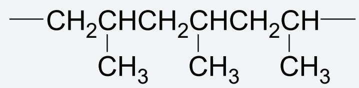
PP, iso isotactic-polypropylene

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	isotactic polypropylene	
CAS name	-	1-propene, homopolymer, isotactic	
Acronym	-	iso-PP	
CAS number	-	25085-53-4	
RTECS number	-	UD1842000	
Formula			
HISTORY			
Person to discover	-	Natta, G; Pino, P; Mazzanti, G	Natta, G; Pino, P; Mazzanti, G, US Patent 3,112,300, Montecatini, Nov. 26, 1963.
Date	-	1963	
Details	-	isotactic polypropylene	
SYNTHESIS			
Monomer(s) structure	-	$H_2C{=}CHCH_3$	
Monomer(s) CAS number(s)	-	115-07-1	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	42.08	
Monomer(s) expected purity(ies)	%	99	
Monomer ratio	-	100% and less	
Formulation example	-	hydrogen is used to control molecular weight	Harding, G W; van Reenen, A J, Eur. Polym. J., 47, 70-77, 2011.
Method of synthesis	-	polymerization carried in the liquid propylene or in a gas-phase reactors	
Temperature of polymerization	^{o}C	40	
Catalyst	-	titanium halide/aluminum alkyl or metallocene	
Number average molecular weight, M_n	dalton, g/mol, amu	5,000-166,000	Fayolle, B; Tchakhtchi, A; Verdu, J, Polym. Testing, 23, 939-47, 2004.
Mass average molecular weight, M_w	dalton, g/mol, amu	158,000-580,000	Fayolle, B; Tchakhtchi, A; Verdu, J, Polym. Testing, 23, 939-47, 2004.
Polydispersity, M_w/M_n	-	1.9-9.7; 3.0-3.9 (metallocene)	Hanyu, A; Wheat, R, J. Plast. Film Sheeting, 15, 2, 109-19, 1999.
Molar volume at 298K	cm^3 mol^{-1}	44.4 (crystalline)	
Van der Waals volume	cm^3 mol^{-1}	30.7 (crystalline)	
Radius of gyration	nm	29.7-30.5	Logotheti, G E; Theodorou, D N, Macromolecules, 40, 2235-45, 2007.
End-to-end distance of unperturbed polymer chain	nm	187-189	Logotheti, G E; Theodorou, D N, Macromolecules, 40, 2235-45, 2007.
STRUCTURE	-		
Crystalline structure			Van der Burgt, F, Crystallization of isotactic polypropylene, Technical University of Eindhoven, 2002.

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PARAMETER	UNIT	VALUE	REFERENCES
Crystallinity	%	29-75; 31-50 (non-spherulitic); 44-67 (non-spherulitic, quenched) 40-57 (spherulitic); 67-69 (uniaxially stretched)	Fayolle, B; Tchakhtchi, A; Verdu, J, Polym. Testing, 23, 939-47, 2004; Mileva, D; Androsch, R; Radusch, H-J, Polym. Bull., 62, 561-71, 2009; Hedesiu, C; Demco, D E; Remerie, K; Bluemich, B; Litvinov, V M, Macromol. Chem. Phys., 209, 734-45, 2008.
Cell type (lattice)	-	monoclinic (α), hexagonal (β), orthorhombic or triclinic (γ; the most thermodynamically stable)	Chen, J-H; Tsai, F-C; Nien, Y-H; Yeh, P-H, Polymer, 46, 5680-88, 2005.
Cell dimensions	nm	a:b:c=0.639:2.044:0.647 (monoclinic); a:b:c=0.854:0.993:4.241 (orthorhombic); a:b:c=0.655:2.157:0.655 (triclinic)	
Unit cell angles	degree	α:β:γ=90:99.2:90 (monoclinic); α:β:γ=90:90:90 (orthorhombic); α:β:γ=97.4:98.8:97.4	
Crystallite size	nm	3.97-6.36 (α); 4-8 (oriented)	Romanos, N A; Theodorou, D N, Macromolecules, 43, 5455-69, 2010; Kang, Y-A; Kim, K-H; Ikehata, S; Ohhoshi, Y; Gotoh, Y; Nagura, M; Urakawa, H, Polymer, 52, 2044-50, 2011.
Polymorphs	-	α, β (metastable), γ	Zhao, S; Xin, Z, J. Polym. Sci. B, 48, 653-65, 2010.
Beta-crystallinity, K value vs. cast roll temperature	-/ºC	0.35/60, 0.78/90, 0.85/104	Kim, S; Townsend, E B, Antec, 2002.
Tacticity	%	90.5-99.5 (isotactic)	Capt, L; Kamal, M R; Rettenberger, S; Muenstedt, H, Antec, 997-1001, 2003; Harding, G W; van Reenen, A J, Eur. Polym. J., 47, 70-77, 2011.
Chain conformation	-	helix, 3/1	
Entanglement molecular weight	dalton, g/mol, amu	6,900 (metallocene)	
Lamellae thickness	nm	15.1-18.5	White, H M; Bassett, D C; Jaaskelainen, P, Polymer, 50, 5559-64, 2009.
Heat of crystallization	kJ kg^{-1}	83.7	Chen, J-H; Tsai, F-C; Nien, Y-H; Yeh, P-H, Polymer, 46, 5680-88, 2005.
Rapid crystallization temperature	ºC	138-144	Pantani, R; Coccorullo, I; Volpe, V; Titomanlio, G, Macromolecules, 43, 9030-38, 2010.
Avrami constants, k/n	-	n=2-3 for monoclinic and 0.45-0.55 for mesomorphic	La Carrubba, V; Piccarolo, S; Brucato, V, J. Appl. Polym. Sci., 104, 1358-67, 2007.
Crystallization activation energy	J mol^{-1}	211.1-316.6	Zhao, S; Xin, Z, J. Polym. Sci. B, 48, 653-65, 2010.
Crystal growth rate	$\mu m\ s^{-1}$	0.1-0.8	Pantani, R; Coccorullo, I; Volpe, V; Titomanlio, G, Macromolecules, 43, 9030-38, 2010.
COMMERCIAL POLYMERS			
Some manufacturers	-	Atofina; Daelin; LyondellBasell; Sunoco	
Trade names	-	Fiinacene; Polypropylene; Moplen; Polypropylene	
PHYSICAL PROPERTIES			
Density at 20ºC	g cm^{-3}	0.90-0.91	
Color	-	white	
Refractive index, 20ºC	-	1.4900-1.503	

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PARAMETER	UNIT	VALUE	REFERENCES
Transmittance	%	60-90 (quenched); 50-65 (slowly cooled)	Mileva, D; Androsch, R; Radusch, H-J, Polym. Bull., 62, 561-71, 2009.
Haze	%	0.3; 0.2-0.9 (biaxially oriented, metallocene)	Hanyu, A; Wheat, R, J. Plast. Film Sheeting, 15, 2, 109-19, 1999.
Gloss, 60°, Gardner (ASTM D523)	%	99; 94-98 (biaxially oriented, metallocene)	
Odor	-	odorless	
Melting temperature, DSC	°C	157-171; 151-166 (commercial); 148-151 (biaxially oriented, metallocene)	Hanyu, A; Wheat, R, J. Plast. Film Sheeting, 15, 2, 109-19, 1999.
Softening point	°C	155-156	
Decomposition temperature	°C	240	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}	265 (TGA); 254 (IR)	He, P; Xiao, Y; Zhang, P; Xing, C; Zhu, N; Zhu, X; Yan, D, Polym. Deg. Stab., 88, 473-79, 2005.
Thermal expansion coefficient, 23-80°C	$°C^{-1}$	1.1-1.4E-4; 6.6E-4 (melt)	
Thermal conductivity, melt	W m^{-1} K^{-1}	0.12-0.22	
Glass transition temperature	°C	-10	
Specific heat capacity	J K^{-1} kg^{-1}	2,500-3,400 (depending on annealing temperature)	Zia, Q; Radusch, H-J; Androsch, R, Polymer, 48, 3504-11, 2007.
Heat of fusion	kJ kg^{-1}	177	Masirek, R; Piorkowska, E, Eur. Polym. J., 46, 1436-45, 2010.
Heat deflection temperature at 0.45 MPa	°C	88-107	
Heat deflection temperature at 1.8 MPa	°C	55	
Vicat temperature VST/A/50	°C	150-155	
Hildebrand solubility parameter	$MPa^{0.5}$	17.2-18.8	
Surface tension	mN m^{-1}	20.2-22.5	
Dielectric constant at 100 Hz/1 MHz	-	2.2-2.3	
Dissipation factor at 100 Hz		0.0003-0.001	
Dissipation factor at 1 MHz		0.0001-0.0003	
Volume resistivity	ohm-m	1E14 to 1E15	
Permeability to oxygen, 25°C	cm^3 m^{-2} day^{-1}	2,600; 2,300-2,900 (biaxially oriented, metallocene)	
Permeability to water vapor, 25°C	cm^3 m^{-2} day^{-1}	3.4; 2.6-3.2 (biaxially oriented, metallocene)	
Contact angle of water, 20°C	degree	116	
Speed of sound	m s^{-1}	2100-125000	
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	30 (commercial); 130 (MD, biaxially stretched); 300 (TD, biaxially stretched); 185-219 (equibiaxially stretched); 140-160 (MD; metallocene); 250-300 (TD; metallocene)	Capt, L; Kamal, M R; Rettenberger, S; Muenstedt, H, Antec, 997-1001, 2003; Hanyu, A; Wheat, R, J. Plast. Film Sheeting, 15, 2, 109-19, 1999.
Tensile modulus	MPa	825 (commercial); 910 (alpha-form); 820 (beta-form)	Mezghani, K S; Gasem, Z; Faheem, M, antec, 2884-91, 2004.
Tensile stress at yield	MPa	33-36	

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PARAMETER	UNIT	VALUE	REFERENCES
Elongation	%	90-500; 100-119 (equibiaxially stretched); 120-170 (MD; biaxially oriented, metallocene); 40-60 (TD; biaxially oriented, metallocene)	Capt, L; Kamal, M R; Rettenberger, S; Muenstedt, H, Antec, 997-1001, 2003; Hanyu, A; Wheat, R, J. Plast. Film Sheeting, 15, 2, 109-19, 1999.
Tensile yield strain	%	10-12	
Flexural strength	MPa	38.9	
Flexural modulus	MPa	1,150-1,570	
Elastic modulus	MPa	2,357-3,450 (equibiaxially stretched)	Capt, L; Kamal, M R; Rettenberger, S; Muenstedt, H, Antec, 997-1001, 2003; Hanyu, A; Wheat, R, J. Plast. Film Sheeting, 15, 2, 109-19, 1999.
Izod impact strength, unnotched, 23°C	$J\ m^{-1}$	33.8; 30.9-74.0 (nucleated)	Zhao, S; Xin, Z, J. Polym. Sci. B, 48, 653-65, 2010.
Izod impact strength, notched, 23°C	$J\ m^{-1}$	25-39	
Poisson's ratio	-	0.38	
Rockwell hardness	-	R95-105	
Shrinkage	%	7; (MD); 10 (TD); 4-11 (MD; biaxially oriented, metallocene); 8-21 (TD; biaxially oriented, metallocene)	
Melt viscosity, shear rate=0 s^{-1}	kPa s	2.9-9.9	
Melt index, 230°C/2.16 kg	g/10 min	1.9-31	
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	
Halogenated hydrocarbons	-	poor	
Ketones	-	good	
Θ solvent, Θ-temp.=122, 206, 142.8, 184°C	-	n-butyl alcohol, p-cresol, diphenyl ether, p-ethyl phenol	
Good solvent	-	1,2,4-trichlorobenzene, decalin, halogenated hydrocarbons, aliphatic ketones, xylene (all above 80°C)	
Non-solvent	-	most common 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 rating	-	HB; V-0 (flame retarded grades)	

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PARAMETER	UNIT	VALUE	REFERENCES
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.
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	-	blown film, extrusion, injection molding	
Additives used in final products	-	antiblocking; slip; antioxidant; nucleating agent	
Applications	-	bags, fibers, film, food packaging	
Outstanding properties	-	clarity, stiffness	
BLENDS			
Suitable polymers	-	EPR, HDPE, PA66, PB, PET, s-PP, PS	
ANALYSIS			
FTIR (wavenumber-assignment)	cm^{-1}/-	isotactic sequences of different length – 808, 841, 900, 973, 998	Li, L; Liu, T; Zhao, L; Yuan, W-k, J. Supercritical Fluids, in press, 2011.
NMR (chemical shifts)	ppm	pentad sequence content determined by C NMR	Harding, G W; van Reenen, A J, Eur. Polym. J., 47, 70-77, 2011.
x-ray diffraction peaks	degree	α-form: 14.08, 16.95, 18.5, 21.2, 21.85 (other forms see reference)	Chen, J-H; Tsai, F-C; Nien, Y-H; Yeh, P-H, Polymer, 46, 5680-88, 2005.