CA cellulose acetate

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	cellulose acetate	
Acronym	-	CA	
CAS number	-	9004-35-7	
HISTORY			
Person to discover	-	Paul Schuetzenberger; Camille & Henri Dreyfus	
Date	-	1865; 1904	
Details	-	Dreyfus brothers begun experimental work on the development of cellulose acetate in 1904. In 1910 they opened a factory capable to produce 3 tons of cellulose acetate per day, mainly used as base for motion picture film and lacquer also used by growing aircraft industry for fabric coatings for wings and fuselage covering	
SYNTHESIS			
Monomer(s) structure	-	$(CH_3CO)_2O$; cellulose	
Monomer(s) CAS number(s)	-	108-24-7; 9004-34-6	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	102.09	
Acetyl content	%	32.0-60.9	
Hydroxyl content	%	3.5-8.7	
Formulation example	-	cellulose/acetic anhydride ratio = 3.43-10.29	Daud, W R W; Djuned, F M, Carbohydrate Polym., 132, 252-60, 2015.
Method of synthesis	-	cellulose derived from wood pulp is reacted with acetic anhydride in the presence of sulfuric acid, followed by the controlled partial hydrolysis in which sulfuric acid and some acetic acid groups are removed to achieve required degree of acetylation	
Temperature of polymerization	^{o}C	0-5 (1 h), 30 (3 h)	Shaikh, H M; Pandare, K V; Nair, G; Varma, A J, Carbohydrate Polym., 76, 23-29, 2009.
Time of polymerization	h	4-6; 1.5-3	Daud, W R W; Djuned, F M, Carbohydrate Polym., 132, 252-60, 2015.
Number average molecular weight, M_n	dalton, g/mol, amu	30,000-125,000	
Mass average molecular weight, M_w	dalton, g/mol, amu	45,000-237,000	Fischer, S; Thuemmler, K; Volkert, B; Hettrich, K; Schmidt, I; Fischer, K, Macromol. Symp., 262, 89-96, 2008.
Polydispersity, M_w/M_n	-	1.47-3.25	Fischer, S; Thuemmler, K; Volkert, B; Hettrich, K; Schmidt, I; Fischer, K, Macromol. Symp., 262, 89-96, 2008.
Polymerization degree (number of monomer units)	-	175-360	
Molar volume at 298K	$cm^3 mol^{-1}$	246-264	Necula, A M; Olaru, N; Olaru, L; Homocianu, M; Ioan, S, J. Appl. Polym. Sci., 115, 1751-57, 2010.

CA cellulose acetate

PARAMETER	UNIT	VALUE	REFERENCES
STRUCTURE			
Crystallinity	%	12; 28 (bacterial cellulose based)	Sousa, M; Bras, A R; Veiga, H I M; Ferreira, F C; de Pinho, M N; Correela, N T; Dionision, M, J. Phys. Chem. B, 114, 10939-53, 2010; Barud, H S; de Araujo, A M; Santos, D B; de Assuncao, R M N; Meireles, C S; Cerquira, D A; Filho, G R; Ribeiro, C A; Messsaddeq, Y; Ribeiro, S J L, Themochim. Acta, 471, 61-69, 2008.
Cell type (lattice)	-	orthorhombic	
Cell dimensions	nm	a:b:c=0.594:1.143:1.046	Perez, S; Samain, D, Adv. Carbohydrate Chem. Biochem., 64, 25-116, 2010.
Unit cell angles	degree	γ=95.4	
Number of chains per unit cell	-	1	
Chain conformation	-	2_1 helix	
COMMERCIAL POLYMERS			
Some manufacturers	-	Eastman	
Trade names	-	Cellulose Acetate, Estron and Chromspun (yarns)	
PHYSICAL PROPERTIES			
Density at 20°C	g cm^{-3}	1.27-1.34; 1.375 (crystalline)	
Bulk density at 20°C	g cm^{-3}	0.22-0.32; 0.43 (tapped)	
Color	-	white flakes	
Refractive index, 20°C	-	1.46-1.49	
Birefringence	-	0.005	
Transmittance	%	>90	
Haze	%	4-8.5	
Gloss, 60°, Gardner (ASTM D523)	%	95	
Odor	-	odorless	
Melting temperature, DSC	°C	230-260	
Softening point	°C	190-229	
Decomposition temperature	°C	304	
Thermal expansion coefficient, 23-80°C	10^{-4} °C^{-1}	0.8-1.8	
Thermal conductivity, melt	W m^{-1} K^{-1}	0.17-0.33	
Glass transition temperature	°C	173-203; 197 (DMTA); 190 (DSC); 185-193 (film); 136-148 (bagasse cellulose)	Sousa, M; Bras, A R; Veiga, H I M; Ferreira, F C; de Pinho, M N; Correela, N T; Dionision, M, J. Phys. Chem. B, 114, 10939-53, 2010; Yuan, J; Dunn, D; Clipse, N M; Newton, R J, Pharm. Technol., 88-100, 2009.
Specific heat capacity	J K^{-1} kg^{-1}	1,260-1,670	
Activation energy of thermal degradation	kJ mol^{-1}	83.9	
Long term service temperature	°C	-20 to 70	
Heat deflection temperature at 0.45 MPa	°C	52-105	

CA cellulose acetate

PARAMETER	UNIT	VALUE	REFERENCES
Heat deflection temperature at 1.8 MPa	°C	46-87	
Hansen solubility parameters, δ_D, δ_P, δ_H	$MPa^{0.5}$	17.1, 13.1, 9.4; 18.6, 12.73, 11.01	
Interaction radius		10.6;-	
Hildebrand solubility parameter	$MPa^{0.5}$	23.5-27.83	
Surface tension	$mN\ m^{-1}$	calc.=45.9	
Dielectric constant at 100 Hz/1 MHz	-	2.15-7/3.3-7	
Dissipation factor at 1 MHz	E-4	1500	
Volume resistivity	ohm-m	1E8 to 1E11 (varies with humidity)	
Electric strength K20/P50, d=0.60.8 mm	$kV\ mm^{-1}$	11-19	
Coefficient of friction	-	0.6 (dynamic); 0.7 (static)	
Permeability to nitrogen, 25°C	$cm^3\ cm\ cm^{-2}\ s^{-1}\ Pa^{-1} \times 10^{-13}$	0.2	
Permeability to oxygen, 25°C	$cm^3\ cm\ cm^{-2}\ s^{-1}\ Pa^{-1} \times 10^{-13}$	0.6	
Permeability to water vapor, 25°C	$cm^3\ cm\ cm^{-2}\ s^{-1}\ Pa^{-1} \times 10^{-13}$	4,000-5,000	
Contact angle of water, 20°C	degree	44	
Surface free energy	$mJ\ m^{-2}$	41.1	
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	12-95; 100-140 (commercial films)	
Tensile modulus	MPa	2,900-4,000	
Tensile stress at yield	MPa	29.6-124	
Elongation	%	15-70	
Tensile yield strain	%	2-47	
Flexural strength	MPa	41-88	
Flexural modulus	MPa	1,000-2,700	
Compressive strength	MPa	29.76-52.99	
Young's modulus	MPa	2,400-4,100	
Charpy impact strength, un-notched, 23°C	$kJ\ m^{-2}$	NB	
Charpy impact strength, notched, 23°C	$kJ\ m^{-2}$	6-15	
Izod impact strength, unnotched, 23°C	$J\ m^{-1}$	100-450	
Izod impact strength, notched, 23°C	$J\ m^{-1}$	110-450	
Izod impact strength, notched, -40°C	$J\ m^{-1}$	53-64	
Shear modulus	MPa	862-1,474	

CA cellulose acetate

PARAMETER	UNIT	VALUE	REFERENCES
Tenacity (fiber) (standard atmosphere)	cN tex^{-1} (daN mm^{-2})	10-15 (13-20)	Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.
Tenacity (wet fiber, as % of dry strength)	%	50-80	Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.
Fineness of fiber (titer)	dtex	2-10	Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.
Length (elemental fiber)	mm	40-120	Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.
Abrasion resistance (ASTM D1044)	mg/1000 cycles	65	
Poisson's ratio	-	0.3827-0.3989	
Shore D hardness	-	73-82	
Rockwell hardness	-	R34-125	
Shrinkage	%	0.2-0.6	
Melt index, 230°C/3.8 kg	g/10 min	1.4-2.4	
Water absorption, equilibrium in water at 23°C	%	2-6.5	
Moisture absorption, equilibrium 23°C/50% RH	%	3.7-6.5; 2.3-2.6 (24 h)	
CHEMICAL RESISTANCE			
Acid dilute/concentrated	-	poor	
Alcohols	-	poor	
Alkalis	-	poor	
Aliphatic hydrocarbons	-	poor	
Aromatic hydrocarbons	-	poor	
Esters	-	poor	
Greases & oils	-	good	
Halogenated hydrocarbons	-	poor	
Ketones	-	good	
Θ solvent, Θ-temp.=155, 37°C	-	acetone, butanone	
Good solvent	-	acetic acid, acetone, aniline, benzyl alchol, cyclohexanone, diethanolamine, formic acid, methyl acetate, phenols, pyridine	
Non-solvent	-	aliphatic esters, hydrocarbons, weak mineral acids	
FLAMMABILITY			
Ignition temperature	°C	304	
Autoignition temperature	°C	475	
Limiting oxygen index	% O_2	18-19	
Minimum ignition energy	J	0.015	
Burning rate (Flame spread rate)	mm min^{-1}	12.7-50.8	
Char at 500°C	%	12	
Volatile products of combustion	-	CH_3COOH, CO, CO_2	

CA cellulose acetate

PARAMETER	UNIT	VALUE	REFERENCES
UL 94 rating	-	HB	
WEATHER STABILITY			
Stabilizers	-	acid scavenger, antioxidant	
Activation energy of hydrolysis	kJ mol^{-1}	121.8	Miller, R L; Stewart, M E, Antec, 2411-16, 1996.
TOXICITY			
NFPA: Health, Flammability, Reactivity rating	-	0-1/0-2/0; 1/1/0 (HMIS)	
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
TLV, ACGIH	mg m^{-3}/ ppm	10	
MAK/TRK	mg m^{-3}/ ppm	3	
OSHA	mg m^{-3}/ ppm	15	
Oral rat, LD_{50}	mg kg^{-1}	>5,000	Thomas, W C; McGrath, L F; Baarson, K A; Auletta, C S; Daly, I W; McConnell, R F, Fd Chem. Toxic., 29, 7, 453-58, 1991.
PROCESSING			
Typical processing methods	-	extrusion, solution	
Preprocess drying: temperature/ time/residual moisture	^{o}C/h/%	65-70/2-3	
Processing temperature	^{o}C	193-210 (injection)	
Processing pressure	MPa	14.5 (injection), 0.45 (back)	
Process time	s	2-12 (cycle); 10-70 (cure)	
Additives used in final products	-	Plasticizers: acetyl triethyl citrate, di-(2-ethylhexyl) phthalate, diethyl phthalate, dimethyl phthalate, dimethyl sebacate, dioctyl sebacate, polyethylene glycol, polypropylene glycol, sulfolane, toluenesulfonamide derivatives, tri-(2-ethylhexyl) phosphate, triacetin, tributyl citrate, triethyl citrate, triphenyl phosphate; Antistatics: silver-doped vanadium pentoxide, vanadium pentoxide; Antiblocking: hydrogenated tallow amide, laponite, silica, talc; Release: magnesium stearate, sodium benzoate; Slip: silicone oil	
Applications	-	coatings (for glass, paper/paperboard), consumer electronics, electrical, fibers, films, food packaging, lacquers (for electric insulators, glass, paper, plastics, wire), membranes, pharmaceutical (osmotic drug delivery, excepient, tableting, task-masking), pressure-sensitive tape, sealants, wood sealers	
BLENDS			
Suitable polymers	-	PEEK, PSU, TPU, epoxy	
ANALYSIS			
FTIR (wavenumber-assignment)	cm^{-1}/-	major bands: C=O stretch of ester group – 1746-1755; asymmetric stretchning of C-C-O of ester group – 1234-1237; asymmetric stretching of O-C-C bond attached to carbonyl – 915	Schilling, M; Bouchard, M; Khanjian, H; Learner, T; Phenix, A; Rivenc, R, Accounts Chem. Res., 43, 6, 888-96, 2010.
NMR (chemical shifts)	ppm	^{1}H and ^{13}C chemical shifts (comprehensive paper)	Kono, H; Hashimoto, H; Shimizu, Y, Carbohydrate Polym., 118, 91-100, 2015.

CA cellulose acetate

PARAMETER	UNIT	VALUE	REFERENCES
x-ray diffraction peaks	degree	8.2, 11.9, 16.8, 21.5 (bagasse cellulose based); 13 and 17	Shaikh, H M; Pandare, K V; Nair, G; Varma, A J, Carbohydrate Polym., 76, 23-29, 2009; Daud, W R W; Djuned, F M, Carbohydrate Polym., 132, 252-60, 2015.