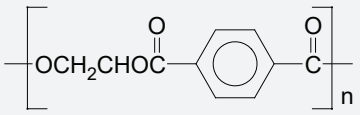
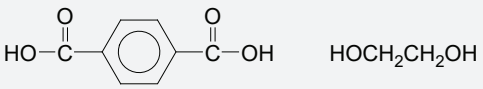
PET poly(ethylene terephthalate)

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	poly(ethylene terephthalate)	
IUPAC name	-	poly(ethylene terephthalate)	
ACS name	-	poly(oxy-1,2-ethanediyloxycarbonyl-1,4-phenylenecarbonyl)	
Acronym	-	PET	
CAS number	-	25038-59-9	
Linear formula			
HISTORY			
Person to discover	-	Whinfield, R J and Dickson, T J	Whinfield, R J and Dickson, T J, US Patent 2,465,319, DuPont, Mar. 22, 1949.
Date	-	1949	
Details	-	first patented by DuPont	
SYNTHESIS			
Monomer(s) structure	-		
Monomer(s) CAS number(s)	-	100-21-0; 107-21-1	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	166.13; 62.07	
Monomer ratio	-	2.676 (72.8:27.2)	
Method of synthesis	-	several processes can be used, including: transesterification, direct esterification, and polycondensation	
Mass average molecular weight, M_w	dalton, g/mol, amu	19,000-66,000; 29,800-45,800 (recycled)	Romao, W; Freanco, M FF; Bueno, M I M S; De Paoli, M-A, Polym. Test., 29, 879-85, 2010.
Molar volume at 298K	cm^3 mol^{-1}	calc.=146.1; 130 (crystalline); 144.5 (amorphous)	
Van der Waals volume	cm^3 mol^{-1}	calc.=96.36; 94.2 (crystalline); 94.2 (amorphous)	
Molecular cross-sectional area, calculated	cm^2 x 10^{-16}	14.0	
STRUCTURE	-		
Crystallinity	%	20-50, 52.5-54.6 (fiber); 85 (oriented film)	Romaao, W; Franco, M F; Corilo, Y E; Ebrlin, M N; Spinace, M A S; De Paoli, M-A, Polym. Deg. Stab., 94, 1849-59, 2009; Blundell, D J; Mahendrasingam, A; Martin, C; Fuller, W; MacKerron, D H; Harvie, J L; Oldman, R J; Riekel, C, Polymer, 41, 7793-7802, 2000.
Cell type (lattice)	-	triclinic	
Cell dimensions	nm	a:b:c=0.448-0.456:0.58-0.594:1.071-1.086	
Unit cell angles	degree	α:β:γ=98-107:118-119:111-112	Kinoshita, Y; Nakamura, R; Kitano, Y; Ashida, T, Polym. Prep., 20, 454, 1979.
Number of chains per unit cell	-	1	

PET poly(ethylene terephthalate)

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Crystallite size	nm	27.8-40.8 (fiber)	
Chain conformation	-	nearly planar	
Entanglement molecular weight	dalton, g/mol, amu	1,936	Barany, T; Czigany, T; Karger-Kotsis, J, Prog. Polym. Sci., 35, 1257-87, 2010.
Crystallization temperature	°C	164	Romaao, W; Franco, M F; Corilo, Y E; Ebrlin, M N; Spinace, M A S; De Paoli, M-A, Polym. Deg. Stab., 94, 1849-59, 2009.
Avrami constants, k/n	-	n=2.4-2.7	Lu, X F; Hay, J N, Polymer, 42, 9423-31, 2001.
COMMERCIAL POLYMERS			
Some manufacturers	-	DuPont; Sabic	
Trade names	-	Rynite; PET	
PHYSICAL PROPERTIES			
Density at 20°C	g cm^{-3}	1.3-1.4; 1.455 (crystalline); 1.333 (amorphous); 1.47-1.81 (20-55% glass fiber)	
Bulk density at 20°C	g cm^{-3}	0.795-0.88	
Color	-	white to gray	
Refractive index, 20°C	-	calc.=1.5392-1.5557; exp=1.5750	
Birefringence	-	0.0469 (fiber)	Romaao, W; Franco, M F; Corilo, Y E; Ebrlin, M N; Spinace, M A S; De Paoli, M-A, Polym. Deg. Stab., 94, 1849-59, 2009.
Haze	%	0.6	
Odor	-	none	
Melting temperature, DSC	°C	245-265; 254 (20-55% glass fiber)	
Decomposition temperature	°C	285-329	
Storage temperature	°C	<50	
Thermal expansion coefficient, -40 to 160°C	$°C^{-1}$	1.7E-5 (film); 6.55E-4 (melt); 1.1-9.5E-5 (20-55% glass fiber)	Mark, H F; Gaylord, N G, Encyclopedia of Polymer Science, Vol. 11, Interscience, New York, 1969.
Thermal conductivity, melt	W m^{-1} K^{-1}	calc.=0.1888; exp.=0.147 (melt); 0.29-0.33 (20-55% glass fiber)	
Glass transition temperature	°C	calc.=76-88; exp.=60-85; 60-76 (amorphous)	
Specific heat capacity	J K^{-1} kg^{-1}	1,170	
Heat of fusion	kJ mol^{-1}	24.1	
Maximum service temperature	°C	-60 to 105	
Temperature index (50% tensile strength loss after 20,000 h/5000 h)	°C	140 (20-55% glass fiber)	
Heat deflection temperature at 0.45 MPa	°C	63.9; 240-248 (20-55% glass fiber)	
Heat deflection temperature at 1.8 MPa	°C	61.1; 210-229 (20-55% glass fiber)	
Vicat temperature VST/B/50	°C	77	
Enthalpy of melting	J g^{-1}	27	Romaao, W; Franco, M F; Corilo, Y E; Ebrlin, M N; Spinace, M A S; De Paoli, M-A, Polym. Deg. Stab., 94, 1849-59, 2009.

PET poly(ethylene terephthalate)

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Hansen solubility parameters, δ_D, δ_P, δ_H	$MPa^{0.5}$	18.7, 6.3, 6.7	
Interaction radius		6.5	
Hildebrand solubility parameter	$MPa^{0.5}$	calc.=14.65-17.15; exp.=17.1-20.8	
Surface tension	mN m^{-1}	calc.=38.7-47.3; exp.=39.5-42.1	
Dielectric constant at 100 Hz/1 MHz	-	3.0-3.3/3.2-3.3; 3.2-4.0/3.0-3.9 (20-55% glass fiber)	
Dissipation factor at 100 Hz	E-4	20-25; 50-100 (20-55% glass fiber)	
Dissipation factor at 1 MHz	E-4	30; 110-150 (20-55% glass fiber)	
Volume resistivity	ohm-m	1E13; 1E13 (20-55% glass fiber)	
Surface resistivity	ohm	1E14 (20-55% glass fiber)	
Electric strength K20/P50, d=0.60.8 mm	kV mm^{-1}	22-26; 24.5-25.5 (20-55% glass fiber)	
Comparative tracking index, CTI, test liquid A	-	175-400	
Arc resistance	s	120-360	
Power factor	-	0.019	
Coefficient of friction	-	0.45 (film to film); 0.17-0.21 (20-55% glass fiber, self); 0.14 (film to steel); 0.17-0.20 (20-55% glass fiber, steel)	
Permeability to oxygen, 25°C	m^3 m m^{-2} s^{-1} Pa^{-1} x 10^{18}	0.4	Colomiones, G; Ducruet, V; Courgneau, C; Guinault, A; Domenek, S, Polym. Int., 59, 818-26, 2010.
Permeability to water vapor, 25°C	cm^3 cm cm^{-2} s^{-1} Pa^{-1} x 10^{12}	11.3	
Contact angle of water, 20°C	degree	72.0-75.0	Donelli, I; Freddi, G; Niefstrasz, V A; Taddei, Polym. Deg. Stab., 95, 1542-50, 2010.
Surface free energy	mJ m^{-2}	44.0	
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	24-41.4; 590 (fiber); 114-189 (20-55% glass fiber)	
Tensile modulus	MPa	2,300; 7,240-17,900 (20-55% glass fiber)	
Tensile stress at yield	MPa	36.5-62.7; 327 (fiber)	
Elongation	%	100-250; 1.6-2.3 (20-55% glass fiber)	
Tensile yield strain	%	4	
Flexural strength	MPa	68.9-78; 172-290 (20-55% glass fiber)	
Flexural modulus	MPa	1,560-2,650; 6,480-17,900 (20-55% glass fiber)	
Compressive strength	MPa	80; 172-241 (20-55% glass fiber)	
Young's modulus	MPa	2,000-2,700	
Izod impact strength, notched, 23°C	J m^{-1}	640	
Izod impact strength, notched, -30°C	J m^{-1}	190	
Shear strength	MPa	79.0-86.5 (20-55% glass fiber)	
Tenacity (fiber) (standard atmosphere)	cN tex^{-1} (daN mm^{-2})	25-95 (35-130)	Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.

PET poly(ethylene terephthalate)

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Tenacity (wet fiber, as % of dry strength)	%	95-100	Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.
Fineness of fiber (titer)	dtex	0.6-44	Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.
Length (elemental fiber)	mm	38-200, filament	Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.
Abrasion resistance (ASTM D1044)	mg/1000 cycles	30-44	
Poisson's ratio	-	0.421-0.430; 0.39-0.41 (20-55% glass fiber)	
Rockwell hardness	-	R110; M95-100 (20-55% glass fiber); R120 (20-55% glass fiber)	
Shrinkage	%	0.7-1.2; 0.18-0.35 (20-55% glass fiber, flow); 0.7-0.9 (20-55% glass fiber, transverse)	
Intrinsic viscosity, 25°C	dl g^{-1}	0.75-0.84	
Melt index, 230°C/3.8 kg	g/10 min	7	
Water absorption, 24h at 23°C	%	0.04-0.14 (24 h); 0.6 (eq)	
Moisture absorption, equilibrium 23°C/50% RH	%	0.35	
CHEMICAL RESISTANCE			
Acid dilute/concentrated	-	good/fair	
Alcohols	-	good/fair	
Alkalis	-	poor	
Aliphatic hydrocarbons	-	good	
Aromatic hydrocarbons	-	good	
Esters	-	fair-poor	
Greases & oils	-	good	
Halogenated hydrocarbons	-	poor	
Ketones	-	fair	
Good solvent	-	DMSO (hot), halogenated aliphatic carboxylic acids, nitrobenzene, phenol	
Non-solvent	-	aliphatic alcohols, carboxylic esters, chlorinated hydrocarbons, ether, hydrocarbons, ketones	
FLAMMABILITY			
Ignition temperature	°C	390	
Autoignition temperature	°C	508	
Limiting oxygen index	% O_2	20-23; 20 (20-55% glass fiber)	
Char at 500°C	%	5.1	Lyon, R E; Walters, R N, J. Anal. Appl. Pyrolysis, 71, 27-46, 2004.
Heat of combustion	J g^{-1}	24,130	Walters, R N; Hacket, S M; Lyon, R E, Fire Mater., 24, 5, 245-52, 2000.
Volatile products of combustion	-	CO, CO_2, acrolein, formaldehyde, ethanol, methanol, acetic acid, acetone	
UL rating	-	HB (20-55% glass fiber); V-0 (20-55% glass fiber and flame retardant)	

PET poly(ethylene terephthalate)

PARAMETER	UNIT	VALUE	REFERENCES
WEATHER STABILITY			
Spectral sensitivity	nm	290-325; 270-325	Yang, J; Xia, Z; Kong, F; Ma, X, Polym. Deg. Stab., 95, 53-8, 2010.
Activation wavelengths	nm	305, 325	
Excitation wavelengths	nm	280, 320, 344, 357; 300 and 330	Yang, J; Xia, Z; Kong, F; Ma, X, Polym. Deg. Stab., 95, 53-8, 2010.
Emission wavelengths	nm	370, 389, 405, 425, 460; 328 and 387+460	Yang, J; Xia, Z; Kong, F; Ma, X, Polym. Deg. Stab., 95, 53-8, 2010.
Important initiators and accelerators	-	ferrocene, cobalt octoates and naphthenates, compounds containing aromatic keto-ester groups	
Products of degradation	-	radicals, crosslinks, hydroperoxides, hydroxyl and carbonyl groups, CO, CO_2	
Stabilizers	-	UVA: 2-hydroxy-4-octyloxybenzophenone; 2-hydroxy-4-methoxybenzophenone; 2,4-dihydroxybenzophenone; 2,2',4,4'-tetrahydroxybenzophenone; 2,2'-dihydroxy-4-methoxybenzophenone; 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-(2H-benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl) phenol; 2,4-di-tert-butyl-6-(5-chloro-2H-benzotriazole-2-yl)-phenol; 2-(3-sec-butyl-5-tert-butyl-2-hydroxyphenyl) benzotriazole; 2-[4-[(2-hydroxy-3-(2'-ethyl)hexyl)oxy]-2-hydroxyphenyl]-4,6-bis(2,4-dimethylphenyl)-1,3,5-triazine; 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; (2-ethylhexyl)-2-cyano-3,3-diphenylacrylate; 1,3-bis-[(2'-cyano-3',3'-diphenylacryloyl)oxy]-2,2-bis-{[(2'-cyano-3',3'-diphenylacryloyl)oxy]methyl}-propane; propane-dioic acid, [(4-methoxyphenyl)-methylene]-dimethyl ester; 2,2'-(1,4-phenylene)bis[4H-3,1-benzoxazin-4-one]; Screener: carbon black, zinc oxide; Acid scavenger: hydrotalcite; HAS: 1,3,5-triazine-2,4,6-triamine, N,N'''[1,2-ethane-diyl-bis[[[4,6-bis[butyl(1,2,6,6-pentamethyl-4-piperidinyl)amino]-1,3,5-triazine-2-yl]imino]-3,1-propanediyl]bis[N',N''-dibutyl-N',N''-bis(1,2,2,6,6-pentamethyl-4-piperidinyl)-; decanedioic acid, bis(2,2,6,6-tetramethyl-1-(octyloxy)-4-piperidinyl)ester, reaction products with 1,1-dimethylethylhydroperoxide and octane; bis(1,2,2,6,6-pentamethyl-4-piperidyl)sebacate + methyl-1,2,2,6,6-pentamethyl-4-piperidyl sebacate; alkenes, C20-24-. alpha.-, polymers with maleic anhydride, reaction products with 2,2,6,6-tetramethyl-4-piperidinamine; 1, 6-hexanediamine, N, N'-bis(2,2,6,6-tetramethyl-4-piperidinyl)-, polymers with 2,4-dichloro-6-(4-morpholinyl)-1,3,5-triazine; 1,6-hexanedi-amine, N,N'-bis(2,2,6,6-tetramethyl-4-piperidinyl)-, polymers with morpholine-2,4,6-trichloro-1,3,5-triazine reaction products, methylated; Phenolic antioxidants: ethylene-bis(oxyethylene)-bis(3-(5-tert-butyl-4-hydroxy-m-tolyl)-propionate); N,N'-hexane-1,6-diylbis(3-(3,5-di-tert-butyl-4-hydroxy-phenylpropionamide)); 3,3',3',5, 5',5'-hexa-tert-butyl-a,a',a'-(mesitylene-2,4,6-triyl)tri-p-cresol; 1,3,5-tris(3,5-di-tert-butyl-4-hydroxybenzyl)-1,3,5-triazine-2,4,6(1H,3H,5H)- trione; Phosphite: bis-(2,4-di-t-butylphenol) pentaerythritol diphosphite; tris (2,4-di-tert-butylphenyl)phosphite; phos-phoric acid, (2,4-di-butyl-6-methylphenyl)ethylester; distearyl pentaerythritol diphosphite; Optical brightener: 2,2'-(2,5-thio-phenediyl)bis(5-tert-butylbenzoxazole)	

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PARAMETER	UNIT	VALUE	REFERENCES
BIODEGRADATION			
Typical biodegradants	-	abiotic hydrolysis is the most important reaction for initiating the environmental degradation of poly(ethylene terephthalate). Also cutinases and carboxylesterases have both shown the potential to hydrolyze polyester bonds similarly to lipases	Donelli, I; Freddi, G; Niefstrasz, V A; Taddei, Polym. Deg. Stab., 95, 1542-50, 2010.
Stabilizers	-	2,4,4'-trichloro-2'-hydroxydiphenyl ether, N-hexyl-N'-(4-vinylbenzyl)-4,4'-bipyridinium bromide chloride	
TOXICITY			
HMIS: Health, Flammability, Reactivity rating	-	1/1/0	
Carcinogenic effect		not listed by ACGIH, NIOSH, NTP	
Oral rat, LD_{50}	mg kg^{-1}	>10,000	
ENVIRONMENTAL IMPACT			
Cradle to grave non-renewable energy use	MJ/kg	69.7-85.5	
Cradle to pellet greenhouse gasses	kg CO_2 kg^{-1} resin	2.5-3.5	
PROCESSING			
Typical processing methods	-	blow molding, extrusion, injection blow molding, injection molding, monofilament extrusion	
Preprocess drying: temperature/time/residual moisture	°C/h/%	110-175/2-16/0.003-0.02	
Processing temperature	°C	260-300	
Additives used in final products	-	Fillers: antimony doped tin oxide, aramid, carbon black, carbon fiber, clays, fly ash, glass fiber, glass spheres, mica, montmorillonite, multiwalled carbon nanotubes, silica, talc, titanium dioxide, wollastonite; Antistatics: antimony-doped tin oxide, carbon nanotubes, polyaniline, polyisonaphthalene; Antiblocking: calcium carbonate, diatomaceous earth, silicone fluid, spherical silicone resin, synthetic silica; Release: calcium stearate, fluorine compounds, glycerol bistearate, pentaerythritol ester, silane modified silica, zinc stearate; Slip: spherical silica, silicone oil	
Applications	-	automotive, bottles, brush bristles, composites, electrical, fiber, film, housings, housewares, lighting, medical (orthopaedic bandages, artificial kindneys, sutrures, artificial tendons, cardioviscular implants), motor parts, packaging, plumbing, power tools, sporting goods, support brackets, textiles	
Outstanding properties	-	high strength, stiffness, excellent, dimensional stability, outstanding chemical, excellent flow characteristics, and heat resistance, and good electrical properties	
ANALYSIS			
FTIR (wavenumber-assignment)	cm^{-1}/-	detailed assignment for amorphous and crystalline in ref.	Donelli, I; Freddi, G; Niefstrasz, V A; Taddei, Polym. Deg. Stab., 95, 1542-50, 2010.
NMR (chemical shifts)	ppm	H NMR: terephthalic acid – 4.80; ethylene glycol – 8.13; isophthalic acid – 8.71, 8.29, 7.60; diethylene glycol – 4.64, 4.13	Romaao, W; Franco, M F; Corilo, Y E; Ebrlin, M N; Spinace, M A S; De Paoli, M-A, Polym. Deg. Stab., 94, 1849-59, 2009.
x-ray diffraction peaks	degree	21.3	Sun, B; Lu, Y; Ni, H; Wang, C, Polymer, 39, 1, 159-63, 1998.