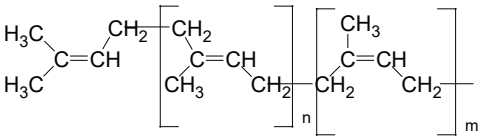
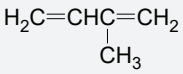
PIB, *cis* *cis*-polyisoprene

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	*cis*-polyisoprene, natural rubber	
CAS name	-	natural rubber; 1,3-butadiene, 2-methyl-, homopolymer	
Acronym	-	*cis*-PIP	
CAS number	-	9003-31-0; 9006-04-6 (natural rubber); 104389-31-3	
Linear formula			
HISTORY			
Person to discover	-	Horne, S E	Horne, S E, US Patent 3,114,743, Goodrich-Gulf Chemicals, Dec. 17, 1963.
Date	-	1963 (filling 1954)	
SYNTHESIS			
Monomer(s) structure	-		
Monomer(s) CAS number(s)	-	78-79-5	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	68.12	
Monomer(s) expected purity(ies)	%	99	
Rubber content	%	94 (natural), >99 synthetic	
Method of synthesis	-	solvent, monomer and catalyst (all high purity) are added to reactor, polymerization is stopped by addition of catalyst deactivator, and rubber protected by addition of a non-staining antioxidant	
Catalyst	-	organoaluminum	
Mass average molecular weight, M_w	dalton, g/mol, amu	40,000-1,240,000 (natural rubber); 1,500,000-2,500,000 (synthetic)	
Polydispersity, M_w/M_n	-	1.02-1.04	
Molar volume at 298K	$cm^3 mol^{-1}$	68.1 (crystalline)	
Van der Waals volume	$cm^3 mol^{-1}$	47.5 (crystalline)	
STRUCTURE			
Crystallinity	%	30	
Cell type (lattice)	-	orthorhombic	
Cell dimensions	nm	a:b:c=1.241:0.881:0.843	
Unit cell angles	degree	β=94.6	
Number of chains per unit cell	-	4	
Crystallite size	nm	6-25 (filaments)	
Tacticity	%	69.5-98	Hyun, K; Hoefl, S; Kahle, S; Wilhelm, M, J. Non-Newtonian Fluid Mech., 160, 93-103, 2009; Bussiere, P-O; Gardette, J-L; Lacoste, J; Baba, M, Polym. Deg. Stab., 88, 182-88, 2005.

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PARAMETER	UNIT	VALUE	REFERENCES
Cis content	%	100 (natural rubber); 90-98 (synthetic)	
Chain conformation	-	$P2_{1/a}$-C_{2h}	
Rapid crystallization temperature	°C	-25	
PHYSICAL PROPERTIES			
Density at 20°C	g cm^{-3}	0.906-0.93; 0.95 (vulcanized)	
Color	-	nearly colorless	
Refractive index, 20°C	-	1.5191-1.52	
Odor	-	odorless	
Melting temperature, DSC	°C	30-35.5	
Thermal expansion coefficient, 23-80°C	$°C^{-1}$	6.7E-4	
Thermal conductivity, melt	W m^{-1} K^{-1}	0.134	
Glass transition temperature	°C	-75 (natural rubber), -70 to -72 (polyisoprene)	
Specific heat capacity	J K^{-1} kg^{-1}	1905	
Maximum service temperature	°C	-50 to 50; (unvulcanized); -55 to 80 (vulcanized)	
Hansen solubility parameters, δ_D, δ_P, δ_H	$MPa^{0.5}$	18.1, 2.4, 2.3	
Interaction radius		10.3	
Hildebrand solubility parameter	$MPa^{0.5}$	17-18.4	
Surface tension	mN m^{-1}	32	Lee, L H, J. Polym. Sci. A-2, 5, 1103, 1967.
Dielectric constant at 1 Hz/1 MHz	-	2.37-2.45/2.6; 2.9 (vulcanized)	
Dielectric loss factor at 1 kHz	-	0.001-0.003	
Dissipation factor at 1000 Hz	E-4	20	
Volume resistivity	ohm-m	1E13	
Electric strength K20/P50, d=0.60.8 mm	kV mm^{-1}	17; 50 (vulcanized)	
Permeability to oxygen, 25°C	cm^3 cm cm^{-2} s^{-1} Pa^{-1} x 10^{12}	1.76	
Diffusion coefficient of oxygen	cm^2 s^{-1} $x10^6$	1.73	
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	28 (vulcanized)	
Tensile stress at yield	MPa	21.6	
Elongation	%	100-800	
Shore A hardness	-	30-90 (unvulcanized); 30-100 (vulcanized)	
Shore D hardness	-	30-45 (vulcanized)	
CHEMICAL RESISTANCE			
Acid dilute/concentrated	-	poor	
Alkalis	-	fair	
Aliphatic hydrocarbons	-	poor	
Aromatic hydrocarbons	-	poor	

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PARAMETER	UNIT	VALUE	REFERENCES
Esters	-	poor	
Greases & oils	-	poor	
Halogenated hydrocarbons	-	poor	
Ketones	-	fair	
Θ solvent, Θ-temp.=25, 32.1, 14.5°C	-	butanone, dioxane, 2-pentanone	
Good solvent	-	chlorinated hydrocarbons, cyclohexane, hydrocarbons, MIBK, toluene	
Non-solvent	-	acetone, alcohols, carboxylic acids	
FLAMMABILITY			
Ignition temperature	°C	>113	
Heat of combustion	J g^{-1}	45,200	
WEATHER STABILITY			
Important initiators and accelerators	-	ozone, singlet oxygen, mechanical stress, $FeCl_3$ (photo-Fenton process)	
Products of degradation	-	radicals, hydroperoxides, epoxy groups, ketone groups, crosslinking, chain scission	
Stabilizers	-	cabon black, antioxidants, antiozonants, 3-mercapto-1,2,4-triazin-5-one derivatives, encapsulated butylated hydroxy toluene	
TOXICITY			
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
PROCESSING			
Typical processing methods	-	Banbury mixer, calendering, coating, Gordon plasticator, sheeting, skim coating, tubing, vulcanization	
Additives used in final products	-	Fillers: barium and strontium ferrites, boron carbide, calcinated clays, calcium carbonate, carbon black, carbon-silica dual phase filler, clays, dolomite, fumed silica, iron oxide, magnesium aluminum silicate, magnesium carbonate, mica, montmorillonite, nickel zinc ferrite, nylon fibers, pulverized polyurethane foam, quartz, silica carbide, soapstone, talc, zinc oxide; Plasticizers: naphthenic oil, polybutene, aromatic oil, esters of dicarboxylic acid; Plasticizers: adipates, aromatic mineral oil, paraffin oil, phosphates, phthalates, polyethylene glycol, processing oil, sebacates; Antistatics: dihydrogen phosphate of ε-aminocaproic acid, iodine doping; Antistatics: carbon black, quaternary ammonium salt, zinc oxide whisker; Antiblocking: diatomaceous earth; Release: propylene wax; Slip: erucamide+stearamide	
Applications	-	boots, conveyor belts, electrician's gloves, gloves, heels and soles, hoses, instrument panels, latex foams, machined components, pipes, plugs, pumps, shock absorbers, sockets, storage-battery cases, switchboard panels, telephone receivers, tire cord impregnation, tires, toys, tubes, valves, vibration dampers, waterproof clothing and bathing apparel, wire and cables	
ANALYSIS			
NMR (chemical shifts)	ppm	H NMR: CH_2 – 4.7; CH – 5.18; C NMR: *cis* – 26.5 and 31.1, *trans* – 32.1	Pilichowski, J-F; Morel, M; Tamboura, F; Chmela, S; Baba, M; Lacoste, J, Polym. Deg. Stab., 95, 1575-80, 2010.