% RH	%	0.5	
CHEMICAL RESISTANCE			
Acid dilute/concentrated	-	good	
Alcohols	-	very good	
Alkalis	-	good	
Aliphatic hydrocarbons	-	very good	
Aromatic hydrocarbons	-	very good	
Esters	-	very good	
Greases & oils	-	very good	
Halogenated hydrocarbons	-	very good	
Ketones	-	very good	
FLAMMABILITY			
Limiting oxygen index	% O_2	21	
UL rating	-	HB	
PROCESSING			
Preprocess drying: temperature/ time/residual moisture	°C/h/%	blow molding, electrospinning, extrusion, injection molding, melt spinning	
Processing temperature	°C	240-260; 220-260 (injection)	
Processing pressure	MPa	55 (holding); 40-80 (injection)	
Process time	s	23 (cycle time)	
Applications	-	appliance, automotive, bottles, electrical, fibers, nanofibers, powder coatings, support for enzyme immobilization	
Outstanding properties	-	chemical resistance, fast crystallization, stiffness, toughness	
BLENDS			
Suitable polymers	-	CSR (core-shell rubber), PF, PP, PVC	
ANALYSIS			
FTIR (wavenumber-assignment)	cm^{-1}/-	CH_2 – 1408, 1331, 1261	Ohsawa, O; Lee, K-H; Kim, B-S; Lee, S; Kim, I-S, Polymer, 2007-12, 2010.
Raman (wavenumber-assignment)	cm^{-1}/-	CH_2 – 1260, 1350-1500; C=O – 1710	Lagaron, J M; Powell, A K; Davidson, N S, Macromolecules, 33, 1030-35, 2000.
NMR (chemical shifts)	ppm	C NMR: -CO- – 208.1; -Ph – 139.9, 133.1, 128.5, 16.6, -$CHCH_2$- – 54.2, 45.4 (product of copolymerization of CO and styrene)	Guo, J T; Ye, Y Q; Gao, S; Feng, Y K, J. Molecular Catalysis, 307A, 121-27, 2009.
x-ray diffraction peaks	degree	17.38, 21.75, 24.65, 25.97, 31.47, 37.87, 39.38, 41.84	Ohsawa, O; Lee, K-H; Kim, B-S; Lee, S; Kim, I-S, Polymer, 2007-12, 2010.