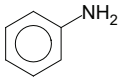
PANI polyaniline

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	polyaniline	
IUPAC name	-	poly(imino-1,4-phenylene)	
ACS name	-	benzenamine, homopolymer	
Acronym	-	PANI	
CAS number	-	25233-30-1	
HISTORY			
Person to discover	-	C J Fritzsche	
Date	-	1841	
Details	-	treating indigo with potassium hydroxide obtained oil which he named aniline; he then oxidized it to PANI	
SYNTHESIS			
Monomer(s) structure	-		
Monomer(s) CAS number(s)	-	62-53-3	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	93.13	
Monomer(s) expected purity(ies)	%	99.5	Zhou, Z; Wang, J; Wang, Z; Zhang, F, Mater. Lett., 65, 2311-14, 2011.
Method of synthesis	-	p-toluenesulfonic acid protonated aniline is used to make anilinium complexes; slow addition of ammonium peroxydisulfate caused formation of polyaniline in the micelles and grew to needle-like aggregates potentially useful as conductive fillers	Jung, W-H; Kim, D-Y; Lee, Y-M; McCarthy, S P, Antec, 1786-90, 2006.
Temperature of polymerization	°C	18 (M_w=29,700); 0 (M_w=122,000); -35 (M_w=166,000)	Yilmaz, F; Kucukyavuz, Z, Polym. Int., 59, 552-56, 2010.
Number average molecular weight, M_n	dalton, g/mol, amu	25,000-127,000	
Mass average molecular weight, M_w	dalton, g/mol, amu	5,000-440,000	
Polydispersity, M_w/M_n	-	2.55-3.46	
Radius of gyration	nm	20-40	
STRUCTURE	-		
Crystallinity	%	30-50	Saxena, V; Malhotra, B D, Handbook of polymers in Elecronics, Ed. Malhotra, B D, Rapra, 2002.
Cell type (lattice)	-	orthorhombic	Pouget, J P; Josefowicz, M E; Epstein, A J; Tang, X; MacDiarmid, A G, Macromolecules, 24, 779, 1991.
Cell dimensions	nm	a:b:c=0.765:0.575:1.02	Pouget, J P; Josefowicz, M E; Epstein, A J; Tang, X; MacDiarmid, A G, Macromolecules, 24, 779, 1991.
Crystallite size	nm	2.8-7.2	

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PARAMETER	UNIT	VALUE	REFERENCES
COMMERCIAL POLYMERS			
Some manufacturers	-	Panipol	
Trade names	-	Panipol	
Composition information	-	water dispersion; NMP, Solvesso, toluene, and xylene solutions, melt processable grade, and masterbatches	
PHYSICAL PROPERTIES			
Density at 20°C	g cm^{-3}	1.36-1.4; 1.245 (emeraldine base)	
Color	-	dark green to black (emeraldine base)	
Refractive index, 20°C	-	1.85	
Transmittance	%	97	Bae, S; Lee, J U; Park, H-s; Jung, E H; Jung, J W; Jo, W H, Solar En. Mater. Solar Cells, 130, 599-604, 2014.
Melting temperature, DSC	°C	385	
Glass transition temperature	°C	100-190	
Long term service temperature	°C	>300	
Hansen solubility parameters, δ_D, δ_P, δ_H	$MPa^{0.5}$	17.4, 8.1, 10.7 (emeraldine base), 17.0, 8.9, 13.7 (emeraldine salt), 21.1, 5.6, 7.3 (leucoemeraldine base)	Shacklette, L W; Han, C C, Mat. Res. Soc. Symp. Proc., 328, 157, 1994.
Hildebrand solubility parameter	$MPa^{0.5}$	22.2 (emeraldine base), 23.6 (emeraldine salt), 23.25 (leucoemeraldine base)	Shacklette, L W; Han, C C, Mat. Res. Soc. Symp. Proc., 328, 157, 1994.
Electric conductivity	Siemens cm^{-1}	6-300; 100,000 (theoretically possible)	MacDiarmid, A G; Zhou, Y; Feng, J; Furst, G T; Shedlow, Antec, 1563-67, 1999.
Volume resistivity	ohm-m	2.5E-3	Saxena, V; Malhotra, B D, Handbook of polymers in Elecronics, Ed. Malhotra, B D, Rapra, 2002.
Surface resistivity	ohm	>1000	
Optical absorption edge	eV	1.6	Saxena, V; Malhotra, B D, Handbook of polymers in Elecronics, Ed. Malhotra, B D, Rapra, 2002.
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	40-168 (non crosslinked); 60-430 (crosslinked)	Oh, E J; Min, Y; Wiesinger, J M; Manohar, S K; Scherr, E M; Prest, P J; MacDiarmid, A G; Epstein, A J, Synthetic Metals, 55-57, 977-82, 1993.
Tensile stress at yield	MPa	120	
Young's modulus	MPa	900 (PANI HCl); 1,300 (PANI base); 1,260-1,750 (fibers)	Valentova, H; Stejskal, J, Synthetic Metals, 160, 832-34, 2010; Wang, H-L; Zhu, Y; Valdez, J A; Mattes, B R, Conductive Polymers and Plastics in Industrial Applications, Rupprecht, L, Ed., WilliamAndrew, 1999.
Intrinsic viscosity, 25°C	dl g^{-1}	0.42-1.42	Yilmaz, F; Kucukyavuz, Z, Polym. Int., 59, 552-56, 2010.
Charpy impact, notched	J cm^{-2}	900	
CHEMICAL RESISTANCE			
Alcohols	-	good	
Aliphatic hydrocarbons	-	good	
Aromatic hydrocarbons	-	good	

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PARAMETER	UNIT	VALUE	REFERENCES
Esters	-	good	
Halogenated hydrocarbons	-	good	
Ketones	-	good	
Good solvent	-	DMAC, DMF, DMSO, NMP (emeraldine base); DMPU (N,N'-dimethyl propylene urea)	
FLAMMABILITY			
Ignition temperature	°C	535	
Volatile products of combustion	-	CO, CO_2, NO_x	
WEATHER STABILITY			
Spectral sensitivity	nm	290, 325, 350, 400; 380-400 (photobleaching); 331 (emeraldine base)	Teo, C H; Rahman, F, Appl. Phys. A, 99, 311-16, 2010; Wang, H-L; Zhu, Y; Valdez, J A; Mattes, B R, Conductive Polymers and Plastics in Industrial Applications, Rupprecht, L, Ed., WilliamAndrew, 1999.
Activation wavelengths	nm	280	Lakshmi, G B V S; Dhillon, A; Siddiqui, A M; Zulfequar, M; Avasthi, D K, Eur. Polym. J., 45, 2873-77, 2009.
Stabilizers	-	Tinuvin 213	Teo, C H; Rahman, F, Appl. Phys. A, 99, 311-16, 2010.
TOXICITY			
NFPA: Health, Flammability, Reactivity rating	-	0/0/0-1	
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
PROCESSING			
Typical processing methods	-	compounding, melt processing (PE, PP, PS, SEBS, EMA, EPDM/PP), *in situ* polymerization, spin coating, surface grafting	Perento, J, Polymers in Electronics 2007, Rapra, 2007, paper 5.
Additives used in final products	-	Fillers: carbon black, montmorillonite, multiwalled carbon nanotubes, silica; Plasticizers: hydroquinone, resorcinol, tert-butyl hydroquinone, 4-hexyl resorcinol, bisphenol-A, sulfonic acids, phosphonic acids (phenyl phosphonic acid), and aliphatic diesters of phosphoric acid (diphenyl, dioctyl and dibutyl); UV absorber: Tinuvin 213	
Applications	-	corrosion protection, EMI shielding, filler to make plastic conductive, materials having electric conductivity, montmorillonite-PANI coated, protection against static electricity, synthesis of carbon black coated by PANI (Eonomer), synthesis of hybrid filler (multiwalled carbon nanotubes+PANI particles); plastics: addition of 8-15 wt% lowers surface resistivity of plastics to 1E4-1E9 ohm; coatings and inks	Perento, J, Polymers in Electronics 2007, Rapra, 2007, paper 5.
Outstanding properties	-	chemical resistance, electrical conductivity	Perento, J, Polymers in Electronics 2007, Rapra, 2007, paper 5.
BLENDS			
Suitable polymers	-	PA, PCL, PEO, PET, PVC	

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PARAMETER	UNIT	VALUE	REFERENCES
ANALYSIS			
FTIR (wavenumber-assignment)	cm^{-1}/-	H-H – 3389, 3270; C-H – 3024; C-N – 1297	Ragachev, A A; Yarmolenko, M A; Xiaohong, J; Shen, R; Luchnikov, P A; Rogachev, A V, Appl. Surf. Sci., 351, 811-8, 2015.
Raman (wavenumber-assignment)	cm^{-1}/-	C-C – 1597-1603, 1563-1566; C=N – 1489	Annapoorni, M J S, Synthetic Metals, 160, 1727-32, 2010.
x-ray diffraction peaks	degree	8.9, 14.8, 20.8, 25.3, 26.7	Zhou, Z; Wang, J; Wang, Z; Zhang, F, Mater. Lett., 65, 2311-14, 2011.