A DFT STUDY OF MODELLING CELLULOSE RADICALS

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Cellulose is one of the most abundant renewable biopolymers, which consists of linear chains of D-glucose units linked β(1-4) glycosidic bonds. Different basic crystalline forms of cellulose have been studied so far. Native cellulose I, occuring in wood cell walls, is found in two different forms, Iα and Iβ. Nishiyama et al. have been identified the crystal structure of cellulose Iα and Iβ by means of X-ray and neutron fiber diffraction.

Although the structure of cellulose has been studied for years, mechanism of cellulose reactions for example radicals occuring during graft copolymerization with vinyl monomers have not been identified fully. In order to provide insight into these mechanisms theoretically, this preliminary study has focused on investigation of the electronic structure of glucose free radicals. Conformational analysis of the unit structure of cellulose has been performed by SPARTAN using semi-empirical PM3 method. The most stable conformer has been optimized by UB3LYP/6-31G** method. The calculated spin densites and charges were interpreted in terms ofthe proposed radical mechanism. The effect of additional units on the spin density has been investigated by increasing the number of unit structure.

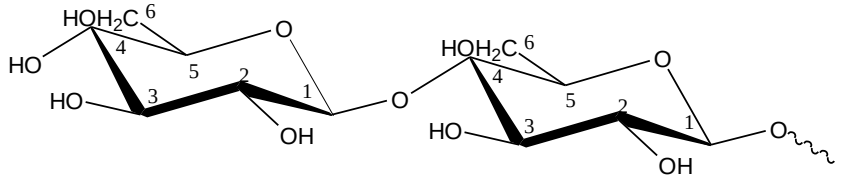

Figure I. The structure of cellulose unit.

References

[1] Krässig, H.A., *Cellulose: Structure and accesibility and reactivity*, Gordon and Breach Scie. Publishers, Yverdon, İsviçre, **2-6, 1993**

[2]Nishiyama, Y., Langan, P., Chanzy, H., "Crystal Structure and Hydrogen bonding System in Cellulose I_β from Synchrotron X-Ray and Neutron Fiber Diffraction", *Journal of American Chemical Society*, **124, 9074, 2002**