Towards Identifying the All Known Stable Radical Species in X-irradiated Sucrose

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Sucrose – the main component of table sugar – is a commonly used food and drinks sweetener. Less known is its fundamental and practical impotence in radiation sciences. On the one hand, it is regarded as a model system to study radiation damage of sugar-containing macrobiomolecules, while on the other, it is a viable alternative to alanine as a solid state/EPR dosimeter. In recent years considerable progress has been made in determining the location and molecular structure of radiation-induced radicals, with special attention to the stable species. One – and to our knowledge last – radical (T4) with a non-negligible contribution to the stable EPR spectrum has remained unidentified and in this contribution we present results of our efforts towards understanding its chemical structure.

Powder spectra of sucrose, exposed to ~100 kGy and ~100 Gy doses of X-rays at room temperature, were analyzed using experimental data from our previous work (J. Phys. Chem. B, 2013, 117, 7169-7178 and poster at IXth EF-EPR conference, Marseille, 2014). Relative contributions of dominant stable radical species at higher and lower doses are compared and discussed. Main features of the chemical structure of T4 have been devised using semi-empirical theory and a number of possible model structures were proposed and tested with periodic Density Functional Theory calculations. Unfortunately, no correspondence with experimental data has been found. This suggests that severe alterations to the molecule occur during reactions leading to this radical. To gain deeper insight into the dependencies of hyperfine tensors on geometry of the radical, a study of a well-chosen molecular fragment has been initiated. Results of calculations are summarized and discussed.