

MODELLING STRUCTURES AND PROPERTIES OF POLYSACCHARIDES

Karim Mazeau *

*CERMAV Centre de Recherches sur les Macromolécules Végétales
BP 53 38041 Grenoble Cedex 9 France
Karim.Mazeau@cermav.cnrs.fr*

Physical and biological properties of biopolymers are closely related on their three-dimensional structures and on recognition phenomena with other molecules. Conformational analysis is performed following two complementary approaches. Experiments suffer from intrinsic average whereas molecular modelling relies on human choices. Only the concerted approach allows a realistic characterisation of the shape of macromolecules and a reliable understanding of how they interact.

The presentation will focus on the application of new molecular modelling methods in order to describe different levels of architectural features of the main cell wall biopolymers: cellulose, hemicelluloses and lignin.

Models of crystalline and amorphous supramolecular architectures of cellulose complete crystallographic studies in revealing a structural microheterogeneity of the crystalline phase. The estimated dependence of the organisation on the bulk cohesive property is in agreement with the thermal conversion of I α to I β allomorphs. Finally, the glass transition temperature of dry amorphous cellulose, which has never could be measured, can be predicted.

Idealised models of different surfaces of cellulose fibres compare favourably well to the structural and thermodynamic data obtained on the real ones. Then, molecular modelling of the physisorption process of various molecules on the surface of cellulose fibres does reveal energetic and structural details of the interaction. Estimated adsorption enthalpies of aromatic molecules are in quantitative agreement with gas chromatography data. Therefore, a confident modelling of the cellulose lignin complexes gives a reasonable explanation for the apparent contradiction between the experimental reports. Similarly, models of the cellulose xyloglucan network disprove the generally accepted hypothesis that optimal interaction requires the perfect 2₁ helical conformation of the cellulose molecules and of the xyloglucan backbone, which should be perfectly aligned along the fibre. Finally, implications for biomimetic nanomaterials having controlled mechanical properties will be given.