CR polychloroprene

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	polychloroprene, neoprene	
CAS name	-	1,3-butadiene, 2-chloro-, homopolymer	
Acronym	-	CR	
CAS number	-	9010-98-4	
RTECS number	-	EI9640000	
HISTORY			
Person to discover	-	Wallace Carothers and Julius Arthur Nieuwland	
Date	-	April 17, 1930	
Details	-	polychloroprene was invented by DuPont scientists on April 17, 1930 after Dr. Elmer K. Bolton of DuPont laboratories attended a lecture by Fr. Julius Arthur Nieuwland, a professor of chemistry at the University of Notre Dame. Fr. Nieuwland's research was focused on acetylene chemistry and during the course of his work he produced divinyl acetylene, a jelly that firms into an elastic compound similar to rubber when passed over sulfur dichloride. After DuPont purchased the patent rights from the university, Wallace Carothers of DuPont took over commercial development of Nieuwland's discovery in collaboration with Nieuwland himself. DuPont focused on monovinyl acetylene and reacted the substance with hydrogen chloride gas, manufacturing chloroprene.	
SYNTHESIS			
Monomer(s) structure	-	chloroprene, C_4H_5Cl	
Monomer(s) CAS number(s)	-	126-99-8	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	88.54	
Monomer ratio	-	100%	
Formulation example	-	n-dodecyl mercaptan (and sometimes xanthogen disulfide) is used as a chain transfer agent in linear grades; slow crystallizing grades are copolymerized with 2,3-dichloro-1,3-butadiene	
Method of synthesis	-	butadiene is converted into the monomer 2-chlorobutadiene-1,3 (chloroprene) via 3,4-dichlorobutene-1, and monomer is then polymerized by free radical emulsion polymerization using batch or continuous process. The polymerization is stopped at desired conversion by stopping agent. Finally the latex is freeze-coagulated to form a thin sheet. After washing and drying, it is shaped into a rope and chopped to chips or granules.	
Heat of polymerization	J g^{-1}	768	
Mass average molecular weight, M_w	dalton, g/mol, amu	140,000	Le Gac, P Y; Roux, G; Verdu, J; Davies, P; Fayolle, B, Polym. Deg. Stab., 109, 175-83, 2014.
Molar volume at 298K	cm^3 mol^{-1}	65.0 (crystalline)	
Van der Waals volume	cm^3 mol^{-1}	45.6 (crystalline)	
STRUCTURE			
Crystallinity	%	18-34	
Cell type (lattice)	-	monoclinic	

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Cell dimensions	nm	a:b:c=1.325:0.763:1.415 (macromer); 0.917:0.992:1.22 (crosslinked rubber)	
Crosslink density	mol kg^{-1}	0.18	Le Gac, P Y; Roux, G; Davies, P; Fayolle, B; Verdu, J, Polymer, 55, 2861-6, 2014.
Tacticity	%	trans: 70-90 (cis - 5-10)	
Rapid crystallization temperature	^oC	-5	
COMMERCIAL POLYMERS			
Some manufacturers	-	DuPont, Bayer, EniChem, Denki Kagaku Kogyo	
Trade names	-	Neoprene	
PHYSICAL PROPERTIES			
Density at 20^{o}C	g cm^{-3}	1.22-1.25	
Color	-	white, amber, gray	
Refractive index, 20^{o}C	-	1.552-1.558	
Odor	-	odorless, mild	
Melting temperature, DSC	^oC	45-92; 70 (cis); 80-115 (trans)	
Decomposition temperature	^oC	>200	
Thermal expansion coefficient, 23-80^{o}C	$^oC^{-1}$	6E-4	
Thermal conductivity, 20^{o}C	W m^{-1} K^{-1}	0.15-0.19	
Glass transition temperature	^oC	-25 to -46; -20 (cis)	
Specific heat capacity	J K^{-1} kg^{-1}	2200	
Heat of fusion	kJ mol^{-1}	8.37	
Hansen solubility parameters, δ_D, δ_P, δ_H	$MPa^{0.5}$	18.1, 4.3, 6.7	
Interaction radius		8.9	
Hildebrand solubility parameter	$MPa^{0.5}$	calc.=16.59-19.19; exp.=17.6-19.13	
Surface tension	mN m^{-1}	43.8	Wu, S, Adhesion, 5, 39, 1973.
Dielectric constant at 100 Hz/1 MHz	-	5-9	
Surface resistivity	ohm	9E6 to 8.4E10 (antistatic)	
Permeability to nitrogen, 25^{o}C	cm^3 cm cm^{-2} s^{-1} Pa^{-1} x 10^{12}	0.088	
Permeability to oxygen, 25^{o}C	cm^3 cm cm^{-2} s^{-1} Pa^{-1} x 10^{12}	0.296	
Permeability to water vapor, 25^{o}C	cm^3 cm cm^{-2} s^{-1} Pa^{-1} x 10^{12}	68.3	
Diffusion coefficient of nitrogen	cm^2 s^{-1} $x10^6$	0.24	
Diffusion coefficient of oxygen	cm^2 s^{-1} $x10^6$	0.38	

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PARAMETER	UNIT	VALUE	REFERENCES
Surface free energy	mJ m^{-2}	40.9	
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	10.3-20.9	
Tensile stress at yield	MPa	0.57	
Elongation	%	380-955	
Tear strength	N mm^{-1}	8.8-50	
Compression set, 24h 70°C	%	10-32	
Shore A hardness	-	42-85	
Brittleness temperature (ASTM D746)	°C	-35 to -55	
Mooney viscosity	-	34-59	
Water absorption, equilibrium in water at 23°C	%	0.9	
CHEMICAL RESISTANCE			
Acid dilute/concentrated	-	good	
Alcohols	-	good	
Alkalis	-	good	
Aliphatic hydrocarbons	-	good	
Aromatic hydrocarbons	-	fair to poor	
Esters	-	fair to poor	
Greases & oils	-	poor	
Ketones	-	fair to poor	
Θ solvent, Θ-temp.=	-	butanone, cyclohexane, trans-decalin	
FLAMMABILITY			
Ignition temperature	°C	>260	
Limiting oxygen index	% O_2	28-47; 46-59 (with FR)	Hornsby, P R, Cusack, P A, Antec, 3310-12, 1998; Hornsby, P R; Mitchell, P A; Cusack, P A, Polym. Deg. Stab., 32, 299-312, 1991.
Heat release	kW m^{-2}	314	
NBS smoke chamber	Ds	800	Hornsby, P R; Mitchell, P A; Cusack, P A, Polym. Deg. Stab., 32, 299-312, 1991.
Char at 500°C	%	12.9	Lyon, R E; Walters, R N, J. Anal. Appl. Pyrolysis, 71, 27-46, 2004.
WEATHER STABILITY			
Important initiators and accelerators	-	$FeCl_3$	Freitas, A R; Vidotti, G J; Rubira, A F; Muniz, E C, Polym. Deg. Stab., 87, 425-32, 2005.
Products of degradation	-	conjugated double bonds	
Stabilizers	-	UVA: dialkyl aryl substituted triazine; Screener: carbon black; Phenolic antioxidant: isotridecyl-3-(3,5-di-tert-butyl-4-hydroxy-phenyl) propionate; 2,2'-isobutylidenebis(2,4-dimethylphenol); phenol, 4-methyl-, reaction products with dicyclopentadiene and isobutene; Thiosynergist: 4,6-bis(dodecylthiomethyl)-o-cresol; Amine: nonylated diphenylamine	

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PARAMETER	UNIT	VALUE	REFERENCES
TOXICITY			
NFPA: Health, Flammability, Reactivity rating	-	0/1/0	
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
TLV, ACGIH	mg m^{-3}	2 (talc)	
OSHA	mg m^{-3}	3.3 (talc)	
Oral rat, LD_{50}	mg kg^{-1}	>5,000; >20,000	
PROCESSING			
Typical processing methods	-	calendering, compounding in solution, dip coating, extrusion, molding (compression, injection), sheeting, vulcanization	
Processing temperature	^{o}C	50-100 (sheet calendering), 40-100 (extrusion)	
Additives used in final products	-	Fillers: carbon black, fumed silica, magnesium oxide, zinc oxide in EMI shielding field: montmorillonite, nickel and carbon black, silver, silver coated glass spheres, silver plated copper, silver plated aluminum, silver plated nickel; Other: acid acceptors (MgO, red lead), vulcanizing agent (ZnO), vulcanization accelerator (thioureas, sulfur-based), vulcanization retarder (MBTS, CBS, TMTD), antioxidant (octylated diphenylamine), antiozonant (diaryl-p-phenylene diamines with selected waxes up to 3 phr), plasticizers (aromatic or naphthenic process oils, mono esters, polyester, chlorinated waxes) processing aids (stearic acid, waxes, low molecular weight polyethylene, high-cis polybutadiene, special factices)	Neoprene, a guide to grades, compounding and processing neoprene rubber, DuPont, Oct. 2008.
Applications	-	adhesives, automotive gaskets, bitumen additive, cellular products, construction applications (bridge pads/seals, soil pipe gaskets, waterproof membranes, asphalt modification), CVJ boots and air springs, foamed wet suits, hose, foam, latex dipped goods (gloves, weather balloons, automotive), paper, and industrial binders (shoe board), molded and extruded goods, protective coatings, power transmission belts, sealants, seals, tear-resistant rubber, tubes and covers (auto and industrial), water-swellable rubber, wire and cable jacketing	
Outstanding properties	-	mechanical strength, ozone and weather resistance, low flammability, chemical resistance, good adhesion	
BLENDS			
Suitable polymers	-	NR, epoxidized polyisoprene	Freitas, A R; Gaffo, L; Rubira, A F; Muniz, E C, J. Molec. Liq., 190, 146-50, 2014.
ANALYSIS			
FTIR (wavenumber-assignment)	cm^{-1}/-	C=O – 1725, C=C – 1695, 1660; CH_2 – 1444, 1431, C-Cl – 658, 602	O'Keefe, J F, Rubber World, June 2004, 27-37.
x-ray diffraction peaks	degree	see reference	Sathasivam, K; Haris, M; Mohan, S, Intl. J. Chem. Res., 2, 3, 1780-85, 2010.