

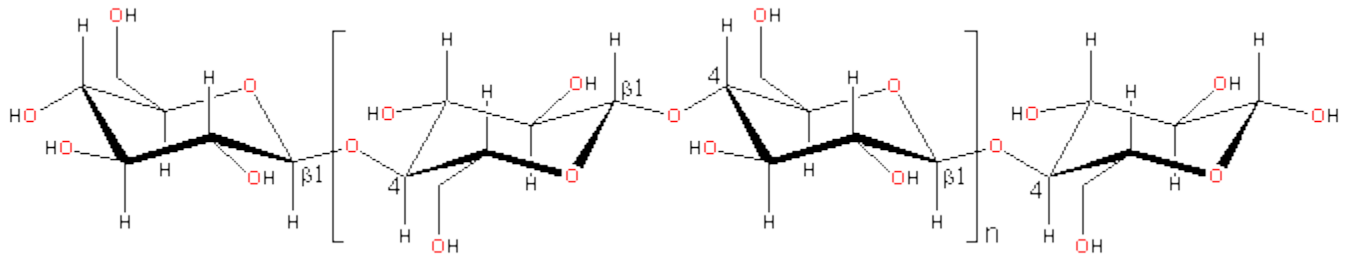
Cellulose

- ▼ [Sources for cellulose](#)
- ▼ [Structural unit](#)
- ▼ [Molecular structure](#)
- ▼ [Functionality](#)

Sources for cellulose

Cellulose is found in plants as microfibrils [1598] (2-20 nm diameter and 100 - 40 000 nm long). These form the structurally strong framework in the cell walls. Cellulose (E460) is mostly prepared from wood pulp. Cellulose is also produced in a highly hydrated form by some bacteria (for example, *Acetobacter xylinum*).

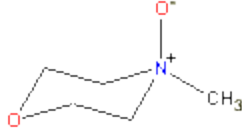
Structural unit



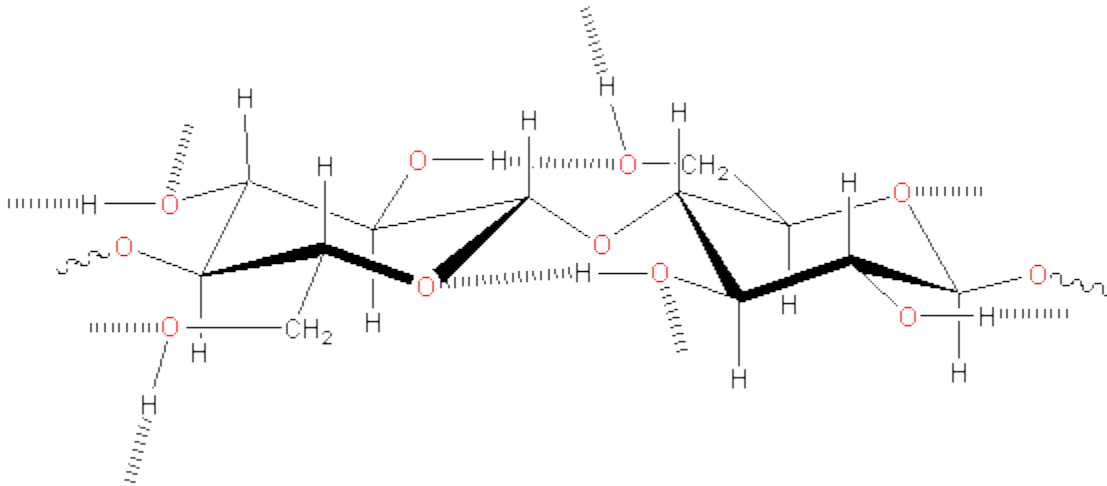
Cellulose is a linear polymer of β -(1 \rightarrow 4)-D-glucopyranose units in 4C_1 conformation. The fully equatorial conformation of β -linked glucopyranose residues stabilizes the chair structure, minimizing its flexibility (for example, relative to the slightly more flexible α -linked glucopyranose residues in amylose). Cellulose preparations may contain trace amounts (\sim 0.3%) of [arabinoxylans](#).^a

Molecular structure

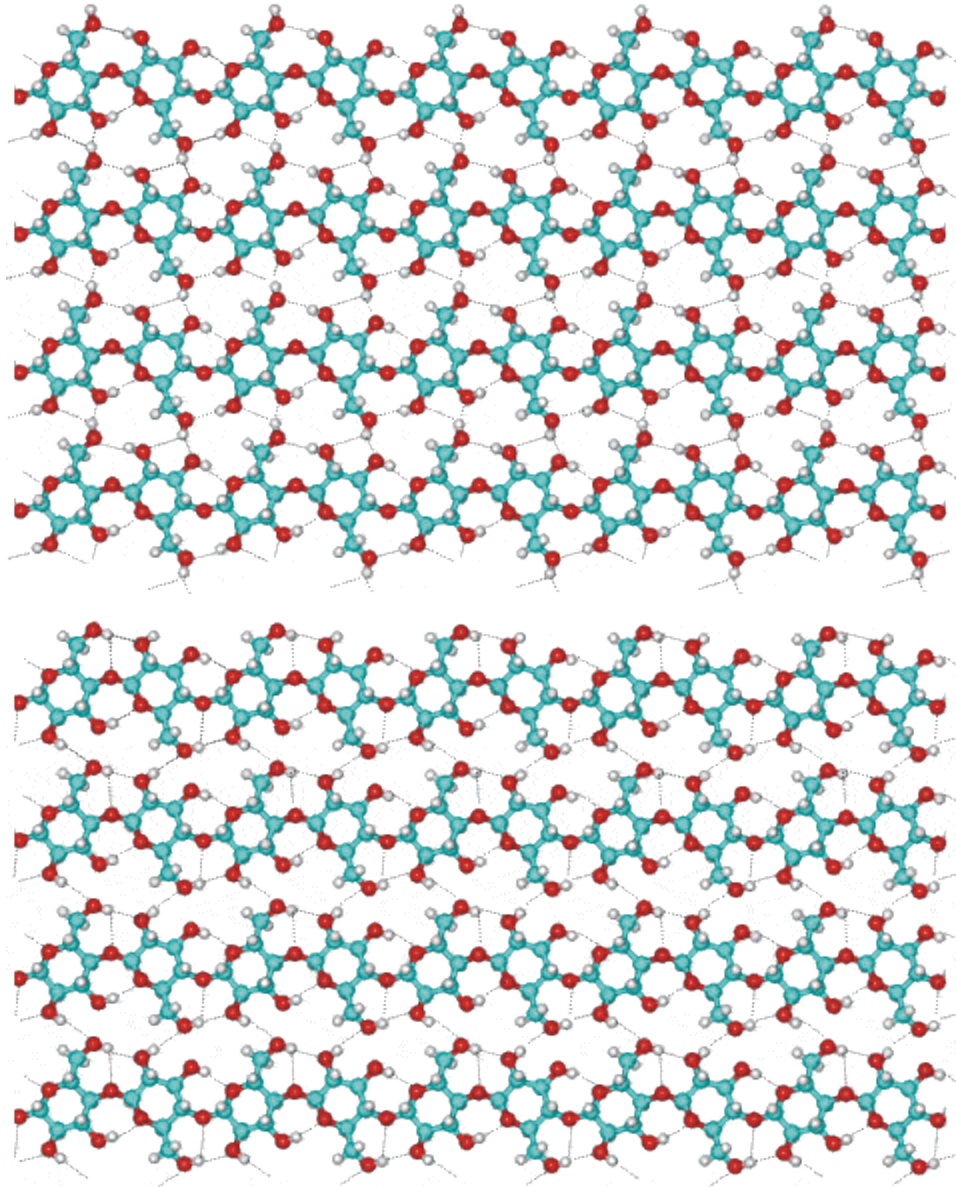
Cellulose is an insoluble molecule consisting of between 2000 - 14000 residues with some preparations being somewhat shorter. It forms crystals (cellulose I_0) where intra-molecular (O3-H \rightarrow O5' and O6 \rightarrow H-O2') and intra-strand (O6-H \rightarrow O3') hydrogen bonds holds the network flat allowing the more hydrophobic ribbon faces to stack. Weak C6-H \rightarrow O2' hydrogen bonds may also make some contribution to the crystal stability. Each residue is oriented 180° to the next with the chain synthesized two residues at a time. Although individual strand of cellulose are intrinsically no less hydrophilic, or no more hydrophobic, than some other soluble polysaccharides (such as [amylose](#)) this tendency to form crystals utilizing extensive hydrophobic interactions [1645] in addition to intra- and intermolecular hydrogen bonding makes it completely insoluble in normal aqueous solutions (although it is soluble in more exotic solvents [2055] such as aqueous



N-methylmorpholine-N-oxide (NMNO, ~0.8 mol water/mol, then up to 30% by wt cellulose at 100 °C [1060]), CdO/ethylene-diamine (cadoxen), LiCl/*N,N*-dimethylacetamide or near-supercritical water [1070]). It is thought that water molecules catalyze the formation of the natural cellulose crystals by helping to align the chains through hydrogen-bonded bridging.



Part of a cellulose preparation is amorphous between these crystalline sections. The overall structure is of aggregated particles with extensive pores capable of holding relatively large amounts of water by capillarity. The natural crystal is made up from metastable **Cellulose I** with all the cellulose strands parallel and no inter-sheet hydrogen bonding. This cellulose I (that is, natural cellulose) contains two coexisting phases cellulose I_α (triclinic) and cellulose I_β (monoclinic) in varying proportions dependent on its origin; I_α being found more in algae and bacteria whilst I_β is the major form in higher plants.

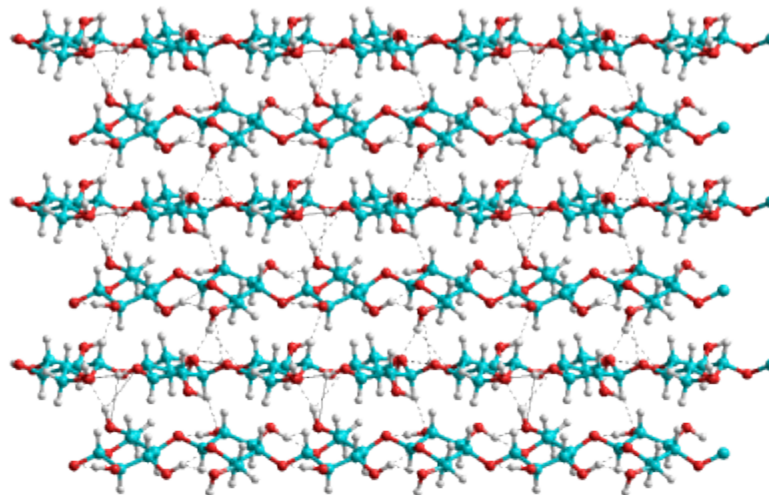


Cellulose I_α and cellulose I_β have the same fibre repeat distance (1.043 nm for the repeat dimer interior to the crystal, 1.029 nm on the surface [721]) but differing displacements of the sheets relative to one another. The neighboring sheets of cellulose I_α (consisting of identical chains with two alternating glucose conformers **-A-B-**) are regularly displaced from each other in the same direction whereas sheets of cellulose I_β (consisting of two conformationally distinct alternating sheets, (as shown right where the 2-OH and 6-OH groups both change orientations so altering the hydrogen bonding pattern) each made up of crystallographically identical glucose conformers) are staggered [559]. It has been found that cellulose (I_β) significantly alters the water structuring at its surface out to about 10 Å, which may affect its enzymatic digestion [905].

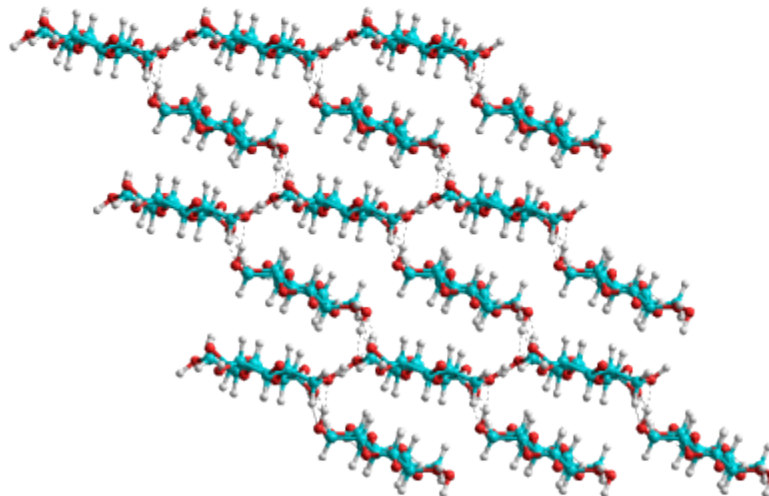
Cellulose I_{α} and cellulose I_{β} are interconverted by bending during microfibril formation [418] and metastable cellulose I_{α} converts to cellulose I_{β} on annealing.

Interactive structures are available ([Jmol](#)).

If it can be recrystallized (for example, from base or CS_2) cellulose I gives the thermodynamically more stable monoclinic **Cellulose II** structure with an antiparallel arrangement of the strands and intermolecular and both intra- and inter-sheet hydrogen-bonding.



View down x axis



View down z axis

This crystalline form of cellulose II, shown left, may also be prepared by deacetylation of cellulose acetate [2039]. Cellulose II contains two different types of anhydroglucose (**A** and **B**) with different backbone structures; the chains consisting of **-A-A-** or **-B-B-** repeat units [627], shown alternating from the top in the x-axis view. Both have intra-chain hydrogen bonding but only the **-A-A-** one has inter-chain hydrogen bonding. There are also hydrogen bonds between the **A** and **B** sheets such that an additional sheet structure consists of alternant **A** and **B** strands, with these sheets joined by hydrogen bonds, shown as diagonal sheets in the z-axis view. In the x-axis view the cellulose molecules go across the view (6 molecules shown) whereas in the z-axis view they disappear into the cartoon (18 molecules shown).

The interactive structure of cellulose II is available ([Jmol](#)).

Cellulose II hydrate may be prepared by immersion of mercerized cellulose II in anhydrous hydrazine followed by washing with water [1736]. It is similar to Cellulose II but has a larger unit cell containing the extra water molecules between the layers.

Cellulose III is formed from cellulose mercerized in ammonia and is similar cellulose II but with the chains parallel, as in cellulose I_α and cellulose I_β [753]. For a review of cellulose structure, see [288]. Microcrystalline cellulose gives needle-shaped nanocrystals (microfibrillated cellulose [1902]) of a relative uniform size with length of 90 ± 50 nm and width of 10 ± 4 nm [1690]. [[Back to Top](#) ▲]

Functionality

Cellulose has many uses as an anticake agent, emulsifier, stabilizer, dispersing agent, thickener, and gelling agent but these are generally subsidiary to its most important use of holding on to water. Water cannot penetrate crystalline cellulose but dry amorphous cellulose absorbs water becoming soft and flexible. Some of this water is non-freezing but most is simply trapped. Less water is bound by direct hydrogen bonding if the cellulose has high crystallinity but some fibrous cellulose products can hold on to considerable water in pores and its typically straw-like cavities; water holding ability correlating well with the amorphous (surface area effect) and void fraction (that is, the porosity). As such water is supercoolable, this effect may protect against ice damage. Cellulose can give improved volume and texture particularly as a fat replacer in sauces and dressings but its insolubility means that all products will be cloudy.

Swelled bacterial cellulose (*ex. Acetobacter xylinum*), in its never-dried state with much smaller fibrils (~1%) than from plants, exhibits pseudoplastic viscosity like [xanthan](#) gels but this viscosity is not lost at high temperatures and low shear rates as the cellulose can retain its structure. Where individual cellulose strands are surrounded by water they are flexible and do not present contiguous hydrophobic surfaces. Bacterial cells may be removed by hot alkali and the clean wet cellulose used as a substrate for immobilizing biomolecules [843] or for covering wounds [844]. On drying the properties of bacterial cellulose irreversibly lose their hydrated properties and tend to those of plant cellulose.

About a third of the world's production of purified cellulose is used as the base material for a number of water-soluble derivatives with pre-designed and wide-ranging properties dependent on groups involved and the degree of derivatization (for an extensive review see [287]). Derivatizing

cellulose interferes with the orderly crystal-forming hydrogen bonding, described above, so that even hydrophobic derivatives may increase the apparent solubility in water. Methyl cellulose (E461) [231] (made by methylating about 30% of the hydroxyl groups) is thermogelling, forming gels above a critical temperature due to hydrophobic interactions between high-substituted regions and consequentially stabilized intermolecular hydrogen bonding. Such gels break down on cooling in a manner similar to that causing the solubility minimum for non-polar gases; hydrophobic saccharides becoming less soluble as the temperature increases [187]. This property is useful in forming films as barriers to water loss and for holding on to small gas bubbles.

Hydroxypropylmethylcellulose (HPMC, E464) has similar properties and uses but with added water interaction and surface activity [1292]. Both methylcellulose and HPMC may be used in gluten-free bakery products as gluten substitutes. Hydroxypropyl cellulose (E463) possesses good surface activity but does not gel as it forms open helical coils. It is a water-soluble thickener, emulsifier and film-former often used in tablet coating. Another important derivative of cellulose is carboxymethylcellulose.

Interactive structures are available (Jmol).

Source : <http://www1.lsbu.ac.uk/water/hycel.html>