Electron magnetic resonance study of primary free radicals in trehalose single crystals

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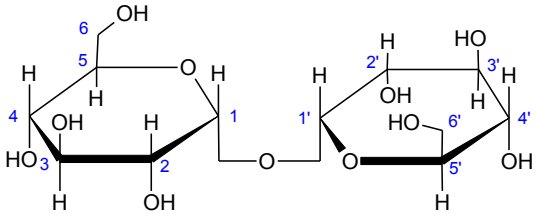
Radiation-induced radicals in sugars have recently gained considerable interest with respect to both fundamental and applied research. A number of studies are available that focus on the dosimetric characteristics of sugar systems. Other studies, like ours, aim to understand the identity and the structural properties of the involved radicals, and the radical reactions in which the primary or secondary products can be linked to the stable radicals.

Furthermore, carbohydrates represent extremely suitable model systems in which primary radiation-induced events may be studied. For instance, the detection of a trapped electron center in organic solids was first made in carbohydrate single crystals[1,2] and the nature of alkoxy radicals is readily investigated in these systems [3].

We present here experimental results obtained for low temperature radiation-induced radicals in trehalose single crystals. After 10 K *in situ* X-irradiation of trehalose single crystals four dominant radicals are present. Two radical species, labeled R1 and R2 are characterized by anisotropic g factors typical for the alkoxy type radicals. The R1 EPR spectrum is a broad singlet for most orientations, indicating only small proton hyperfine couplings. The direction of the maximum g value (g_{max}) indicates that O4' is the most likely site for the unpaired electron. R2 mainly exhibits a quartet EPR spectrum and the g_{max} direction favours O2 as the site of the unpaired electron. The other two radicals, R3 and R4, are characterized by a rather isotropic g tensor typical of alkyl radicals. R3 is characterized by a rather isotropic triplet in EPR which suggests two almost equivalent β proton hyperfine interactions. It is obtained by a net hydrogen abstraction from the C3' position. The second alkyl radical has most likely the unpaired electron localized at the C2 position.

A major purpose of this study is to compare the obtained results with the results reported by De Cooman et al[4] for 10 K X-irradiated sucrose single crystals. Trehalose and sucrose have a close structural similarity: they both are disaccharides composed of two units linked by a glycosidic oxygen bridge between their two anomeric carbon atoms, C1 and C1'. The study of very similar products may lead to a better general understanding of the radiation chemistry of carbohydrates.



Chemical Structure of Trehalose

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