

# CHI chitosan

PARAMETER	UNIT	VALUE	REFERENCES
<b>GENERAL</b>			
Common name	-	chitosan, poly-D-glucosamine	
Acronym	-	CHI	
CAS number	-	9012-76-4; 1398-61-4 (chitin)	
EC number	-	222-311-2	
RTECS number	-	FM6300000	
<b>HISTORY</b>			
Person to discover	-	Bracconot; Ledderhose; Rammelberg	
Date	-	1811; 1878; 1930	
Details	-	Bracconot discovered chitin in 1811; Ledderhose, determined composition of chitin in 1878; and, in 1930, Rammelberg obtained chitosan from chitin	
<b>SYNTHESIS</b>			
Monomer(s) structure	-	D-glucosamine; N-acetyl-D-glucosamine	
Monomer(s) CAS number(s)	-	3416-24-8; 7512-17-6	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	161.156; 221.21	
Method of synthesis	-	commercially produced by deacetylation of chitin (chitin is a structural element of shrimp and crab shells); deacetylation can be accomplished by treating chitin with an aqueous 40-45% NaOH for 4-5 h	
Degree of deacetylation	%	65-95; 90	Hu, J; Wang, X; Xiao, Z; Bi, W, LTW Food Sci. Technol., 63, 519-26, 2015.
Number average molecular weight, $M_n$	dalton, g/mol, amu	33,700-99,400	
Mass average molecular weight, $M_w$	dalton, g/mol, amu	20,000-190,000 (low $M_w$ chitosan); 190,000-375,000 (high $M_w$ chitosan); 1,000,000-2,500,000 (chitin); 150,000	Hu, J; Wang, X; Xiao, Z; Bi, W, LTW Food Sci. Technol., 63, 519-26, 2015.
Polydispersity, $M_w/M_n$	-	3.3-8.1	
<b>STRUCTURE</b>			
Crystallinity	%	35-50 (chitosan fibers)	
Cell type (lattice)	-	orthorhombic	Okuyama, K; Noguchi, K; Miyazawa, T; Yui, T; Ogawa, K, Macromolecules, 30, 19, 5849-55, 1997.
Cell dimensions	nm	a=0.895, b=1.697, c=1.037	Okuyama, K; Noguchi, K; Miyazawa, T; Yui, T; Ogawa, K, Macromolecules, 30, 19, 5849-55, 1997.
Number of chains per unit cell	-	4 (8 water molecules)	Okuyama, K; Noguchi, K; Miyazawa, T; Yui, T; Ogawa, K, Macromolecules, 30, 19, 5849-55, 1997.
Crystallite size	nm	1.04	Ogawa, K, J. Metals, Materials, Minerals, 15, 1, 1-5, 2005.
Polymorphs	-	$\alpha$ , $\beta$ , $\gamma$	Dash, M; Chiellini, F; Ottenbrite, R M; Chiellini, E, Prog. Polym. Sci., 36, 981-1014, 2011.
Chain conformation	-	2-fold helix	
<b>COMMERCIAL POLYMERS</b>			
Some manufacturers	-	BASF, Cognis	
Trade names	-	Chitopharm	

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<b>PHYSICAL PROPERTIES</b>			
Density at 20°C	g cm <sup>-3</sup>	1.4-1.42	
Bulk density at 20°C	g cm <sup>-3</sup>	0.4-0.68	
Color	-	off-white to gray	
Refractive index, 20°C	-	1.52-1.54	
Birefringence	-	0.012	
Melting temperature, DSC	°C	199-230	
Decomposition temperature	°C	313-317	
Glass transition temperature	°C	163-172	Martinez-Camacho, A P; Cortez-Rocha, M O; Ezquerro-Brauer, J M; Graciano-Verdugo, A Z; Rodriguez-Felix, F; Castillo-Ortega, M M; Yepiz-Gomez, M S; Plascencia-J; M, Carbohydrate Polym., 82, 305-15, 2010.
Volume resistivity	ohm-m	1.25E-7	
Permeability to water vapor, 25°C	g m <sup>-1</sup> s <sup>-1</sup> Pa <sup>-1</sup> x 10 <sup>11</sup>	7.24	Pinotti, A; Garcia, M A; Martino, M N; Zaritzky, Food Hydrocolloids, 21, 66-72, 2007.
<b>MECHANICAL &amp; RHEOLOGICAL PROPERTIES</b>			
Tensile strength	MPa	6.7-150.2	Park, S Y; Marsh, K S; Rhim, J W, J. Foo Sci., Food Eng. Phys. Properties, 67, 1, 194-97, 2002.
Elongation	%	4.1-117.8	Park, S Y; Marsh, K S; Rhim, J W, J. Foo Sci., Food Eng. Phys. Properties, 67, 1, 194-97, 2002.
Young's modulus	MPa	32.6	
Tenacity (fiber)	cN tex <sup>-1</sup>	10-15; 3-7 (wet)	Pillai, C K S; Paul, W; Sharma, C P, Prog. Polym. Sci., 34, 641-78, 2009.
Moisture absorption, equilibrium 23°C/50% RH	%	10	
<b>CHEMICAL RESISTANCE</b>			
Acid dilute/concentrated	-	poor	
Alcohols	-	poor	
Alkalis	-	poor	
Esters	-	poor	
Halogenated hydrocarbons	-	poor	
Ketones	-	poor	
Good solvent	-	acetic acid, formic acid, concentrated mineral acids, water	
<b>FLAMMABILITY</b>			
Autoignition temperature	°C	>530	
<b>WEATHER STABILITY</b>			
Activation wavelengths	nm	320	

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<b>BIODEGRADATION</b>			
Typical biodegradants	-	chitosan can be degraded by enzymes able to hydrolyze glucosamine–glucosamine, glucosamine and N-acetylglucosamine–N-acetylglucosamine; it can also be degraded by lysozyme	
Stabilizers	-	chitosan itself has antimicrobial properties	Kong, M; Chen, X G; Xing, K; Park, H J, Int. J. Food Microbiol., 144, 1, 51-63, 2010.
<b>TOXICITY</b>			
NFPA: Health, Flammability, Reactivity rating	-	0-2/0-1/0-1	
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
Oral mouse, LD <sub>50</sub>	mg kg <sup>-1</sup>	>16,000	
<b>ENVIRONMENTAL IMPACT</b>			
Aquatic toxicity, <i>Daphnia magna</i> , LC <sub>50</sub> <sup>a</sup> 48 h	% survival	100	Protech, Techn. Rep. TR01.1, Jul. 2004.
Aquatic toxicity, <i>Fathead minnow</i> , LC <sub>50</sub> <sup>a</sup> 48 h	% survival	100	Protech, Techn. Rep. TR01.1, Jul. 2004.
Aquatic toxicity, <i>Rainbow trout</i> , LC <sub>50</sub> <sup>a</sup> 48 h	% survival	100; LC <sub>50</sub> : >10,000 mg/l	Protech, Techn. Rep. TR01.1, Jul. 2004.
<b>PROCESSING</b>			
Typical processing methods	-	electrospinning, extrusion, hydrogel formation, precipitation, preparation (deminalarization, deproteinazation, decoloration, and deacetylation), spinning, spray drying	Youn, D K; No, H K; Prinyawiwatkul, W, Carbohydrate Polym., 69, 707-12, 2007.
Applications	-	agriculture (biopesticide, seed treatment, plant growth enhancement), fibers, medical (wound treatments, artificial skin, hemostatic agent), pharmaceutical (drug delivery systems); textile industry, veterinary medicine, water filtration (helps to remove turbidity), beer clarification	Dash, M; Chiellini, F; Ottenbrite, R M; Chiellini, E, Prog. Polym. Sci., 36, 981-1014, 2011; Gassara, F; Antzak, C; Ajila, C M; Sarma, S J; Brar, S K; Verma, M, J. Food Eng., 166, 80-85, 2015.
Outstanding properties	-	accelerates wound healing, anti-itching effect, antimicrobial agent, moisturizing action; antioxidant activity, fat-binding, antimicrobial activity	Zou, P; Yang, X; Wang, J; Li, Y; Yu, H; Zhang, Y; Liu, G, Food Chem., 190, 1174-81, 2016.
<b>BLENDS</b>			
Suitable polymers	-	C, CMC, PAM, PEG, PEO, PMMA, PVOH, PVP, polylysine	Lewandowska, K, J. Mol. Liquids, 209, 301-5, 2015.
<b>ANALYSIS</b>			
FTIR (wavenumber-assignment)	cm <sup>-1</sup> /-	N-H – 332-3349; amide – 1646-1648	Cardenas, G; Miranda, S P, J. Chilean Chem. Soc., 49, 4, 291-95, 2004.