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Modeling radiation-damage processes in organic solids via DFT calculations of EMR parameters

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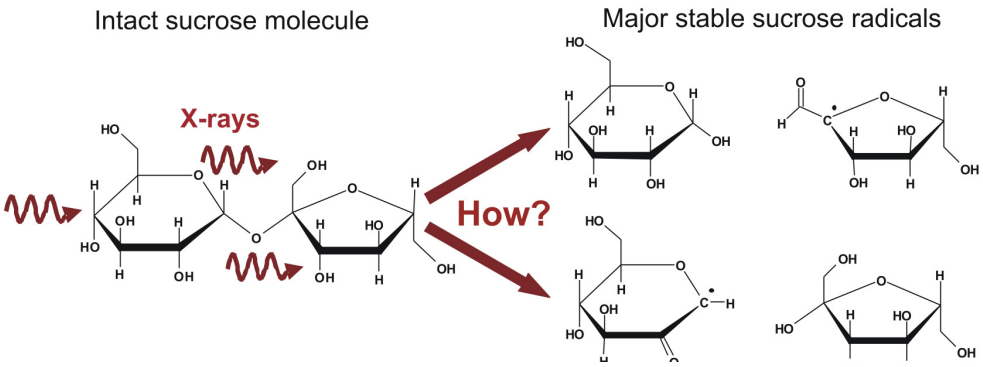
High-energy radiation induces radicals in organic materials. When created in biological macromolecules such as DNA, these can cause harm to living organisms. This detrimental effect is also exploited for the sterilisation of e.g. foodstuffs, and radiation-induced radicals are used for dosimetry purposes. Knowledge of the structure of the radicals and their formation mechanisms is therefore of fundamental importance.

In particular, radiation-induced radicals in solid sugars are studied (i) as model systems to gain insight into the precise role of the deoxyribose unit in the radiation chemistry of DNA and (ii) because of their potential as (emergency) dosimeters. X-irradiation typically gives rise to a variety of primary radicals in these systems, which then transform into stable radicals or diamagnetic species via one or more radical reactions. A prerequisite for unraveling the formation mechanisms is the identification of the different intermediate (semistable) radicals.

Experimentally, solid-state sugar radicals can be characterised in detail by electron magnetic resonance (EMR) experiments. These allow determination of *EMR parameters* which describe the interaction of the unpaired-electron spin with its lattice environment, e.g. with (nearby) nuclear spins. Theoretical calculations of EMR parameters with DFT codes are increasingly being used to help clarify, interpret and explain experimental results.



Recently we have managed, in a combined experimental and theoretical approach, to identify the structure of the major radiation-induced stable radicals in solid sucrose [1,2,3] (see Figure). We currently are investigating their formation mechanism, also via both EMR experiments and DFT modeling. A summary of the results obtained so far are presented.

Keywords: magnetic resonance, DFT, radiation, radicals, organic, solid state

[1] H. De Cooman, E. Pauwels, H. Vrielinck, A. Dimitrova, N. Yordanov, E. Sagstuen, M. Waroquier and F. Callens, *Spectrochim. Acta A*, **69**, 1372 (2008)
[2] H. De Cooman, E. Pauwels, H. Vrielinck, E. Sagstuen, F. Callens and M. Waroquier, *J. Phys. Chem. B*, **112**, 7298 (2008)
[3] H. De Cooman, E. Pauwels, H. Vrielinck, E. Sagstuen, S. Van Doorslaer, F. Callens and M. Waroquier, *Phys. Chem. Chem. Phys.*, **11**, 1105 (2009).