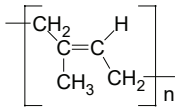
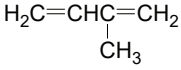
PIP, *trans* *trans*-polyisoprene

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	*trans*-polyisoprene, guttapercha	
CAS name	-	1,3-butadiene, 2-methyl-, homopolymer	
Acronym	-	*trans*-PIP	
CAS number	-	104389-32-4	
Linear formula			
HISTORY			
Person to discover	-	Saltman, W M	Saltman, W M, US Patent 3,008,945, Goodyear Tire & Rubber Company, Nov. 14, 1961.
Date	-	1961	
Details	-	patented polymerization permits synthesis of product containing 97% *trans*-form	
SYNTHESIS			
Monomer(s) structure	-		
Monomer(s) CAS number(s)	-	78-79-5	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	68.12	
Method of synthesis	-	bulk precipitation polymerization of isoprene catalyzed by supported titanium catalyst $TiCl_4/MgCl_2$	
Biosynthesis		few species of higher plants have been shown to produce polyisoprene in the all *trans*-l,4 configuration; these include Gutta Percha from *Palaqium gutta* and Balata from *Mimusops balata* which are typical high molecular weight trans-polyisoprenes occurring as latex; *Achras sapota* produces low molecular-weight *trans*-polyisoprene as a mixture with high molecular weight *cis*-polisoprene in latex form	
Temperature of polymerization	°C	20-40	
Time of polymerization	h	40	
Catalyst	-	$TiCl_4/MgCl_2$	Huang, B; Zhao, Z; Yao, W; Du, A; Zhao, Y, US Patent 7,718,742, Qingdao Qust Fangtai Material Engineering, 2010.
Yield	%	95	
Number average molecular weight, M_n	dalton, g/mol, amu	2,560-1,199,400	
Mass average molecular weight, M_w	dalton, g/mol, amu	5,000-500,000	
Polydispersity, M_w/M_n	-	1.04-1.11	
Molar volume at 298K	cm^3 mol^{-1}	64.7 (crystalline)	
Van der Waals volume	cm^3 mol^{-1}	47.5 (crystalline)	
STRUCTURE			
Crystallinity	%	34	

PIP, *trans* *trans*-polyisoprene

PARAMETER	UNIT	VALUE	REFERENCES
Cell type (lattice)	-	monoclinic (α), orthorhombic (β)	
Trans content	%	97 (guttapercha); 92-99+ (synthetic)	
COMMERCIAL POLYMERS			
Some manufacturers	-	Kuraray	
PHYSICAL PROPERTIES			
Density at 25°C	g cm^{-3}	0.90-0.95	
Color	-	white	
Odor		odorless	
Melting temperature, DSC	°C	58-67	
Glass transition temperature	°C	-63 to -68	
Surface tension	mN m^{-1}	31	Lee, L H, J. Polym. Sci. A-2, 5, 1103, 1967.
Permeability to nitrogen, 25°C	cm^3 cm cm^{-2} s^{-1} Pa^{-1} x 10^{12}	0.711	
Permeability to water vapor, 25°C	cm^3 cm cm^{-2} s^{-1} Pa^{-1} x 10^{12}	172	
Diffusion coefficient of nitrogen	cm^2 s^{-1} $x10^6$	1.17	
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	19.6-36.7 (vulcanized)	
Elongation	%	250-400 (vulcanized)	
Shore A hardness	-	90-95 (vulcanized)	
Mooney viscosity	-	20-90	
CHEMICAL RESISTANCE			
Acid dilute/concentrated	-	poor	
Alkalis	-	fair	
Aliphatic hydrocarbons	-	poor	
Aromatic hydrocarbons	-	poor	
Esters	-	poor	
Greases & oils	-	poor	
Halogenated hydrocarbons	-	poor	
Ketones	-	fair	
Θ solvent, Θ-temp.=47.7, 60.0°C	-	dioxane, n-propyl acetate	
Good solvent	-	chlorinated hydrocarbons, cyclohexane, hydrocarbons, MIBK, toluene	
Non-solvent	-	acetone, alcohols, carboxylic acids	
TOXICITY			
HMIS: Health, Flammability, Reactivity rating	-	0/1/0	

PIP, *trans* *trans*-polyisoprene

PARAMETER	UNIT	VALUE	REFERENCES
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
OSHA	mg m^{-3}	5	
PROCESSING			
Typical processing methods	-	calendering, extrusion, mixing, molding, vulcanization	
Additives used in final products	-	Fillers: calcium carbonate, carbon black, carbon fiber, graphite, kaolin, montmorillonite, silica, silicates, titanium dioxide, zinc oxide	
Applications	-	use in more than 40,000 products; ablatives, aircraft tires, dental (root filling material), electrochemical cell components, pressure-sensitive adhesives, and many more	
ANALYSIS			
FTIR (wavenumber-assignment)	cm^{-1}/-	C=O: 1690 (carboxyl), 1720 (aldehyde), 1745 (ketone); 855 - *trans*-isoprenyl unit	
Raman (wavenumber-assignment)	cm^{-1}/-	CH_3 – 2970, 2960; CH_2 – 2932, 2906; C=C – 1662; C-C – 1098, 1010, 985	Arjunan, Subramanian, S; Mohan, S; Spectrochim. Acta, 57A, 2547-54, 2001.