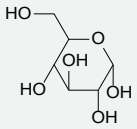
C cellulose

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	cellulose	
IUPAC name	-	cellulose; 2-(hydroxymethyl)-6-[4,5,6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy-oxane-3,4,5-triol	
Acronym	-	C	
CAS number	-	9004-34-6	
EC number	-	232-674-9	
RTECS number	-	FJ5691460	
HISTORY			
Person to discover	-	Emil Fischer	
Date	-	1891-1894	
Details	-	in 1902 Fischer received Nobel Price for establishing structure of carbohydrates, including cellulose	
SYNTHESIS			
Monomer(s) structure	-		
Monomer(s) CAS number(s)	-	50-99-7	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	180.16	
Monomer ratio	-	100%	
Number-average molecular weight		36000-40000	Roig, F; Dantras, E; Dandurand, J; Lacabanne, C, J. Phys. D: Appl. Phys., 44, 045403, 2011.
Particle length	nm	700-1100 (nanofibrils)	Ladhar, A; Arous, M; Kaddami, H; Raihane, M; Kallel, A; Graca, M P F; Costa, L C, J. Mol. Liq., 209, 272-9, 2015.
Particle diameter	nm	8-12.5 (nanofibrils)	Ladhar, A; Arous, M; Kaddami, H; Raihane, M; Kallel, A; Graca, M P F; Costa, L C, J. Mol. Liq., 209, 272-9, 2015.
Cellulose content in some natural products	%	cotton – 94, hemp – 77, flax, kapok, sisal – 75, wood – 40-50, straw – 40-50	
Method of synthesis	-	bacterial cellulose can be biosynthesized by *Gluconacetobacter* sp. and some other bacteries	Pokalwar, S U; Mishra, M K; Manwar, A V, Recent Res. Sci. Technol., 2, 7, 14-19, 2010.
Mass average molecular weight, M_w	dalton, g/mol, amu	160,000-560,000	
Polymerization degree (number of monomer units)	-	300-1700 (wood); 800-10,000 (cotton), 1,000-3,000 (purified cotton); 200-600 (regenerated cellulose; e.g., rayon)	
STRUCTURE			
Crystallinity	%	40-60 (typical); 75 (cotton); 60 (wood pulp); 46-51 (switchgass leaves); 35 (regenerated cellulose); 25 (viscose)	
Cell type (lattice)	-	triclinic/monoclinic (I); monoclinic (II)	
Cell dimensions	nm	a:b:c=0.835:0.70:1.03 (I); a:b:c=0.81:0.904:1.036 (II); a:b:c=1.025:0.778:1.034 (III); a:b:c=0.803:0.813:1.034 (allomorph IV/I); a:b:c=0.799:0.81:1.034 (allomorph IV/II)	Perez, S; Samain, D, Adv. Carbohydrate Chem. Biochem., 64, 25-116, 2010.
Unit cell angles	degree	γ= 84 (I); γ=117 (II); γ=122.4	

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PARAMETER	UNIT	VALUE	REFERENCES
Number of chains per unit cell	-	2 (I); 2 (II)	
Crystallite size	nm	5-6 (cotton); 5.8-7 (wood pulps); 2-3.1 (viscose)	
Polymorphs	-	I, II (marine algae; occurs when form I is treated with NaOH), III (ammonia treatment of I and II gives III), and IV (heating of III generates IV)	
Chain conformation	-	gauche-gauche, gauche-trans, trans-gauche; P2/1 (I); P2/1 (II)	
Heat of crystallization	kJ kg^{-1}	105-134	
COMMERCIAL POLYMERS			
Some manufacturers	-	Sigma-Aldrich	
PHYSICAL PROPERTIES			
Density at 20°C	g cm^{-3}	1.54-1.57; 1.59-1.63 (crystalline); 1.482-1.489 (amorphous)	
Bulk density at 20°C	g cm^{-3}	0.3	
Color	-	white	
Refractive index, 20°C	-	1.534-1.618	
Birefringence	-	1.573-1.595/1.527-1.534	
Haze	%	4	
Gloss, 60°, Gardner (ASTM D523)	%	90	
Odor	-	none	
Melting temperature, DSC	°C	260-270 (decomp.)	
Thermal expansion coefficient, 23-80°C	$°C^{-1}$	0.2-1.6E-5	
Thermal conductivity, melt	W m^{-1} K^{-1}	0.054-0.13	
Glass transition temperature	°C	220-245	
Specific heat capacity	J K^{-1} kg^{-1}	1364 (wood); 1318 (cotton)	
Activation energy of thermal degradation	kJ mol^{-1}	225-238 (pellets and powder); 120 (fiber)	Roig, F; Dantras, E; Dandurand, J; Lacabanne, C, J. Phys. D: Appl. Phys., 44, 045403, 2011.
Maximum service temperature	°C	225	
Hildebrand solubility parameter	$MPa^{0.5}$	18.03-32.02	
Surface tension	mN m^{-1}	36-42 (regenerated from pulp); 42 (regenerated from cotton)	
Dielectric constant at 100 Hz/1 MHz	-	3-7.5	
Dielectric loss factor at 1 kHz	-	0.02	
Surface resistivity	ohm	1E16 (pure cellulose); 2.4E7 (raw cotton); 1E4 (viscose)	
Electric strength K20/P50, d=0.60.8 mm	kV mm^{-1}	30-50	
Coefficient of friction	-	0.2 (dynamic); 0.25 (static)	
Permeability to nitrogen, 25°C	cm^3 cm cm^{-2} s^{-1} Pa^{-1} x 10^{-13}	0.02-0.06	
Permeability to oxygen, 25°C	cm^3 cm cm^{-2} s^{-1} Pa^{-1} x 10^{-13}	0.004-0.04	

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PARAMETER	UNIT	VALUE	REFERENCES
Permeability to water vapor, 25°C	cm^3 cm cm^{-2} s^{-1} Pa^{-1} x 10^{-13}	20,000	
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	69-170 (regenerated); 50-120 (cellophane); 2.2-5.9 (pulp handsheets)	Spence, K L; Venditti, R A; Habibi, Y; Rojas, O J; Pawlak, J J, Bio-resource Technol., 101, 5961-68, 2010.
Tensile modulus	MPa	3,000-5,000	
Tensile creep modulus, 1000 h, elongation 0.5 max	MPa	70-125	
Elongation	%	18-70 (film); 6-10 (fiber); 22-70 (regenerated)	
Young's modulus	MPa	137,000 (crystalline microfibril); 3,490-9,080 (microcrystalline)	Orts, W J; Imam, S H; Glenn, G M; Inglesby, M K; Guttman, M E; Nguyen, A; Revol, J-F, Antec, 2427-31, 2004; Roberts, R J; Rowe, R C; York, P, Int. J. Pharmaceutics, 105, 177-80, 1994.
Tenacity (fiber) (standard atmosphere)	cN tex^{-1} (daN mm^{-2})	18-75 (25-125)	Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.
Tenacity (wet fiber, as % of dry strength)	%	40-110	Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.
Fineness of fiber (titer)	dtex	1.3-3.6	Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.
Length (elemental fiber)	mm	25-220	Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.
Poisson's ratio	-	0.30 (microcrystalline)	Roberts, R J; Rowe, R C; York, P, Int. J. Pharmaceutics, 105, 177-80, 1994.
CHEMICAL RESISTANCE			
Acid dilute/concentrated	-	good-poor	
Alcohols	-	good	
Alkalis	-	poor	
Aliphatic hydrocarbons	-	good	
Aromatic hydrocarbons	-	good	
Esters	-	good	
Greases & oils	-	good	
Halogenated hydrocarbons	-	good	
Ketones	-	good	
Good solvent	-	alkalies, calcium thiocyanate, sodium xantanate, phosphoric acid, sulfuric acid	
Non-solvent	-	diluted alkalies and acis, hydrocarbons, mineral oils, water, organic solvents	

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PARAMETER	UNIT	VALUE	REFERENCES
FLAMMABILITY			
Ignition temperature	°C	390-420	
Autoignition temperature	°C	400-410	
Limiting oxygen index	% O_2	18-20; 22.8-30.3 (treated cellulose)	Gaan, S; Rupper, P; Salimova, V; Heuberger, M, Polym. Deg. Stab., 94, 1125-34, 2009.
Heat release	kW m^{-2}	197; 130-190 (treated cellulose)	Gaan, S; Rupper, P; Salimova, V; Heuberger, M, Polym. Deg. Stab., 94, 1125-34, 2009.
Burning rate (Flame spread rate)	mm min^{-1}	195-399	Flisi, U, Polym. Deg. Stab., 30, 153-68, 1990.
Char at 500°C	%	7.8; 8-22.6 (treated cellulose)	
Heat of combustion	J g^{-1}	15,090-18,855	
WEATHER STABILITY			
Spectral sensitivity	nm	328 (rayon); 290-340 (without oxygen), 290-380 (with oxygen)	
Activation energy of photo-oxidation	kJ mol^{-1}	79 (bond scission)	Hill, D J T; Lee, T T; Darveniza, M; Saha, T, Polym. Deg. Stab., 48, 79, 1995.
Depth of UV penetration	μm	500-2500 (depth of lignin degradation)	
Important initiators and accelerators	-	nitroxyl radicals, ozone, thermal degradation	Biliuta, G; Fras, L; Strnad, S; Harabagiu, V; Coseri, S, J. Polym. Sci., Part A: Polym. Chem., 48, 4790-99, 2010.
Products of degradation	-	bond scission	
Stabilizers	-	UVA: 2-(2H-benzotriazol-2-yl)-p-cresol; phenol, 2-(5-chloro-2H-benzotriazole-2-yl)-6-(1,1-dimethylethyl)-4-methyl-; 2-(2H-benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl)phenol; isopropenyl ethinyl trimethyl piperidol (cellulose diacetate), biphenyl cellulose (UV absorber fro paper), phenylbenzimid-azole (reactive stabilizer for application in cellulosic textiles); Optical brighteners: 2,2'-(2,5-thiophenediyl)bis(5-tert-butyl-benzoxazole); Mixtures: an ortho-hydroxy tris-aryl-s-triazine compound+hindered hydroxybenzoate compound+hindered amine compound containing a 2,2,6,6-tetraalkylpiperidine or 2,2,6,6-tetraalkylpiperazinone radical	
BIODEGRADATION			
Typical biodegradants	-	β-glucosidase	
Stabilizers	-	borate base supplemented with azole or thujaplicin; guar gum benzamide is water resistant biocide	Clausen, C A; Yang, V, Int. Biode-ter. Biodeg., 59, 20-24, 2007Das, D; Ara, T; Dutta, S; Mukherjee, A, Bioresource Technol., 102, 5878-83, 2011.
TOXICITY			
NFPA: Health, Flammability, Reactivity rating	-	0-2/1-2/0	
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
TLV, ACGIH	mg m^{-3}	3 (respirable), 10 (total)	
NIOSH	mg m^{-3}	5 (respirable), 10 (total)	
OSHA	mg m^{-3}	5 (respirable), 15 (total)	
Oral rat, LD_{50}	mg kg^{-1}	>5,000	
Skin rabbit, LD_{50}	mg kg^{-1}	>2,000	

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PARAMETER	UNIT	VALUE	REFERENCES
ENVIRONMENTAL IMPACT			
Aquatic toxicity, Daphnia magna, LC_{50}, 48 h	mg l^{-1}	<1,000 to 111,000	Dave, G; Aspegren, P, Ecotoxicology Env. Safety, 73, 1629-32, 2010.
Biological oxygen demand, BOD_5	mg l^{-1}	148-163	Boroski, M; Rodriques, A C; Carcia, J C; Gerola, A P; Nozaki, J; Hioka, N, J. Hazardous Mater., 160, 135-41, 2008.
Chemical oxygen demand	mg O_2 g^{-1}	1193	Raposo, F; de la Rubia, M A; Borja, R; Alaiz, M, Talanta, 76, 448-53, 2008.
Theoretical oxygen demand	mg O_2 g^{-1}	1184	Raposo, F; de la Rubia, M A; Borja, R; Alaiz, M, Talanta, 76, 448-53, 2008.
PROCESSING			
Typical processing methods	-	paper and pulp processing methods, chemical processing methods used to produce cellulose derivatives, spinning (rayon), compounding (adhesives and binders), extrusion (cellophane)	
Applications	-	conversion products (e.g., cellophane, rayon, etc.), derivatives (e.g., cellulose acetate, nitrocellulose, etc), fiber, medical (wound dressings, bandages), paper, reinforcement, textiles, thickeners, and many other	
ANALYSIS			
Raman (wavenumber-assignment)	cm^{-1}/-	C-H – 2800-3000; O-H – 1475, 1640; water – 1640	Fechner, P M; Wartewig, S; Füting, M; Heilmann, A; Neuber,t R H H; Kleinebudde, P, AAPS PharmaSci., 5, 4, art. 31, 2003.