

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 | - | $\text{HC}\equiv\text{CH}$ | |
| 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 | °C | -78 | |
| Catalyst | - | Zigler-Natta; $\text{Pd}(\text{OAc})_2$ | 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 Electronics, Ed. Malhotra, B D, Rapra, 2002. |
| Cell type (lattice) | - | orthorhombic, hexagonal | |
| Cell dimensions | nm | a:b:c=0.720-0.741:0.406-0.492:0.245-0.260 (<i>trans</i> , orthorhombic); 0.761-0.768:0.430-0.446:0.436-0.447 (<i>cis-transoid</i> , orthorhombic); 0.512:0.512:0.484 (<i>cis-cisoid</i> , 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 (<i>cis</i>); 100 (<i>trans</i>) at 150°C; 98.1 (<i>cis</i>) at -78°C | Shrikawa, H, Synthetic Metals, 125, 3-10, 2002. |
| Cis content | % | depends on polymerization temperature; <i>cis</i> , which is insulator-like state, can be converted to <i>trans</i> 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 <i>cis</i> -isomer | °C | 0 (beginning), 100 (complete isomerization to <i>trans</i>) | |
| Glass transition temperature | °C | 200 | Fink, J K, High Performance Polymers, William Andrew, 2008. |
| Surface tension | mN m ⁻¹ | 51 (<i>cis</i>); 52 (<i>trans</i>) | Schonhorn, H; Baker, G L; Bates, F S, J. Polym. Sci., Polym. Phys. Ed., 23, 1555, 1985. |
| Volume resistivity | ohm-m | 1E2 (<i>trans</i> -rich); 2.4E6 (<i>cis</i> 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 (<i>trans</i>), 2.0 (<i>cis</i>) | Saxena, V; Malhotra, B D, Handbook of polymers in Electronics, 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 | |

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| 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 /- | <i>trans</i> -PAC – 1150 and 1450 | Oshiro, T; Yamazato, M; Higa, A; Toguchi, M, Jpn J. Appl. Phys., 46, 2, 756-60, 2007. |