CTA cellulose triacetate

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	cellulose triacetate	
Acronym	-	CTA	
CAS number	-	9012-09-3	
HISTORY			
Person to discover	-	Walker, W H	Walker, W H, US Patent, 774,714, Nov. 8, 1904.
Date	-	1904; 1954	
Details	-	Walker patented production of cellulose acetate; first commercially produced by Celanese and Eastman Chemical	
SYNTHESIS			
Monomer(s) structure	-	cellulose; acetic acid	
Monomer(s) CAS number(s)	-	9004-34-6; 64-19-7	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	depends on raw material; 60.05	
Acetyl content	%	42.5-43.6; 60.7-61.2 (combined)	
Hydroxy content	%	0.82 (min. 92% hydroxyl groups must be acetylated)	
Degree of substitution		0.89-2.84	El Nemr, A; Ragab, S; El Sikaily, A; Khaled, A, Carbohydrate Polym., 130, 41-8, 2015.
Method of synthesis	-	see cellulose acetate	
Catalyst	-	N-iodosuccinimide	El Nemr, A; Ragab, S; El Sikaily, A; Khaled, A, Carbohydrate Polym., 130, 41-8, 2015.
Number average molecular weight, M_n	dalton, g/mol, amu	30,000-350,000	Fredercik, T J; Godfrey, D A, US Patent 6,683,174, Eastman, 2004; Shimada, H; Nobucawa, S; Yamaguchi, M, Carbohydrate Polym., 120, 22-8, 2015.
Mass average molecular weight, M_w	dalton, g/mol, amu	14,000-408,000	Fredercik, T J; Godfrey, D A, US Patent 6,683,174, Eastman, 2004.
Polydispersity, M_w/M_n	-	3.32-6.11	
Polymerization degree (number of monomer units)	-	165-1670	
Radius of gyration	nm	7.01-7.55	Nair, P R M; Gohil, R M; Patel, K C; Patel, R D, Eur. Polym. J., 13, 273-76, 1977.
STRUCTURE	-		
Crystallinity	%	24-40; 42 (210°C), 72.2 (250°C), 99.5 (290°C)	Hindeleh, A M; Johnson, D J, Polymer, 11, 12, 666-680, 1970.
Cell type (lattice)	-	monoclinic	
Cell dimensions	nm	a=0.5939, b=1.1431, c=1.046	Sikorski, P; Wada, M; Heux, L; Shintani, H; Stokke, B T, Macromolecules, 37, 12, 4547-53, 2004.
Unit cell angles	degree	γ=95.4	Sikorski, P; Wada, M; Heux, L; Shintani, H; Stokke, B T, Macromolecules, 37, 12, 4547-53, 2004.
Number of chains per unit cell	-	2	
Crystallite size	nm	10-20 molecules	

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Polymorphs	-	I (one chain monoclinic), II, N	Zugenmaier, P, Macromol. Symp., 208, 81-166, 2004; Numata, Y; Kumagai, H; Kono, H; Erata, T; Takai, M, Sen'I Gakkaishi, 60, 3, 75-80, 2004.
Chain conformation	-	2/1 helix	Sikorski, P; Wada, M; Heux, L; Shintani, H; Stokke, B T, Macromolecules, 37, 12, 4547-53, 2004.
COMMERCIAL POLYMERS			
Some manufacturers	-	Eastman	
Trade names	-	Cellulose Triacetate	
PHYSICAL PROPERTIES			
Density at 20°C	g cm^{-3}	1.28-1.34	
Color	-	off white	
Refractive index, 20°C	-	1.472-1.475	
Birefringence	-	-0.003; 0.051 to -0.30 (elongation ratio 0 to 30%)	Hayakawa, D; Ueda, K, Carbohydrate Res., 402, 146-51, 2015.
Transmittance	%	89-93	
Haze	%	0.2-7.6	
Odor	-	odorless	
Melting temperature, DSC	°C	230	
Softening point	°C	190-205	
Decomposition temperature	°C	>240	
Fusion temperature	°C	260	
Thermal expansion coefficient, 23-80°C	10^{-4} $°C^{-1}$	1.-1.5	
Glass transition temperature	°C	120-195	
Specific heat capacity	J K^{-1} kg^{-1}	1,500	
Molar volume	kmol m^{-3}	3.6; 5.0	
Hildebrand solubility parameter	$MPa^{0.5}$	18.84-19.4	Shimada, H; Nobucawa, S; Yamaguchi, M, Carbohydrate Polym., 120, 22-8, 2015.
Dielectric constant at 100 Hz/1 MHz	-	3.0-4.5	
Dielectric loss factor at 1 kHz	-	0.01-0.02	
Volume resistivity	ohm-m	1E11 to 1E13	
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	28-56	
Elongation	%	20-50	
Flexural strength	MPa	42-69	
Izod impact strength, notched, 23°C	J m^{-1}	1.1-4.5	
Intrinsic viscosity, 25°C	dl g^{-1}	1.7	
Water absorption, equilibrium in water at 23°C	%	2-7	
Moisture absorption, equilibrium 23°C/50% RH	%	3	

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PARAMETER	UNIT	VALUE	REFERENCES
CHEMICAL RESISTANCE			
Acid dilute/concentrated	-	good/poor	
Aliphatic hydrocarbons	-	resistant	
Aromatic hydrocarbons	-	resistant	
Esters	-	non-resistant	
Greases & oils	-	resistant	
Ketones	-	non-resistant	
Θ solvent, Θ-temp.=27	-	acetone	
Good solvent	-	chloroform, dioxane, ethyl acetate, ethylene carbonate, methyl acetate, methylene chloride, THF, trichloroethane	
Non-solvent	-	aliphatic hydrocarbons, aliphatic ethers, chlorobenzene, dichloroethane, ethanol (absolute), MIBK, weak mineral acids	
FLAMMABILITY			
Ignition temperature	°C	>540	
Limiting oxygen index	% O_2	18.4	
Heat of combustion	J g^{-1}	20,230	
BIODEGRADATION			
Typical biodegradants	-	bacterium *Sphingomonas paucimobilis*	Abrusci, C; Marquina, D; Santos, A; Del Amo, A; Corralees, T; Catalina, F, Int. Biodet. Biodeg., 63, 759-64, 2009.
TOXICITY			
NFPA: Health, Flammability, Reactivity rating	-	0/2/0; 1/1/0 (HMIS)	
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
OSHA	mg m^{-3}	5 (respirable dust) 15 t(total dust)	
PROCESSING			
Additives used in final products	-	glycerin, triethyl citrate, dioctyl phthalate, diisodecyl adipate	Azadimanesh, F; Mohammadi, N, Carbohydrate Polym., 130, 316-24, 2015; Shimada, H; Nobucawa, S; Yamaguchi, M, Carbohydrate Polym., 120, 22-8, 2015.
Applications	-	clothing, coatings, consumer electronics, LCD displays, photo-graphic films, protective film for polarizing plate	
Outstanding properties	-	low shrinkage, wrinkle resistant, optical clarity	
ANALYSIS			
FTIR (wavenumber-assignment)	cm^{-1}/-	C=O – 1735; C-O – 1216, 1029	
NMR (chemical shifts)	ppm	carbonyl carbon 170.9, 172.2; ring carbon 80.6, 76.3, 72.9, 62.7; methyl carbon 23.2, 22.3	