CN cellulose nitrate

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	cellulose nitrate, nitrocellulose	
CAS name	-	cellulose, nitrate	
Acronym	-	CN	
CAS number	-	9004-70-0	
RTECS number	-	QW0970000	
HISTORY			
Person to discover	-	Henri Braconnot; Alexander Parker	
Date	-	1832; 1855	
Details	-	Henri Braconnot discovered that nitric acid with starch or wood fibers produces explosive material; Alexander Parker invented celluloid	
SYNTHESIS			
Monomer(s) structure	-	cellulose; HNO_3	
Monomer(s) CAS number(s)	-	9004-34-6; 7697-37-2	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	depends on raw material; 63.012	
Nitrification degree	%	76-89 (lacquer grades); >87 (explosive grades)	
Nitrogen content	%	11.1-12.2 (non-explosive because their nitrogen content is less than 12.%) 12.55-13.42 (explosive)	Alinat, E; Delaunay, N; Archer, X; Gareil, P, Carbohydrate Polym., 128, 99-104, 2015; Alinat, E; Delaunay, N; Archer, X; Vial, J; Gareil, P, Forensic Sci. Int., 250, 68-76, 2015.
Method of synthesis	-	concentrated sulfuric acid and 70% nitric acid are mixed with cellulose at 0°C to produce nitrocellulose	
Temperature of polymerization	°C	0	
Yield	%	35-100	Adekunle, I M, E-J. Chem., 7, 3, 709-16, 2010.
Mass average molecular weight, M_w	dalton, g/mol, amu	125,000-150,00; 750,000-875,000 (dynamite) 20,000-312,000 (non-explosive) 69,000-200,000	Alinat, E; Delaunay, N; Archer, X; Gareil, P, Carbohydrate Polym., 128, 99-104, 2015; Alinat, E; Delaunay, N; Archer, X; Vial, J; Gareil, P, Forensic Sci. Int., 250, 68-76, 2015.
Polymerization degree (number of monomer units)	-	500-600; 3,000-5,000 (dynamite)	
Radius of gyration	nm	6.3-34.1	Alinat, E; Delaunay, N; Archer, X; Gareil, P, Carbohydrate Polym., 128, 99-104, 2015.
STRUCTURE			
Cell type (lattice)	-	orthorhombic	Meader, D; Atkins, E; Happey, T, Polymer 19, 1371, 1978.
Cell dimensions	nm	a:b:c=1.22:2.54:0.90	Meader, D; Atkins, E; Happey, T, Polymer 19, 1371, 1978.
PHYSICAL PROPERTIES			
Density at 20°C	g cm^{-3}	1.35-1.40	
Color	-	white to yellow	
Refractive index, 20°C	-	1.49-1.51	
Odor	-	odorless	

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PARAMETER	UNIT	VALUE	REFERENCES
Melting temperature, DSC	^oC	142-170 (ignites); 169-170	Kim, D H, Reference Module in Biochemical Science from Encyclopedia of Toxicology, 3rd Ed., Elsevier, 2014, pp. 540-42.
Decomposition temperature	^oC	>170	
Thermal expansion coefficient, 23-80^{o}C	$^oC^{-1}$	0.8-1.2E-4	
Thermal conductivity, melt	W m^{-1} K^{-1}	0.23	
Glass transition temperature	^oC	53-66	
Heat of fusion	kJ mol^{-1}	3.8-6.3	
Long term service temperature	^oC	-20 to 70	
Heat deflection temperature at 1.8 MPa	^oC	60-71	
Hansen solubility parameters, δ_D, δ_P, δ_H	$MPa^{0.5}$	16.2, 14.1, 9.5; 15.4, 14.7, 8.8	
Interaction radius		10.7; 11.5	
Hildebrand solubility parameter	$MPa^{0.5}$	21.4-23.5	
Surface tension	mN m^{-1}	calc.=38.0	
Dielectric constant at 100 Hz/1 MHz	-	7/6	
Power factor	-	3-5	
Permeability to nitrogen, 25^{o}C	cm^3 cm cm^{-2} s^{-1} Pa^{-1} x 10^{12}	0.0087	
Permeability to oxygen, 25^{o}C	cm^3 cm cm^{-2} s^{-1} Pa^{-1} x 10^{12}	0.146	
Permeability to water vapor, 25^{o}C	cm^3 cm cm^{-2} s^{-1} Pa^{-1} x 10^{12}	472	
Diffusion coefficient of nitrogen	cm^2 s^{-1} $x10^6$	0.0193	
Diffusion coefficient of oxygen	cm^2 s^{-1} $x10^6$	0.15	
Diffusion coefficient of water vapor	cm^2 s^{-1} $x10^6$	0.0262	
Contact angle of water, 20^{o}C	degree	54.7	
Surface free energy	mJ m^{-2}	42.7	
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	35-70	
Elongation	%	10-40	
Flexural strength	MPa	62-76	
Flexural modulus	MPa	1,300-1,500	
Compressive strength	MPa	14-55	
Izod impact strength, notched, 23^{o}C	J m^{-1}	270-370	

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PARAMETER	UNIT	VALUE	REFERENCES
Rockwell hardness	-	R95-115	
Water absorption, equilibrium in water at 23°C	%	0.6-2.0	
Moisture absorption, equilibrium 23°C/50% RH	%	1	
CHEMICAL RESISTANCE			
Acid dilute/concentrated	-	poor	
Alcohols	-	good	
Aromatic hydrocarbons	-	fair	
Esters	-	poor	
Halogenated hydrocarbons	-	poor	
Ketones	-	poor	
Good solvent	-	acetic acid (glacial), acetone, amyl acetate, ethylene glycol ethers	
Non-solvent	-	higher alcohols, higher carboxylic acids, higher ketones	
FLAMMABILITY			
Ignition temperature	°C	140	
Autoignition temperature	°C	140	
Flash point	°C	12.8	Kim, D H, Reference Module in Biochemical Science from Encyclopedia of Toxicology, 3rd Ed., Elsevier, 2014, pp. 540-42.
Volatile products of combustion	-	H_2O, CO, CO_2, NO_x	
WEATHER STABILITY			
Spectral sensitivity	nm	285	
Important initiators and accelerators	-	NO_x (autocatalytic process)	
Products of degradation	-	chain scission, radical formation	
Stabilizers	-	diphenylamine, 2-nitrodiphenylamine	
TOXICITY			
NFPA: Health, Flammability, Reactivity rating	-	2/3/3	
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	Kim, D H, Reference Module in Biochemical Science from Encyclopedia of Toxicology, 3rd Ed., Elsevier, 2014, pp. 540-42.
Mutagenic effect	-	not listed	
TLV, ACGIH	mg m^{-3}/ ppm	n/a	
NIOSH	mg m^{-3}/ ppm	n/a	
MAK/TRK	mg m^{-3}/ ppm	n/a	
OSHA	mg m^{-3}/ ppm	n/a	

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PARAMETER	UNIT	VALUE	REFERENCES
Oral rat, LD_{50}	mg kg^{-1}	>5,000; 8798-10,373 (no observable adverse effect)	Kim, D H, Reference Module in Biochemical Science from Encyclopedia of Toxicology, 3rd Ed., Elsevier, 2014, pp. 540-42.
ENVIRONMENTAL IMPACT			
Aquatic toxicity, algae, LC_{50}, 48 h	mg l^{-1}	579	Kim, D H, Reference Module in Biochemical Science from Encyclopedia of Toxicology, 3rd Ed., Elsevier, 2014, pp. 540-42.
PROCESSING			
Typical processing methods	-	blow molding, casting, compounding, compression molding, machining	
Processing temperature	°C	85-93 (compression molding)	
Processing pressure	MPa	14-34 (compression molding)	
Additives used in final products	-	Plasticizers: 2-ethylhexyl diphenyl phosphate, acetyl tributyl citrate, acrylic resin (Acronal 700 L), aliphatic polyurethane, butyl benzyl phthalate, camphor (plasticizer of celluloid), castor oil, dibutyl phthalate, dimethyl phthalate, diisooctyl phthalate, epoxidized soybean oil, glyceryl triacetate, glyceryl tribenzoate, glyceryl tribenzoate, N-ethyl (o,p)-toluenesulfonamide, octyl diphenyl phosphate, sucrose acetate isobutyrate, tricresyl phosphate, triethylene glycol, urea resin; Antistatics: poly(3,4-ethylenedioxythiophene sulfonate), vanadium pentoxide; Slip: alumina, silica; Amines (stabilizers of gunpowder)	
Applications	-	celluloid, electroexplosive devices, explosives, lacquers	
BLENDS			
Suitable polymers	-	CA, PEG, PMMA	