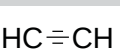
PAC polyacetylene

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	polyacetylene	
IUPAC name	-	poly(ethene-1,2-diyl); polyethyne	
CAS name	-	ethyne, homopolymer	
Acronym	-	PAC	
CAS number	-	25067-58-7	
HISTORY			
Person to discover	-	Natta, G, Mazzanti, G, Corradini, P; Ito, T, Shirakawa, H, and Ikeda, S	Shirakawa, H, Rev. Mod. Phys., 73, 713-18, 2001.
Date	-	1958; 1967	
Details	-	first synthesis; synthesized PAC film	
SYNTHESIS			
Monomer(s) structure	-		
Monomer(s) CAS number(s)	-	74-86-2	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	26.04	
Monomer ratio	-	100%	
Method of synthesis	-	the most common method of synthesis is ring opening metathesis polymerization of molecules such as cyclooctatetraene; simple method of synthesis of cis isomer involves blowing acetylene onto the stationary surface of Ziegler catalyst	
Temperature of polymerization	^{o}C	-78	
Catalyst	-	Zigler-Natta; $Pd(OAc)_2$	Huber, J; Mecking, S, Angew. Chem. Int. Ed., 45, 6314-17, 2006.
Number average molecular weight, M_n	dalton, g/mol, amu	21,500-286,100	
Polydispersity, M_w/M_n	-	1.25-1.46	
STRUCTURE			
Crystallinity	%	80	Saxena, V; Malhotra, B D, Handbook of polymers in Elecronics, Ed. Malhotra, B D, Rapra, 2002.
Cell type (lattice)	-	othorhombic, hexagonal	
Cell dimensions	nm	a:b:c=0.720-0.741:0.406-0.492:0.245-0.260 (*trans*, othorhombic); 0.761-0.768:0.430-0.446:0.436-0.447 (*cis*-transoid, orthorhombic); 0.512:0.512:0.484 (*cis*-cisoid, hexagonal)	Shrikawa, H, Synthetic Metals, 125, 3-10, 2002.
Fibril diameter	nm	20-100	Shrikawa, H, Synthetic Metals, 125, 3-10, 2002.
Tacticity	%	70-95 (*cis*); 100 (*trans*) at 150^{o}C; 98.1 (*cis*) at -78^{o}C	Shrikawa, H, Synthetic Metals, 125, 3-10, 2002.
Cis content	%	depends on polymerization temperature; *cis*, which is insulator-like state, can be converted to *trans* by heating	Skanderi, Z; Djebaili, A; Bouzaher, Y; Belloum, M; Abadie, M J M, Composites, Part A, 36, 497-501, 2005.
Chain conformation	-	helix	Akagi, K; Mori, T, Chem. Record, 8, 395-406, 2008.
Space group		Pnam	Martens, J H F; Pichler, K; Marseglia, E A; Friend, R H; Cramail, H; Khosravi, E; Parker, D; Feast, W J; Polymer, 35, 2, 403-14, 1994.

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PHYSICAL PROPERTIES			
Density at 20°C	g cm^{-3}	1.0-1.23	
Refractive index, 20°C	-	1.7-3	
Isomerization temperature of *cis*-isomer	°C	0 (beginning), 100 (complete isomerization to *trans*)	
Glass transition temperature	°C	200	Fink, J K, High Performance Polymers, William Andrew, 2008.
Surface tension	mN m^{-1}	51 (*cis*); 52 (*trans*)	Schonhorn, H; Baker, G L; Bates, F S, J. Polym. Sci., Polym. Phys. Ed., 23, 1555, 1985.
Volume resistivity	ohm-m	1E2 (*trans*-rich); 2.4E6 (*cis* 80%)	Shrikawa, H, Synthetic Metals, 125, 3-10, 2002.
Contact angle of water, 20°C	degree	72	
Surface free energy	mJ m^{-2}	51.5	
Optical absorption edge	eV	1.4 (*trans*), 2.0 (*cis*)	Saxena, V; Malhotra, B D, Handbook of polymers in Elecronics, Ed. Malhotra, B D, Rapra, 2002.
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	900	
Tensile modulus	MPa	50,000	
Young's modulus	MPa	25,000-30,000	
CHEMICAL RESISTANCE			
Acid dilute/concentrated	-	good	
Alcohols	-	good	
Alkalis	-	good	
Aliphatic hydrocarbons	-	good	
Aromatic hydrocarbons	-	good	
Esters	-	good	
Greases & oils	-	good	
Halogenated hydrocarbons	-	good	
Ketones	-	good	
Good solvent	-	aniline, DMF, isopropylamine	
Non-solvent	-	acetone, carbon tetrachloride, methanol	
BIODEGRADATION			
Stabilizers	-	some polyacetylene derivatives have insecticidal properties especially in the presence of UV	Haouas, D; Guido, F; Monia, B H-K; Habib, B H M, Ind. Crops Products, in press, 2011.
TOXICITY			
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
PROCESSING			
Typical processing methods	-	printing using dispersion	
Additives used in final products	-	Antistatics: carbon black, various doping systems	
Applications	-	antistatics, environmental sensing devices, membranes, rechargeable batteries, semiconductor devices, solar cells	

PARAMETER	UNIT	VALUE	REFERENCES
Outstanding properties	-	Marine polyacetylenes constitute a very structurally diverse and useful class of compounds with important biological activities such as antifungal, antibiotic, anticancer, antitumor, anti-HIV, anti-inflammatory, and antimicrobial properties.	Legrave, N; Elsebai, M F; Mehiri, M; Amade, P, Studies in Natural Products Chemistry, Chapter 8, 251-95, Elsevier, 2015.
BLENDS			
Suitable polymers	-	SBS	
ANALYSIS			
Raman (wavenumber-assignment)	cm^{-1}/-	*trans*-PAC 1150 and 1450	Oshiro, T; Yamazato, M; Higa, A; Toguchi, M, Jpn J. Appl. Phys., 46, 2, 756-60, 2007.