# CHI chitosan

| PARAMETER | UNIT | VALUE | REFERENCES |
|---|---|---|---|
| **GENERAL** | | | |
| **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 | |
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| **HISTORY** | | | |
| **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 | |
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| **SYNTHESIS** | | | |
| **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 | |
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| **STRUCTURE** | | | |
| **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; Ottenbritte, R M; Chiellini, E, Prog. Polym. Sci., 36, 981-1014, 2011. |
| **Chain conformation** | - | 2-fold helix | |
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| **COMMERCIAL POLYMERS** | | | |
| **Some manufacturers** | - | BASF, Cognis | |
| **Trade names** | - | Chitopharm | |

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| **PHYSICAL PROPERTIES** | | | |
| **Density at 20ºC** | g $cm^{-3}$ | 1.4-1.42 | |
| **Bulk density at 20ºC** | g $cm^{-3}$ | 0.4-0.68 | |
| **Color** | - | off-white to gray | |
| **Refractive index, 20ºC** | - | 1.52-1.54 | |
| **Birefringence** | - | 0.012 | |
| **Melting temperature, DSC** | ºC | 199-230 | |
| **Decomposition temperature** | ºC | 313-317 | |
| **Glass transition temperature** | ºC | 163-172 | Martinez-Camacho, A P; Cortez-Rocha, M O; Ezquerra-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, 25ºC** | g $m^{-1}$ $s^{-1}$ $Pa^{-1}$ x $10^{11}$ | 7.24 | Pinotti, A; Garcia, M A; Martino, M N; Zaritzky, Food Hydrocolloids, 21, 66-72, 2007. |
| | | | |
| **MECHANICAL & RHEOLOGICAL PROPERTIES** | | | |
| **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 $tex^{-1}$ | 10-15; 3-7 (wet) | Pillai, C K S; Paul, W; Sharma, C P, Prog. Polym. Sci., 34, 641-78, 2009. |
| **Moisture absorption, equilibrium 23ºC/50% RH** | % | 10 | |
| | | | |
| **CHEMICAL RESISTANCE** | | | |
| **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 | |
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| **FLAMMABILITY** | | | |
| **Autoignition temperature** | ºC | >530 | |
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| **WEATHER STABILITY** | | | |
| **Activation wavelengths** | nm | 320 | |
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| **BIODEGRADATION** | | | |
| **Typical biodegradants** | - | chitosan can be degraded by enzymes able to hydrolyze glucosamine–glucosamine, glucosamine and N-acetyl-glucosamine–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. |
| | | | |
| **TOXICITY** | | | |
| **NFPA: Health, Flammability, Reactivity rating** | - | 0-2/0-1/0-1 | |
| **Carcinogenic effect** | - | not listed by ACGIH, NIOSH, NTP | |
| **Oral mouse, $LD_{50}$** | mg $kg^{-1}$ | >16,000 | |
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| **ENVIRONMENTAL IMPACT** | | | |
| **Aquatic toxicity, Daphnia magna, $LC_{50}$, 48 h** | % survival | 100 | Protech, Techn. Rep. TR01.1, Jul. 2004. |
| **Aquatic toxicity, Fathead minnow, $LC_{50}$, 48 h** | % survival | 100 | Protech, Techn. Rep. TR01.1, Jul. 2004. |
| **Aquatic toxicity, Rainbow trout, $LC_{50}$, 48 h** | % survival | 100; $LC_{50}$: >10,000 mg/l | Protech, Techn. Rep. TR01.1, Jul. 2004. |
| | | | |
| **PROCESSING** | | | |
| **Typical processing methods** | - | electrospinning, extrusion, hydrogel formation, precipitation, preparation (deminaralization, deproteinazation, decoloration, and deacetylation), spinning, spray drying | Youn, D K; No, H K; Prinyawiwatkul, W, Carbohydrate Polym., 69, 707-12, 2007. |
| **Applications** | - | agriculture (biopeticide, 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; Ottenbritte, 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. |
| | | | |
| **BLENDS** | | | |
| **Suitable polymers** | - | C, CMC, PAM, PEG, PEO, PMMA, PVOH, PVP, polylysine | Lewandowska, K, J. Mol. Liquids, 209, 301-5, 2015. |
| | | | |
| **ANALYSIS** | | | |
| **FTIR (wavenumber-assignment)** | $cm^{-1}$/- | N-H – 332-3349; amide – 1646-1648 | Cardenas, G; Miranda, S P, J. Chilean Chem. Soc., 49, 4, 291-95, 2004. |
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