Temperature dependence of the X-irradiated sucrose powder EPR spectrum

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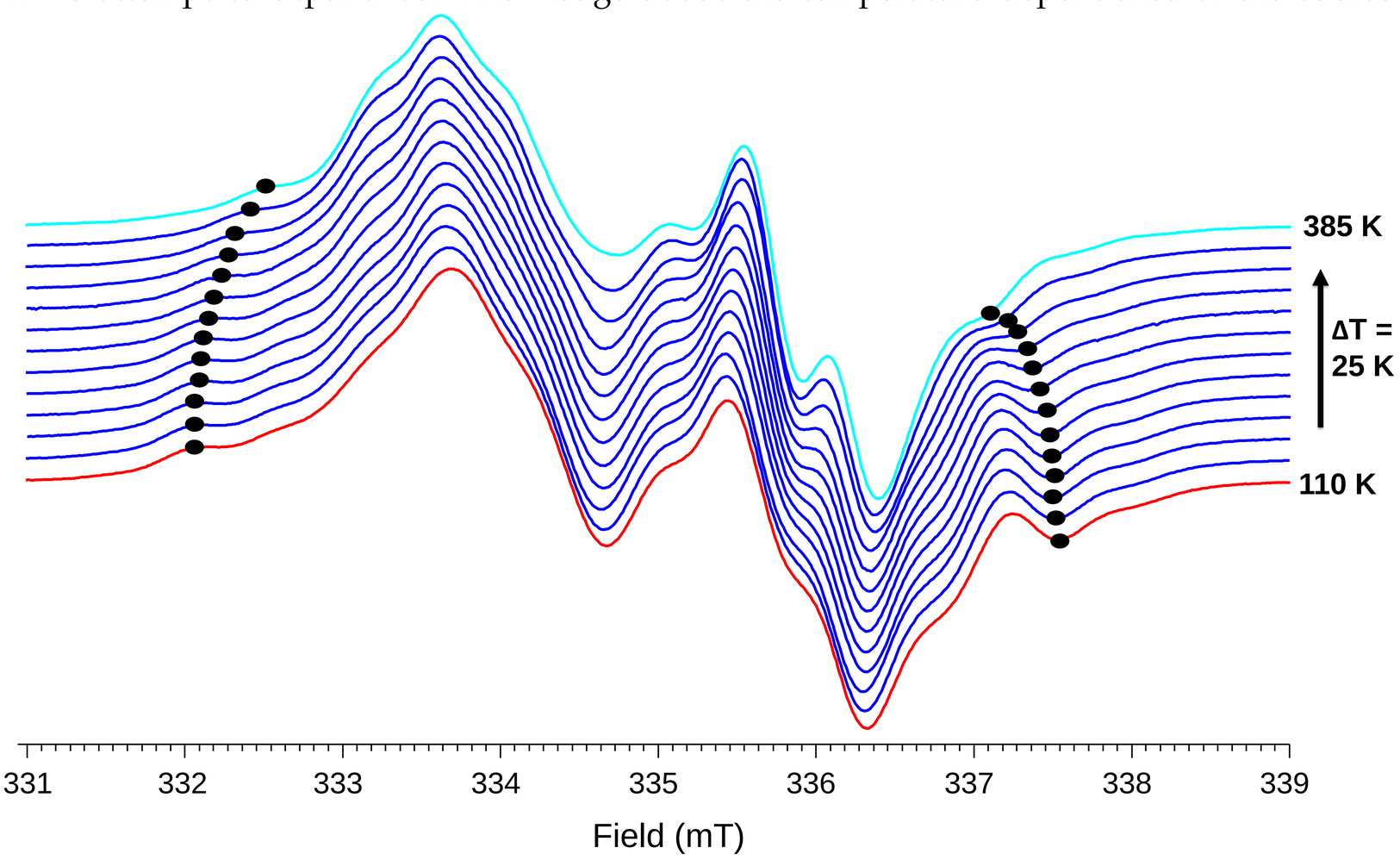
Abstract

Sucrose is the main component of table sugar and it is present in many sugar-containing foodstuffs. High-energy radiation induces stable radicals in sucrose, which are detectable with EPR at room temperature. Multiple radical species contribute to the stable EPR spectrum of irradiated sucrose. Our group identified three radical species (T1,T2,T3) contributing to the centre of the radiation-induced EPR spectrum [1] and recently the fourth species (T4), contributing to the "wings", has been thoroughly characterized and tentatively identified [2]. These results followed from single crystal EPR and ENDOR studies at 110 K, combined with density functional theory calculations. Dosimetric measurements on sucrose, however, are performed at room temperature on powder samples: decomposing and reliably simulating such spectra still presents a challenge. In this work we attempt to expand our knowledge about the temperature dependence of the sucrose powder spectrum.

Temperature dependence

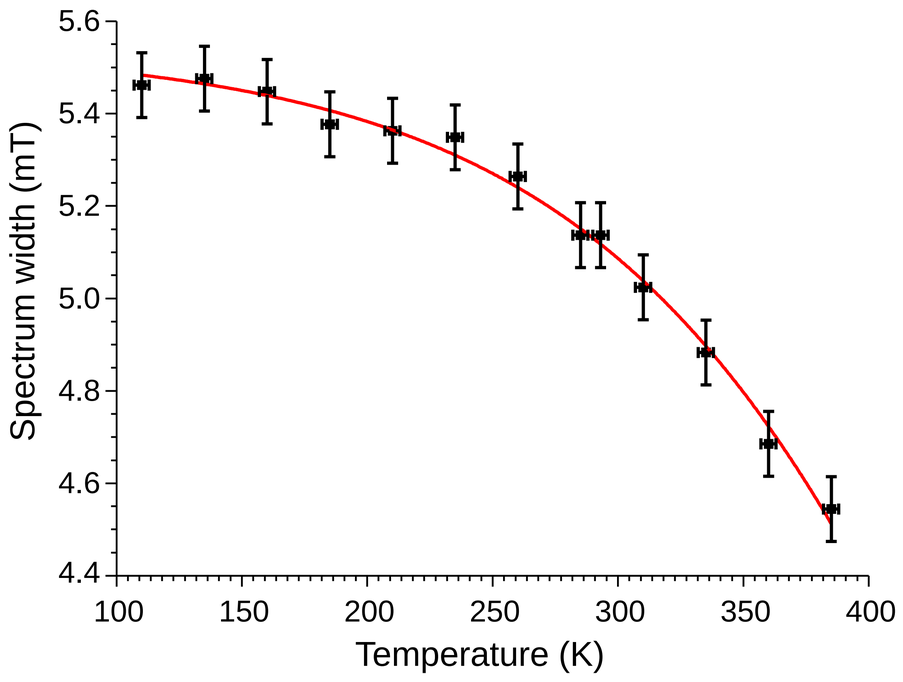
To investigate the temperature dependence we measured X-band EPR powder spectra from 110 K to 385 K in steps of 25 K. Changes are clearly visible.

- The central part of the spectrum shows only small changes.
- The "wings" gradually move closer to the centre. This is highlighted by the dots on the spectra.
- As a result, a narrowing of the total spectrum is observed.

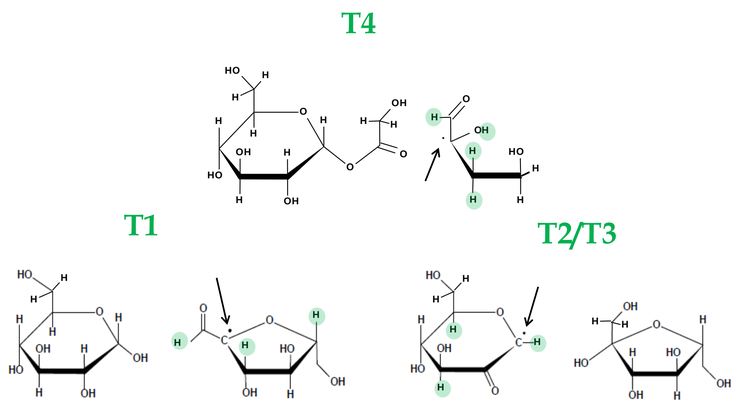


Narrowing of the total spectrum

To quantify the narrowing of the spectrum, the distance between the positions indicated by the dots, is represented in the figure below, as a function of temperature.

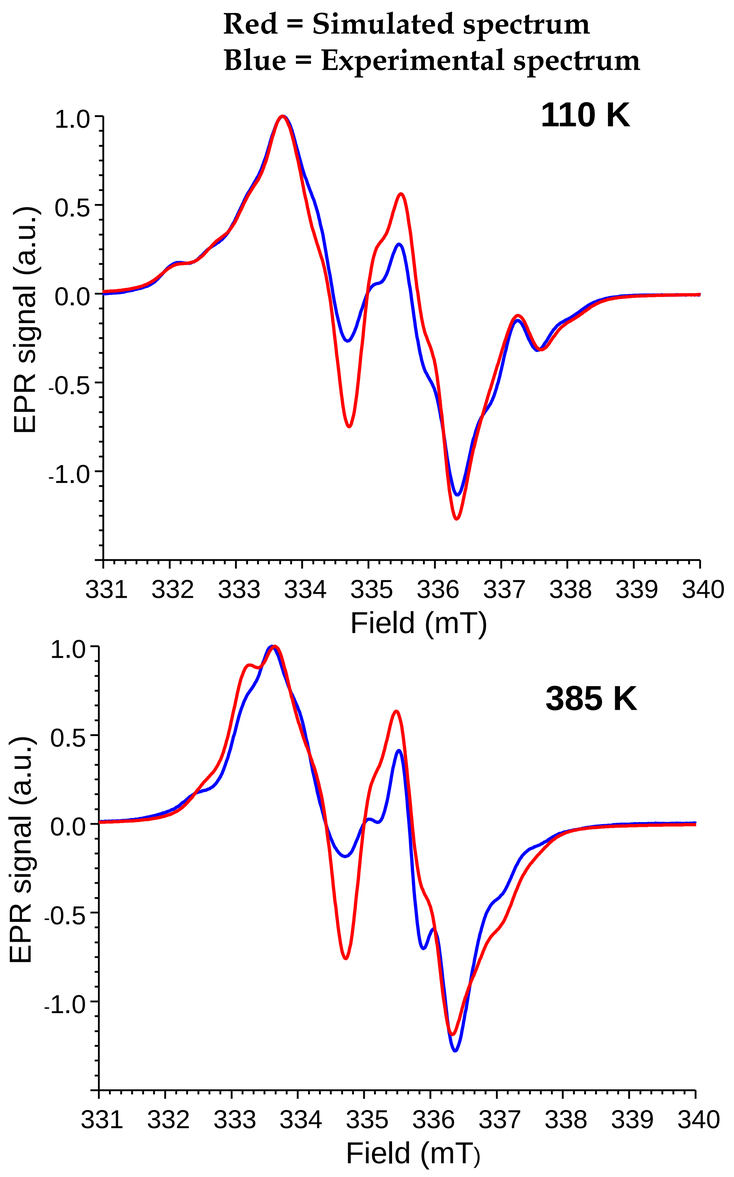


Simulations



110 K
- 4 radicals with ± equal contribution.
- Spin Hamiltonian parameters as determined from 110 K ENDOR and ENDOR-induced EPR study.
- Mixed isotropic Gaussian-Lorentzian linewidth: 3 mT.

385 K
- Only HF interactions of T4 adapted: x0,8.



Conclusions

- The temperature-dependence of the EPR spectrum of irradiated sucrose is nearly exclusively due to the T4 radical component.
- The temperature-evolution of the total width of the EPR spectrum and preliminary spectrum simulations suggest a thermally activated decrease of (a) hyperfine interaction(s) in the T4 radical.

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References

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2. J. Kusakovskij, I. Caretti, S. Van Doorslaer, F. Callens and H. Vrielinck, Phys Chem Chem Phys 18 (16), 10983-10991 (2016).