Radicals in Sucrose Single Crystals Induced by X-rays at Different Temperatures: a Combined EPR and DFT Study

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Understanding the nature of radiation-induced defects in sugar compounds is of importance for dosimetry purposes as well as in the radiation chemistry of DNA. Sucrose (table sugar) is of particular interest for nuclear emergency dosimetry because of its widespread use, its radiation sensitivity, the stability of the induced radicals, and its linear dose response up to 104 Gy. Recent dosimetric studies suggest sugar to be the best, universal material for EPR- (Electron Paramagnetic Resonance) and/or UV-dosimetry in the region 0.44-160 kGy. In sugars and sugar derivatives, X-rays initially create various types of defects which then transform into the final, stable radical products through a generally complex multi-step process. Ultimately, an advanced understanding of the radiation-induced processes in these materials could aid in establishing dosimetry protocols and provide more insight into the exact role of sugar radicals in the radiation chemistry of DNA.

Electron Magnetic Resonance (EMR) experiments on sugar single crystals allow for characterisation of the radicals in a detailed way via hyperfine interactions of the unpaired electron spin with the lattice 1H nuclear spins. The last couple of years, highly accurate Density Functional Theory (DFT) calculations on extended organic solid state systems have become feasible due to advances in computing power and density functionals as well as to the development of new codes for the calculation of EMR parameters. Combining these experimental and theoretical 'tools' has already proven to be a very powerful approach to study the radiation chemistry of sugars [1-3].

We present the results of EMR experiments performed on sucrose single crystals at different temperatures, from 10 K up to room temperature, after in situ irradiation at these temperatures, and of subsequent annealing experiments. Through comparison of experimental and computational DFT results, the most prominent radicals are identified and information is obtained on their formation mechanism. Among others, our study reveals the structure of the three predominant radicals stable at room temperature, that are most relevant in the context of dosimetry.

1. 'Identification and Conformational Study of Stable Radiation-Induced Defects in Sucrose Single Crystals using Density Functional Theory Calculations of Electron Magnetic Resonance Parameters', De Cooman, H.; Pauwels, E.; Vrielinck, H.; Sagstuen, E.; Callens, F.; Waroquier, M., J. Phys. Chem. B, accepted.

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3. Tarpan, M.; Sagstuen, E.; Pauwels, E.; Vrielinck, H.; Waroquier, M. and Callens, F. J. Phys. Chem. A, in press, doi:10.1021/jp7119284.

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