

# PAN polyacrylonitrile

PARAMETER	UNIT	VALUE	REFERENCES
<b>GENERAL</b>			
Common name	-	polyacrylonitrile	
IUPAC name	-	polyacrylonitrile	
ACS name	-	2-propenenitrile, homopolymer	
Acronym	-	PAN	
CAS number	-	25014-41-9; 63908-52-1	
EC number	-	not available	
RTECS number	-	AT6977900	
Linear formula		$(C_3H_3N)_n$	
<b>HISTORY</b>			
Person to discover	-	Herbert Rein (1920, first synthesis); 1942, spinning from dimethylformamide (DuPont chemist Ray Houtz in 1942, used dimethylacetamide for production of spinning solution, which was the base of Orlon production in DuPont)	
Date	-	1920	
Details	-	The name Orlon® has been trademarked by the DuPont company, discovered by a scientist (Ray C. Houtz) working with rayon. Production of the trademarked material began in 1950.	
<b>SYNTHESIS</b>			
Monomer(s) structure	-	$CH_2=CHCN$	
Monomer(s) CAS number(s)	-	107-13-1	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	53.06	
Monomer(s) expected purity(ies)	%	min 99	
Monomer content	%	85-100; 100% - pure PAN; 100-85% - Dralon, Orlon, Acrilan; <85 - modacrylics	
Comonomers		acrylic acid methylester, itaconic acid, methacrylic acid ethyl-ester, styrene, vinyl acetate, vinyl chloride	
Method of synthesis	-	chain growth polymerization (the chain-growth reaction occurs in several steps, including initiation, propagation, and termination). Acrylic fiber is commercially produced by free radical polymerization, initiated by a redox system. Industrial production of polyacrylonitrile is a variant of aqueous dispersion polymerization, which takes place in homogenous phase under isothermal conditions	Long, T E; McGrath, J E; Turner, S R, Encyclopedia of Physical Science and Technology, Elsevier, 2004, 751-74; Atasoy, I; Yuceer, M; Berber, R, Comp. Aided Chem. Eng., 21, 1617-22, 2006.
Temperature of polymerization	°C	50 (emulsion polymerization)	
Yield	%	>90% (emulsion polymerization)	
Activation energy of polymerization	J g <sup>-1</sup>	426 (water), 292 (DMF)	Dainton, F S; Eaton, R S, J. Polym. Sci., 39, 313, 1959; Rabel, W, Ueberreiter, Ber. Bunsenges., 67, 710, 1963
Heat of polymerization	J g <sup>-1</sup>	1450	Joshi, R M, J. Polym. Sci., 56, 313, 1962.
Number average molecular weight, $M_n$	dalton, g/mol, amu	30,000-40,000	
Mass average molecular weight, $M_w$	dalton, g/mol, amu	30,000-230,000; 80,000-100,000 (fiber)	Long, T E; McGrath, J E; Turner, S R, Encyclopedia of Physical Science and Technology, Elsevier, 2004, 751-74.
Polydispersity, $M_w/M_n$	-	1.1-3.5	
Polymerization degree (number of monomer units)	-	700	

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PARAMETER	UNIT	VALUE	REFERENCES
<b>Molar volume at 298K</b>	cm <sup>3</sup> mol <sup>-1</sup>	calc.=45.1-47.7; 41.5 (crystalline); exp.=41.8-44.8	
<b>Van der Waals volume</b>	cm <sup>3</sup> mol <sup>-1</sup>	32.2; 30.7 (crystalline)	
<b>Radius of gyration</b>	nm	1.6-2.3	Karanikas, S; Economou, I G, Eur. Polym. J., 47, 735-45, 2011.
<b>End-to-end distance of unperturbed polymer chain</b>	nm	3.1-5.4	Karanikas, S; Economou, I G, Eur. Polym. J., 47, 735-45, 2011.
<b>STRUCTURE</b>			
<b>Crystallinity</b>	%	18.5-45; 60 (fiber)	Qian, B; Lin, W, J. Polym. Eng., 15, 327, 1995; Esrafilzadeh, D; Morshed, M; Tavanai, H, Synthetic Metals, 159, 267-72, 2009; Jung, B; Yoon, J K; Kim, B; Rhee, H-W, J. Membrane Sci., 246, 67-76, 2005.
<b>Crystalline structure</b>	-	orthorhombic; pseudo-hexagonal; hexagonal	
<b>Cell dimensions</b>	nm	a:b:c=1.055:0.58:0.508; a:b:c=2.148:1.155:0.7096; a:b=1.036:0.598 (hexagonal)	Kobayashi, H J, J. Polym. Sci., B1, 209, 1963; Colvin, B G; Storr, P, Eur. Polym. J., 10, 337, 1974; Allen, R A; Ward, I M; Bashir, Z, Polymer, 35, 10, 2063-71, 1994
<b>Unit cell angles</b>	degree	$\alpha$ : $\beta$ : $\gamma$ =90:90:90; $\alpha$ : $\beta$ : $\gamma$ =90:90:90	
<b>Crystallite size</b>	nm	4.35-7.8; 30.3 (fiber)	Qian, B; Lin, W, J. Polym. Eng., 15, 327, 1995; Esrafilzadeh, D; Morshed, M; Tavanai, H, Synthetic Metals, 159, 267-72, 2009.
<b>Polymorphs</b>	-	hexagonal, orthorhombic	
<b>Tacticity</b>	%	isotactic: 25-29, heterotactic: 47-51, and syndiotactic: 22-27 in radical polymerization; syndiotactic (mainly orthorhombic), isotactic (tetragonal)	
<b>Chain conformation</b>	-	helix	
<b>Entanglement molecular weight</b>	dalton, g/mol, amu	calculated: 1,412-3,486	
<b>Lamellae thickness</b>	nm	11-13	Gohil, R M; Patel, K C; Patel, R D, Polymer, 15, 402-6, 1974.
<b>Heat of crystallization</b>	kJ kg <sup>-1</sup>	22.8	
<b>Rapid crystallization temperature</b>	°C	110-130	
<b>Avrami constants, k/n</b>	-	1.634-1.648	Esrafilzadeh, D; Morshed, M; Tavanai, H, Synthetic Metals, 159, 267-72, 2009.
<b>COMMERCIAL POLYMERS</b>			
<b>Some manufacturers</b>	-	Lenzing Plastics, Montefibre	
<b>Trade names</b>	-	Dolanit, Leacril	
<b>PHYSICAL PROPERTIES</b>			
<b>Density at 20°C</b>	g cm <sup>-3</sup>	1.184 (1.04-1.31), calculated: 1.112-1.177	
<b>Color</b>	-	white	
<b>Refractive index, 20°C</b>	-	1.514-1.52	
<b>Molar polarizability</b>	cm <sup>3</sup> x 10 <sup>-25</sup>	calculated: 19.14-22.51	
<b>Odor</b>	-	odorless	
<b>Melting temperature, DSC</b>	°C	317 (297-341)	

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PARAMETER	UNIT	VALUE	REFERENCES
<b>Temperatures of carbonization</b>	°C	20-300 - stretching and oxidation; 1000 - carbonization; 1500-3000 ordering and orientation	Rahaman, M S A; Ismail, A F; Mustafa, A. Polym. Deg. Stab., 92, 1421-32, 2007.
<b>Thermal expansion coefficient, 23-80°C</b>	°C <sup>-1</sup>	0.3-2E-4	
<b>Thermal conductivity, melt</b>	W m <sup>-1</sup> K <sup>-1</sup>	0.272	Knappe, W; Lohe, P; Wutschig, R, Angew. Makromol. Chem. , 7 , 181-193, 1969.
<b>Glass transition temperature</b>	°C	84-85 (43.8-105); calculated: 89-148	
<b>Specific heat capacity</b>	J K <sup>-1</sup> mol <sup>-1</sup>	0.0688	
<b>Heat of fusion</b>	kJ g <sup>-1</sup>	0.042-5.021	
<b>Maximum service temperature</b>	°C	140	
<b>Hansen solubility parameters, <math>\delta_D</math>, <math>\delta_P</math>, <math>\delta_H</math></b>	MPa <sup>0.5</sup>	21.7, 14.1, 9.1	
<b>Interaction radius</b>		10.9	
<b>Hildebrand solubility parameter</b>	MPa <sup>0.5</sup>	calc.=26.2; exp.=25.27-27.4	
<b>Surface tension</b>	mN m <sup>-1</sup>	calc.= 42.5-61.1; exp.= 44-50	Lee, H-L, J Appl. Polym. Sci., 12, 719, 1968; Wu, S, Polymer Interface and Adhesion, Marcel Dekker, New York, 1982, p. 87.
<b>Dielectric constant</b>	-	calc.=3.01-3.99; exp.=2.87-4.00/4.2	
<b>Dissipation factor at 100 Hz</b>		0.113	
<b>Dissipation factor at 1 MHz</b>		0.033	
<b>Volume resistivity</b>	ohm-m	1E11	
<b>Surface resistivity</b>	ohm	5.5E+7	
<b>Electric strength K20/P50, d=0.60.8 mm</b>	kV mm <sup>-1</sup>	3.6E+8 to 4E+9	
<b>Permeability to oxygen, 25°C</b>	cm <sup>3</sup> cm cm <sup>-2</sup> s <sup>-1</sup> Pa <sup>-1</sup> x 10 <sup>12</sup>	0.000015-0.00041	
<b>Permeability to water vapor, 25°C</b>	cm <sup>3</sup> cm cm <sup>-2</sup> s <sup>-1</sup> Pa <sup>-1</sup> x 10 <sup>12</sup>	23-49	
<b>Surface free energy</b>	mJ m <sup>-2</sup>	46.8	
<b>MECHANICAL &amp; RHEOLOGICAL PROPERTIES</b>			
<b>Tensile strength</b>	MPa	19-72; 133-480 (fiber); 115-117 (film)	Lenzing Plastics; Hu, Y; Sun, T; Wang, H; Wu, D, J. Appl. Polym. Sci., 114, 3668-72, 2009.
<b>Tensile modulus</b>	MPa	3,700	
<b>Elongation</b>	%	15-35	Lenzing Plastics, Montefibre
<b>Elastic modulus</b>	MPa	5,670 (fiber)	Lenzing Plastics
<b>Tenacity (fiber) (standard atmosphere)</b>	cN tex <sup>-1</sup> (daN mm <sup>-2</sup> )	35-45 (40-55)	Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.
<b>Tenacity (wet fiber, as % of dry strength)</b>	%	80-95	Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.

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PARAMETER	UNIT	VALUE	REFERENCES
Fineness of fiber (titer)	dtex	0.6-25	Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.
Length (elemental fiber)	mm	38-200	Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.
Shrinkage	%	14-22; 5.1 (fiber in boiling water)	Wu, G; Lu, C; Wu, X; Zhang, S; He, F; Ling, L, J. Appl. Polym. Sci., 94, 1705-9, 2004.
Melt viscosity, shear rate=1000 s <sup>-1</sup>	Pa s	170	
Water absorption, equilibrium in water at 23°C	%	1.0-1.5	
<b>CHEMICAL RESISTANCE</b>			
Acid dilute	-	good	
Alcohols	-	very good	
Alkalis (weak)	-	good	
Aliphatic hydrocarbons	-	good	
Aromatic hydrocarbons	-	good	
Esters	-	poor	
Halogenated hydrocarbons	-	poor	
⊖ solvent	-	ethyl carbonate	
Good solvent	-	γ-butyrolactone, chloroacetonitrile, dioxanone, DMA, DMF, DMSO, dimethyl phosphite, dimethyl sulfone, ethylene carbonate, nitric acid, sulfuric acid	Iovleva, M M; Smirnova, V N; Budnitskii, G A, Fibre Chem., 33, 4, 262-64, 2001.
Non-solvent	-	acetonitrile, alcohols, chlorinated hydrocarbons, diethyl ether, formamide, hydrocarbons, ketones, methanol	
<b>FLAMMABILITY</b>			
Ignition temperature	°C	480	
Autoignition temperature	°C	560	
Limiting oxygen index	% O <sub>2</sub>	18-18.2	Crook, V; Ebdon, J; Hunt, B; Joesph, P; Wyman, P, Polym. Deg. Stab., 95, 2260-68, 2010.
Char at 500°C	%	31.5; 53 (nitrogen)	Yang, C Q; He, Q; Lyon, R E; Hu, Y, Polym. Deg. Stab., 95, 108-15, 2010; Crook, V; Ebdon, J; Hunt, B; Joesph, P; Wyman, P, Polym. Deg. Stab., 95, 2260-68, 2010.
Volatile products of combustion	-	HCN, NH <sub>3</sub> , H, CO, H <sub>2</sub> O	
<b>WEATHER STABILITY</b>			
Spectral sensitivity	nm	270, 310	
Important initiators and accelerators	-	CO, CO <sub>2</sub> , NH <sub>3</sub> , H <sub>2</sub> O	
Products of degradation	-	polyenes, imides, hydroperoxides, lactones, amides, CO, CO <sub>2</sub> , H <sub>2</sub> O, NH <sub>3</sub>	
Stabilizers	-	benzophenone, benzotriazole, and benzoates	
<b>BIODEGRADATION</b>			
Typical biodegradants	-	considerable resistance	

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PARAMETER	UNIT	VALUE	REFERENCES
<b>TOXICITY</b>			
NFPA: Health, Flammability, Reactivity rating	-	2/0/0	
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
TLV, ACGIH	mg m <sup>-3</sup>	3	
MAK/TRK	ppm	3 (Germany)	
OSHA	ppm	2	
Oral rat, LD <sub>50</sub>	mg kg <sup>-1</sup>	11,000; 3,000	
<b>ENVIRONMENTAL IMPACT</b>			
Aquatic toxicity, <i>Daphnia magna</i> , LC <sub>50</sub> , 48 h	mg l <sup>-1</sup>	1,000-185,000	Lithner, Ph D Thesis, Univrsity of Gothenburg, 2011.
<b>PROCESSING</b>			
Processing temperature	°C	160-175 (filament extrusion)	
Additives used in final products	-	Plasticizers: dibutyl phthalate, propylene carbonate, ethylene carbonate, dimethylformamide, dimethylsulfoxide, glycerin, polyethylene glycol, polypropylene glycol, vegetable and mineral oils, tributyl phosphate; Antistatics: alkylamine salts of branched alkylbenzenesulfonic acids, polyaniline, polymeric quaternary ammonium salt	
Applications	-	concrete, composites, dielectric material, fibers, production of carbon fiber, clothing, awnings, beach umbrellas, boat covers, car tops	
<b>BLENDS</b>			
Suitable polymers	-	gelatin, PANI, PMHS, PVDF-HFP	
<b>ANALYSIS</b>			
FTIR (wavenumber-assignment)	cm <sup>-1</sup> /-	CN – 2240, NH <sub>2</sub> – 3240, NH – 3500	
NMR (chemical shifts)	ppm	rr – 27.31; mr – 26.88; mm – 26.40	Katsuraya, K; Hatanaka, K; Matsuzaki, K; Minagawa, M, Polymer, 42, 6323-26, 2001.
x-ray diffraction peaks	degree	17 (sharp), 20-30 (amorphous), 30 (weak)	Jung, B; Yoon, J K; Kim, B; Rhee, H-W, J. Membrane Sci., 246, 67-76, 2005.