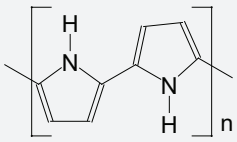
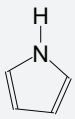
PPy polypyrrole

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	polypyrrole	
IUPAC name	-	poly(pyrrole-2,5-diyl)	
CAS name	-	1H-oyrrole, homopolymer	
Acronym	-	PPy	
CAS number	-	30604-81-0	
Formula			
HISTORY			
Person to discover	-	Bolto, B A; Weiss, D E	
Date	-	1963	
Details	-	published paper on high conductivity of polypyrrole	
SYNTHESIS			
Monomer(s) structure	-		
Monomer(s) CAS number(s)	-	109-97-7	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	67.09	
Method of synthesis	-	dry pyrrole was polymerized in the presence of oxidant and dopant in water medium	
Temperature of polymerization	°C	0	
Time of polymerization	h	40	
Catalyst	-	ammonium persulfate (oxidant)	
Yield	%	42	
Heat of polymerization	J g^{-1}	894-2161	
Number average molecular weight, M_n	dalton, g/mol, amu	240,000	
Mass average molecular weight, M_w	dalton, g/mol, amu	22,000-356,000	Bose, S; Kuila, T; Uddin, M E; Kim, N H; Lau, A K T; Lee, J H, Polymer, 51, 5921-28, 2010.
Polydispersity, M_w/M_n	-	1.48	
Polymerization degree (number of monomer units)	-	303	
Radius of gyration	nm	42.4	Huang, K; Wan, M; Long, Y; Chen, Z; Wei, Y, Synthetic Metals, 155, 495-500, 2005.
STRUCTURE			
Crystallinity	%	50	Saxena, V; Malhotra, B D, Handbook of polymers in Elecronics, Ed. Malhotra, B D, Rapra, 2002.
Cell type (lattice)	-	monoclinic	
Cell dimensions	nm	a:b:c=0.82:0.735:0.682	
Unit cell angles	degree	α:β:γ=90:90:117	

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Chain conformation	-	anti-gauche	Fonner, J M; Schmidt, C E; Ren, P, Polymer, 51, 4985-93, 2010.
PHYSICAL PROPERTIES			
Density at 20°C	g cm^{-3}	1.3-1.48	
Melting temperature, DSC	°C	>300	
Decomposition temperature	°C	290	
Storage temperature	°C	25	
Glass transition temperature	°C	80	
Volume resistivity	ohm-m	50.7	Bose, S; Kuila, T; Uddin, M E; Kim, N H; Lau, A K T; Lee, J H, Polymer, 51, 5921-28, 2010.
Surface resistivity	ohm	4E2 to 2.8E4	Lee, J Y; Kim, K T; Kim, S Y; Kim, C Y, Antec, 1422-26, 1996.
Optical absorption edge	eV	2.5	Saxena, V; Malhotra, B D, Handbook of polymers in Elecronics, Ed. Malhotra, B D, Rapra, 2002.
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	30-68; 25 (fibers); 127 (electrochemical film)	
Elongation	%	2 (fibers); 26 (electrochemical film)	
Elastic modulus	MPa	1,500 (fibers); 1,950 (film)	
CHEMICAL RESISTANCE			
Alcohols	-	very good	
Aliphatic hydrocarbons	-	very good	
Aromatic hydrocarbons	-	very good	
Esters	-	very good	
Greases & oils	-	very good	
Halogenated hydrocarbons	-	very good	
Ketones	-	very good	
FLAMMABILITY			
Volatile products of combustion	-	H_2O, CO, CO_2, HCN, SO_2	
WEATHER STABILITY			
Spectral sensitivity	nm	230, 338, 410, 430, 435, 500, 900	Li, X-G; Li, A; Huang, M-R; Liao, Y; Lu, G-Y, J. Phys. Chem C, 144, 19244-55, 2010.
TOXICITY			
NFPA: Health, Flammability, Reactivity rating	-	0/1/0; 2/0/0 (HMIS)	
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	

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PARAMETER	UNIT	VALUE	REFERENCES
PROCESSING			
Typical processing methods	-	chemical oxidation of pyrrole in carbon black suspension, electrochemical anodic polymerization, Langmuir-Blodgen technique of monolayer production, solution polymerization over the substrate	
Additives used in final products	-	Fillers: carbon black, silica, tin oxide	
Applications	-	battery electrodes, capacitors, controlled release agents for other components, electronic displays, EMI shielding, nonmetallic conductors, optoelectronic systems, sensors	
BLENDS			
Suitable polymers	-	chitosan, PA6, PAN, PANI, PCL, PLA, PP, PU, PVAC, PVDF, PVP, SI	
ANALYSIS			
FTIR (wavenumber-assignment)	cm^{-1}/-	H-O – 3558; N-H – 3377, 3388, 1035, 759, 558; CN – 2219, 2871; C=O – 1698; C-O – 1115 and more in ref.	Zhang, N; van Ooij, W J; Luo, S, Antec, 2495-2501, 1999; Bose, S; Kuila, T; Uddin, M E; Kim, N H; Lau, A K T; Lee, J H, Polymer, 51, 5921-28, 2010.
Raman (wavenumber-assignment)	cm^{-1}/-	polaronic form – 962, 1053; bipolaronic form – 930, 1086; C=C – 1589; skeletal band – 1475	Foroughi, J; Spinks, G M; Wallace, G G, Sensors Actuators, B155, 278-84, 2011.
NMR (chemical shifts)	ppm	C NMR: β carbons – 113.6; α, β carbons - 129.3; α carbons - 123.7, 142.9; OH substituted α carbons - 149.2	Rizzi, M; Trueba, M; Trasatti, S P, Synthetic Metals, 161, 23-31, 2011.
x-ray diffraction peaks	degree	23.5-25.1 (amorphous PPy)	Li, X-G; Li, A; Huang, M-R; Liao, Y; Lu, G-Y, J. Phys. Chem C, 144, 19244-55, 2010; Bose, S; Kuila, T; Uddin, M E; Kim, N H; Lau, A K T; Lee, J H, Polymer, 51, 5921-28, 2010.