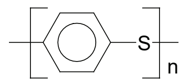
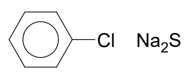
PPS poly(p-phenylene sulfide)

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	poly(p-phenylene sulfide)	
CAS name	-	poly(thio-1,4-phenylene)	
Acronym	-	PPS	
CAS number	-	25212-74-2; 26125-40-6	
Linear formula			
HISTORY			
Person to discover	-	Charles Friedel and James Mason Crafts; Wayne Hill and James Edmonds	
Date	-	1888; 1967, 1972	
Details	-	PPS was discovered by Fridel and Crafts 1888, and method of production was developed by Hill and Edmonds in 1967, and commercialization of PPS by Phillips Petroleum Company in 1972	Fink, J K, High Peformance Polymers, William Andrew, 2008.
SYNTHESIS			
Monomer(s) structure	-		
Monomer(s) CAS number(s)	-	106-46-7; 1313-82-2	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	147. 004; 78.04	
Monomer ratio	-	1.88	
Formulation example	-	reagents, solvent, catalyst, molecular weight modifier	Fink, J K, High Peformance Polymers, William Andrew, 2008.
Method of synthesis	-	PPS is manufactured based on reaction between sodium sulfide and p-dichlorobenzene	Fink, J K, High Peformance Polymers, William Andrew, 2008.
Temperature of polymerization	°C	160-260	
Time of polymerization	h	88	
Catalyst	-	lithium salts, sodium acetate, cyclic amine compounds	Fink, J K, High Peformance Polymers, William Andrew, 2008.
Mass average molecular weight, M_w	dalton, g/mol, amu	12,000-1,400,000	
Polydispersity, M_w/M_n	-	1.4-2.0	
Molar volume at 298K	cm^3 mol^{-1}	75.3 (crystalline)	
Van der Waals volume	cm^3 mol^{-1}	54.1 (crystalline)	
STRUCTURE	-		
Crystallinity	%	40-83	Lu, J; Huang, R; Oh, I-K, Macromol. Chem. Phys., 208, 405-14, 2007.
Cell type (lattice)	-	orthorhombic	Tabor, B J; Magre, E P; Boon, J, Eur. Polym. J., 7, 1127, 1971.
Cell dimensions	nm	a:b:c=0.867:0.561:1.026	Tabor, B J; Magre, E P; Boon, J, Eur. Polym. J., 7, 1127, 1971.
Unit cell angles	degree	$\alpha:\beta:\gamma$=90:90:90	

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Space group	-	Pbcn	Napolitano, R; Pirozzi, B; Iannelli, P, Macromol. Theory Simul., 10, 9, 827-32, 2001.
Tacticity	%	*trans* (100)	
Chain conformation	-	helix 2/1	
Entanglement molecular weight	dalton, g/mol, amu	20,000	
Avrami constant, n	-	1.4-3	Nohara, L B; Nohara, E L; Moura, A; Goncalves, J M R P; Costa, M L; Rezende, M C, Polimeros: Ciencia Tecnologia, 16, 2, 104-110, 2006; D'Ilario, L; Martinelli, A, Eur. Phys. J. E, 19, 37-45, 2006.
Activation energy of molecular motion	kJ mol^{-1}	70 (amorphous); 43 (crystalline)	Jurga, J; Wozniak-Braszak, Fojud, Z; Jurga, K, Solid State Magnetic Resonance, 25, 47-52, 2004.
COMMERCIAL POLYMERS			
Some manufacturers	-	Chevron Phillips; Solvay; Ticona; Toyobo	Fortron, Ticona, May 2007.
Trade names	-	Ryton; Primef; Fortron; Procon (fiber)	
PHYSICAL PROPERTIES			
Density at 20°C	g cm^{-3}	1.34-1.36; 1.425-1.44 (crystalline); 1.32 (amorphous)	
Color	-	white to pale yellow	
Refractive index, 20°C	-	1.83	
Birefringence	-	0.27; 0..3 (theoretical maximum)	
Odor	-	mild	
Melting temperature, DSC	°C	285-295	
Decomposition temperature	°C	450-480; 532	Duan, Y; Cong, P; Liu, X; Li, T, J. Macromol. Sci. B, 48, 604-16, 2009.
Explosion temperature	°C	500	
Thermal expansion coefficient, 23-80°C	$°C^{-1}$	4.9-5.2E5	
Thermal conductivity, melt	W m^{-1} K^{-1}	0.29; 0.20 (40% glass fiber)	
Glass transition temperature	°C	74-92	
Heat of fusion	kJ mol^{-1}	4.5-5.5	
Maximum service temperature	°C	218-232	
Long term service temperature	°C	<240	
Temperature index (50% tensile strength loss after 20,000 h/5000 h)	°C	230	Padey, D; Walling, J; Wood A, Polymers in Defence and Aerospace 2007, Rapra, 2007, paper 15.
Heat deflection temperature at 1.8 MPa	°C	150-263 (depends on mold temperature; 40% glass fiber)	Greer, M R; Reaume, A; Kowalski, G, Antec, 504-8, 2010.
Enthalpy of melting	J g^{-1}	43.1	Nohara, L B; Nohara, E L; Moura, A; Goncalves, J M R P; Costa, M L; Rezende, M C, Polimeros: Ciencia Tecnologia, 16, 2, 104-110, 2006.
Hansen solubility parameters, δ_D, δ_P, δ_H	$MPa^{0.5}$	18.7, 5.3, 3.7	
Interaction radius		6.7	
Hildebrand solubility parameter	$MPa^{0.5}$	19.8	

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Dielectric constant at 100 Hz/1 MHz	-	3.8-5.2/3.8-4.9	
Relative permittivity at 10 kHz	-	2.7-3.2; 4 (40% glass fiber)	
Dissipation factor at 100 Hz	E-4	40-300	
Dissipation factor at 1 MHz	E-4	11; 62 (40% glass fiber)	
Volume resistivity	ohm-m	1E9; >10E13 (40% glass fiber)	
Surface resistivity	ohm	>10E15 (40% glass fiber)	
Electric strength K20/P50, d=0.60.8 mm	kV mm^{-1}	18; 28 (40% glass fiber)	
Comparative tracking index, CTI, test liquid A	-	125	
Arc resistance	s	125-185	
Coefficient of friction	-	0.4 (air); 0.22 (water); 0.6 (40% glass fiber)	Duan, Y; Cong, P; Liu, X; Li, T, J. Macromol. Sci. B, 48, 604-16, 2009.
Contact angle of water, 20°C	degree	80.3	
Surface free energy	mJ m^{-2}	46.8	
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	90; 131-195 (40-65% glass fiber)	
Tensile modulus	MPa	3,800; 14,500-19,100 (40% glass fiber)	
Elongation	%	3-8; 0.9-1.9 (40-65% glass fiber)	
Flexural strength	MPa	125-145; 200-285 (40-65% glass fiber)	
Flexural modulus	MPa	3,750-4,200; 14,500-19,400 (40-65% glass fiber)	
Compressive strength	MPa	112; 260-296 (40-65% glass fiber)	
Charpy impact strength, unnotched, 23°C	kJ m^{-2}	53 (40% glass fiber)	
Charpy impact strength, notched, 23°C	kJ m^{-2}	10 (40% glass fiber)	
Izod impact strength, unnotched, 23°C	J m^{-1}	35-82; 34 (40% glass fiber)	
Izod impact strength, notched, 23°C	J m^{-1}	2.6-3.5; 10 (40% glass fiber)	
Rockwell hardness	-	M90-95; M100 (40% glass fiber)	
Shrinkage	%	1.2-1.8; 0.13-0.7 (40% glass fiber)	Greer, M R; Reaume, A; Kowalski, G, Antec, 504-8, 2010.
Water absorption, equilibrium in water at 23°C	%	0.01-0.03	
CHEMICAL RESISTANCE			
Acid dilute/concentrated	-	very good to fair (nitric acid, see ref.)	Tanthapanichakoon, W; Hata, M; Nitta, K-h; Faruuchi, M; Otani, Y, Polym. Deg. Stab., 91, 2614-21, 2006.
Alcohols	-	very good	
Alkalis	-	very good	
Aliphatic hydrocarbons	-	very good	
Aromatic hydrocarbons	-	very good	
Esters	-	very good	
Greases & oils	-	very good	
Halogenated hydrocarbons	-	good	

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Ketones	-	very good	
Good solvent	-	not soluble below 200°C; above 200°C soluble in 1-chloro-naphthalene and biphenyl	
Non-solvent	-	all solvents below 200°C	
FLAMMABILITY			
Ignition temperature	°C	480-500	
Autoignition temperature	°C	540	
Limiting oxygen index	% O_2	40; 47 (40% glass fiber)	
Char at 500°C	%	41.6	Lyon, R E; Walters, R N, J. Anal. Appl. Pyrolysis, 71, 27-46, 2004.
Heat of combustion	J g^{-1}	28,390-29,620	Walters, R N; Hacket, S M; Lyon, R E, Fire Mater., 24, 5, 245-52, 2000.
Volatile products of combustion	-	CO, CO_2, SO_2, CS	
UL 94 rating	-	V-0	
WEATHER STABILITY			
Spectral sensitivity	nm	290-370	
Activation wavelengths	nm	330	
Excitation wavelengths	nm	300-320; 308	
Emission wavelengths	nm	396; 396	
Products of degradation	-	yellowing, conjugated double bonds, crosslinking, chains scission, carbonyls	
Stabilizers	-	UVA: benzotriazole (derivative of Tinuvin 327 in which chlorine atom is replaced by phenylthio or phenylsulfonyl groups); Screener: carbon black	Das, P K; DesLauriers, P J; Fahey, D R; Wood, F K; Cornforth, F J, Polym. Deg. Stab., 48, 1-10, 1995 and ibid. 11-23.
Effect of exposure	WOM	2,000 h with little change in tensile and impact strength	
TOXICITY			
NFPA: Health, Flammability, Reactivity rating	-	1/0/0	
TLV, ACGIH	mg m^{-3}	3 (respirable), 10 (total)	
OSHA	mg m^{-3}	5 (respirable), 15 (total)	
PROCESSING			
Typical processing methods	-	blending, coating, compression molding, extrusion, injection molding, lamination, thermoforming	
Preprocess drying: temperature/time/residual moisture	°C/h/%	120/1-2 (unfilled); 140/4 (reinforced)	
Processing temperature	°C	300-340 (injection molding); 285-310 (extrusion)	
Processing pressure	MPa	50-110 (injection); 30-70 (holding)	
Additives used in final products	-	Fillers: aramid fiber, calcium carbonate, carbon fiber, ferrosoferric oxide, glass fiber, glass flake, mica, talc, PTFE, zinc oxide; Plasticizers: diphenyl phthalate, hydrogenated terphenyl; Antistatics: carbon nanofiber, expandable graphite, octadecyltriethoxysilane; Other: decolorants; Release, high density polyethylene, silicone	

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Applications	-	aerospace, automotive lighting, carburetor parts, chip carriers, coil bobbins, electrical and electronic parts, food choppers, fuel components, halogen lamp sockets, IC card connectors, ignition and braking systems, impeller diffusers, lamp sockets, magnets, microwave oven components, motor fans, optical drive, phone jacks, oil well valves, plastic housing for a high speed motor, pump housings, relay components, sockets, steam hair drier parts, tape recorder head mounts, technical parts (pumps, automotive, printer components, liquid crystalline display projectors), thermally-conductive materials, transistor encapsulation	
Outstanding properties	-	temperature resistance, chemical resistance, inherently flame retardant, high rigidity	
BLENDS			
Suitable polymers	-	EVA, PA66, PAR, PE, PET, PP, PS	
ANALYSIS			
FTIR (wavenumber-assignment)	cm^{-1}/-	benzene ring – 1574, 1073; SO – 1159, 1320; phenolic group – 3400, more in ref.	Zimmerman, D A; Koenig, J L; Ishida, H, Spectrochim. Acta A51, 2397-2409, 1995.
Raman (wavenumber-assignment)	cm^{-1}/-	C-C – 1574; C-H – 1180, 1074, 840; C-S – 743	Zimmerman, D A; Koenig, J L; Ishida, H, Spectrochim. Acta A51, 2397-2409, 1995.
x-ray diffraction peaks	degree	4.3, 6.2	Langer, L; Billaud, D; Issi, J-P, Solid State Commun., 126, 353-57, 2003.