Radiation-induced radical formation in solid state sugars: a review of recent EMR and DFT results, H. De Cooman, E. Pauwels, H. Vrielinck, E. Sagstuen, M. Waroquier, F. Callens, *11th International Workshop on Electron Magnetic Resonance Of Disordered Systems (EMARDIS)*, Sofia-Boyana, Bulgaria, **11 - 18 June 2009**

Carbohydrates are important constituents of several biological systems, including DNA, and elucidating their radiation chemistry is therefore of general importance. In particular, sugar radicals play a crucial role in radiation-induced single and double strand breaks in DNA, which can lead to mutations and, finally, cancer. Certain sugars such as sucrose (table sugar) are also promising dosimetric materials. An advanced knowledge of the radiation-induced processes in carbohydrates may therefore provide better insight into the DNA radiation chemistry and aid in establishing reliable sugar dosimetry protocols. The first step in acquiring such knowledge is identification of the radical structures.

Electron Magnetic Resonance (EMR) experiments on irradiated sugar single crystals allow a very detailed characterisation of the radicals via the ***g***-tensor and the hyperfine interactions between the unpaired electron spin and the nuclear spins in the lattice. Single crystals also offer the advantage of mimicking to some extent the compact structure of chromosomal DNA. Numerous EMR studies on single crystals of sugars and sugar derivatives have been performed the last decades, but radical identification by EMR experiments alone is often ambiguous and sometimes not feasible. The last few years, highly accurate Density Functional Theory (DFT) calculations on extended organic solid state systems have become possible. These provide a powerful tool to help clarify and interpret experimental results and enable unambiguous structural identifications that were not possible before.

In this talk, an overview will be given of recently identified radiation-induced radicals in single crystals of sugars (e.g. sucrose,[1,2,3] fructose[4]) and sugar derivatives (e.g. glucose 1-phosphate[5,6]). The results pertain to primary as well as intermediate and stable species and the identifications are mainly based on the agreement, both in principal values and directions, between experimentally determined and DFT calculated proton hyperfine tensors. Common structural features are highlighted and possible commonly operative formation mechanisms are discussed.

1. H. De Cooman, E. Pauwels, H. Vrielinck, A. Dimitrova, N. Yordanov, E. Sagstuen, M. Waroquier and F. Callens, *Spectrochim Acta Part A*, **2008**, 69, 1372 – 1383.
2. H. De Cooman, E. Pauwels, H. Vrielinck, E. Sagstuen, F. Callens and M. Waroquier, *J. Phys. Chem. B*, **2008**, 112, 7298-7307.
3. H. De Cooman, E. Pauwels, H. Vrielinck, E. Sagstuen, S. Van Doorslaer, F. Callens and M. Waroquier, *Phys. Chem. Chem. Phys.*, **2008**, DOI:10.1039/B816641B.
4. M. Tarpan, E. Sagstuen, E. Pauwels, H. Vrielinck, M. Waroquier and F. Callens, *J. Phys. Chem. A*, **2008**, 112, 3898-3905.
5. H. De Cooman, G. Vanhaelewyn, E. Pauwels, E. Sagstuen, M. Waroquier and F. Callens, *J. Phys. Chem. B*, **2008**, 112, 15045–15053.
6. H. De Cooman, G. Vanhaelewyn, E. Sagstuen, F. Callens and M. Waroquier, *J. Phys. Chem. B*, **2008**, 112, 15054–15063.

[a]Research Assistant of the Research Foundation - Flanders (FWO - Vlaanderen)
[b]Postdoctoral Fellow of the Research Foundation - Flanders (FWO - Vlaanderen)