

PP, syndio syndiotactic-polypropylene

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	polypropylene, syndiotactic	
CAS name	-	1-propene, homopolymer, syndiotactic	
Acronym	-	s-PP	
CAS number	-	26063-22-9	
RTECS number	-	UD1842000	
Formula		$\text{---CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}(\text{CH}_3)\text{---}$	
HISTORY			
Person to discover	-	Natta, G; Corradini, P; Pasquon, I; Pegoraro, M; Peraldo, M	Natta, G; Corradini, P; Pasquon, I; Pegoraro, M; Peraldo, M, US Patent 3,258,455, Montecatini, June 28, 1966.
Date	-	1966	
Details	-	syndiotactic polypropylene	
SYNTHESIS			
Monomer(s) structure	-	$\text{H}_2\text{C}=\text{CHCH}_3$	
Monomer(s) CAS number(s)	-	115-07-1	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	42.08	
Monomer ratio	-	100% and less	
Temperature of polymerization	°C	-78	
Catalyst	-	special class of metallocene, vanadium-based (Natta)	De Rosa, C; Auriemma, F, Prog. Polym. Sci., 31, 145-237, 2006.
Yield	%	100	
Number average molecular weight, M_n	dalton, g/mol, amu	35,000-119,000	
Mass average molecular weight, M_w	dalton, g/mol, amu	87,000-1,190,000	
Polydispersity, M_w/M_n	-	1.29-6.2	
STRUCTURE			
Crystallinity	%	25-63	
Cell type (lattice)	-	orthorhombic	
Cell dimensions	nm	a:b:c=1.45:1.12:0.74 (form I); a:b:c=1.45:0.6:0.74 (form II); a:b:c=0.522:1.117:0.506 (form III)	Yamashita, K; Fujiwara, N; Fujikawa, Y; Nakaoki, T; Chiu, W-Y; Stroeve, P, Polym. Eng. Sci., 49, 740-46, 2009.
Crystallite size	nm	2.7	Arranz-Andres, J; Guevara, J L; Velilla, T; Quijada, R; Benavente, R; Perez, E; Cerrada, M L, Polymer, 46, 12287-97, 2005.
Space group		lbca (form I); C222/1 (form II)	Razavi, Encyclopedia of Materials: Science and Technology, 7708-11, Elsevier, 2008.
Polymorphs	-	I, II, III, IV	De Rosa, C; Auriemma, F, Prog. Polym. Sci., 31, 145-237, 2006.

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Tacticity	%	90.0-96.8 (syndiotactic)	
Chain conformation	-	helical (t2g2)n (I and II); transplanar (t6g2t2g2)n (III and IV); zigzag (tttt) (on stretching)	Bonnet, M; Yan, S; Petermann, J; Zhang, B; Yang, D, J. Mater. Sci., 36, 3, 635-41, 2001; Tian, N; Lv, R; Na, B; Xu, W; Li, Z, J. Phys. Chem. B, 113, 14920-24, 2009.
Entanglement molecular weight	dalton, g/mol, amu	2,700 (metallocene)	
COMMERCIAL POLYMERS			
Some manufacturers	-	Total	
Trade names	-	Polypropylene	
PHYSICAL PROPERTIES			
Density at 20°C	g cm ⁻³	0.88; 0.856 (amorphous); 0.93 (crystalline)	
Color	-	white	
Transmittance	%	91	
Haze	%	2	
Odor	-	odorless	
Melting temperature, DSC	°C	117-156	
Decomposition temperature	°C	260	He, P; Xiao, Y; Zhang, P; Xing, C; Zhu, N; Zhu, X; Yan, D, Polym. Deg. Stab., 88, 473-79, 2005.
Activation energy of thermal degradation	kJ mol ⁻¹	268 (TGA); 269 (IR)	He, P; Xiao, Y; Zhang, P; Xing, C; Zhu, N; Zhu, X; Yan, D, Polym. Deg. Stab., 88, 473-79, 2005.
Glass transition temperature	°C	-15 to 3	
Heat of fusion	kJ mol ⁻¹	4.4-8.2	
Vicat temperature VST/A/50	°C	111	
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	15.2-25.2	
Tensile modulus	MPa	483	
Elongation	%	250-300	
Tensile yield strain	%	10-11	
Flexural modulus	MPa	345	
Izod impact strength, unnotched, 23°C	J m ⁻¹	640	
Shrinkage	%	33-38 (fibers)	Guadagno, L; D'Aniello, C; Naddeo, C; Vittoria, V, Macromolecules, 34, 2512-21, 2001.
Melt index, 230°C/2.16 kg	g/10 min	2-20	
CHEMICAL RESISTANCE			
Acid dilute/concentrated	-	very good	
Alcohols	-	very good	
Alkalis	-	very good	
Aliphatic hydrocarbons	-	fair to poor	
Aromatic hydrocarbons	-	poor	
Esters	-	fair	
Greases & oils	-	good to fair	

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PARAMETER	UNIT	VALUE	REFERENCES
Halogenated hydrocarbons	-	poor	
Ketones	-	good	
⊖ solvent, ⊖-temp.=45, 36°C	-	i-amyl acetate, cyclohexane	
Good solvent	-	chlorinated hydrocarbons, cyclohexane, diethyl ether, toluene	
Non-solvent	-	many polar solvents	
FLAMMABILITY			
Ignition temperature	°C	>200; 93.3 (fibers & yarns)	
Autoignition temperature	°C	570	
Limiting oxygen index	% O ₂	17	
Heat release	kW m ⁻²	101-727 (with flame retardants)	
Char at 500°C	%	0	Lyon, R E; Walters, R N, J. Anal. Appl. Pyrolysis, 71, 27-46, 2004.
Heat of combustion	J g ⁻¹	45,800	
Volatile products of combustion	-	CO, CO ₂ , soot	
UL 94 rating	-	HB; V-0 (flame retarded grades)	
WEATHER STABILITY			
Effect of tacticity	-	sPP is substantially more stable than iPP	Kato, M; Tsuruta, A; Kuroda, S; Osawa, Z, Polym. Deg. Stab., 67, 1-5, 2000.
Effect of exposure	-	300-500 h in Xenotest decrease tensile strength of sPP by 65-90%	Barany, T; Foldes, E; Czigany, T; Karger-Kocsis, J, J. Appl. Polym. Sci., 3462-3469, 2004.
TOXICITY			
NFPA: Health, Flammability, Reactivity rating	-	1/1/0	
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
Mutagenic effect	-	not known	
Teratogenic effect	-	not known	
Reproductive toxicity	-	not known	
TLV, ACGIH	mg m ⁻³	3 (respiratory), 10 (total)	
OSHA	mg m ⁻³	5 (respiratory), 15 (total)	
Oral rat, LD ₅₀	mg kg ⁻¹	>5,000	
Skin rabbit, LD ₅₀	mg kg ⁻¹	>2,000	
PROCESSING			
Typical processing methods	-	extrusion, injection molding, injection blow molding	
Applications	-	fiber, film, impact modifier, medicine, sheet	
Outstanding properties	-	narrow MW, melt strength	
BLENDS			
Suitable polymers	-	EPR, PE, i-PP	

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ANALYSIS			
FTIR (wavenumber-assignment)	cm ⁻¹ /-	1715 – carbonyl; 3420 – OH; more in refs.	He, P; Xiao, Y; Zhang, P; Xing, C; Zhu, N; Zhu, X; Yan, D, Polym. Deg. Stab., 88, 473-79, 2005; Sevegney, M S; Kannan, R M; Siedle, A R; Percha, P A, J. Polym. Sci. B, 43, 439-61, 2005.
NMR (chemical shifts)	ppm	syndiotacticity index – 303-313; planar zigzag – 375; helical – 537, 550, 776; amorphous – 845, 970, 996 and more	Sevegney, M S; Kannan, R M; Siedle, A R; Naik, R; Naik, V M, Vibrational Spectroscopy, 40, 246-56, 2006.
x-ray diffraction peaks	degree	12.2, 15.8, 18.8, 20.6	Razavi, Encyclopedia of Materials: Science and Technology, 7708-11, Elsevier, 2008.