Electron Paramagnetic Resonance Spectrum of Room Temperature Irradiated Sucrose: Characterization Beyond the Known Stable Radicals

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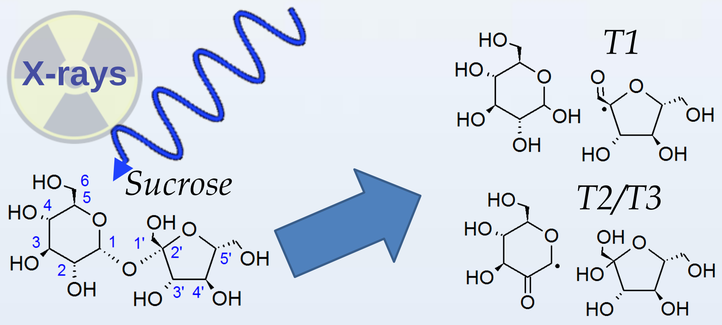
Introduction

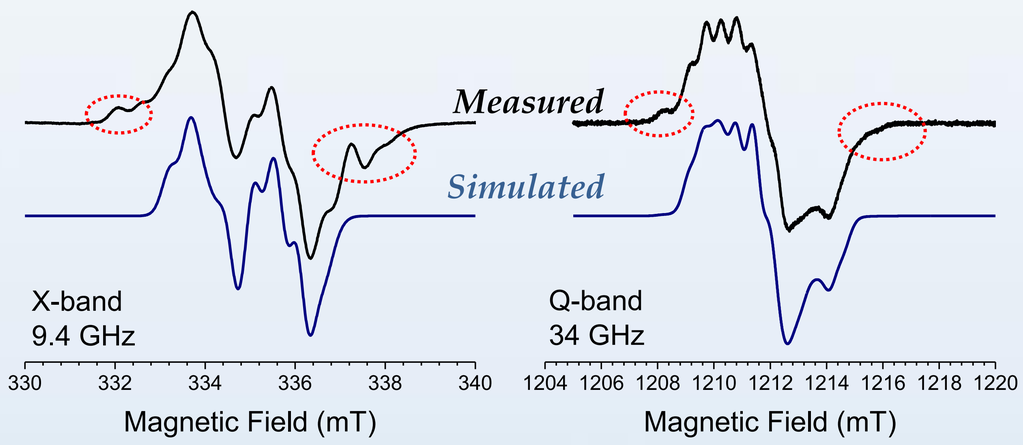
Understanding the stable EPR spectrum of radiation-induced radicals in sucrose has several motivations. From a fundamental scientific viewpoint, identification of the radical structures may provide insight into the radiation chemistry of sugar-containing macrobiomolecules, e.g. DNA. On the other hand, via measurement of signal intensity, the stable EPR signal of sucrose allows to determine radiation doses. Table sugar, that consists for over 90% of sucrose, is present in nearly every household in its pure form or as a foodstuff ingredient. It is therefore considered as a very suitable accident and emergency dosimeter. The composite nature of this powder EPR spectrum, may however complicate dose assessment. Characterization of individual components in this spectrum and determination of their specific dose dependence would present a major step ahead.

Known radicals (T1, T2, T3)

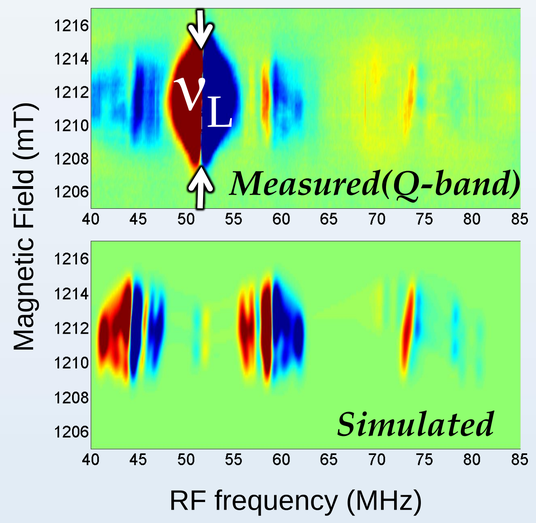
Structure of sucrose and dominating radicals



Powder spectrum simulations including only T1, T2 and T3

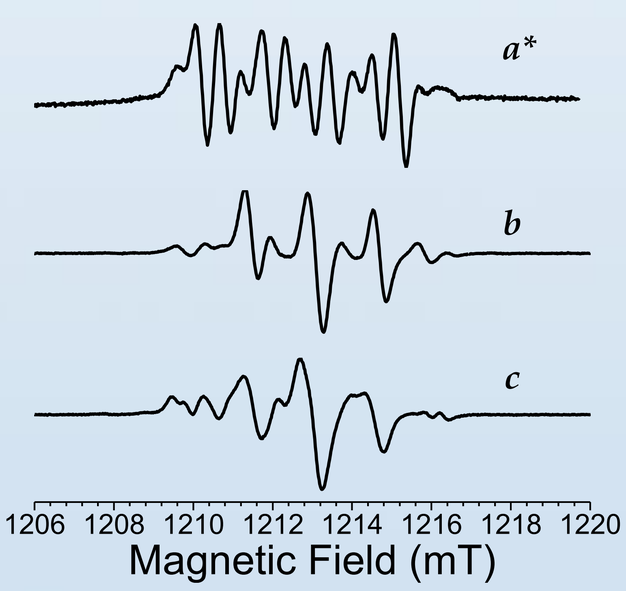


FF-ENDOR of powder sucrose

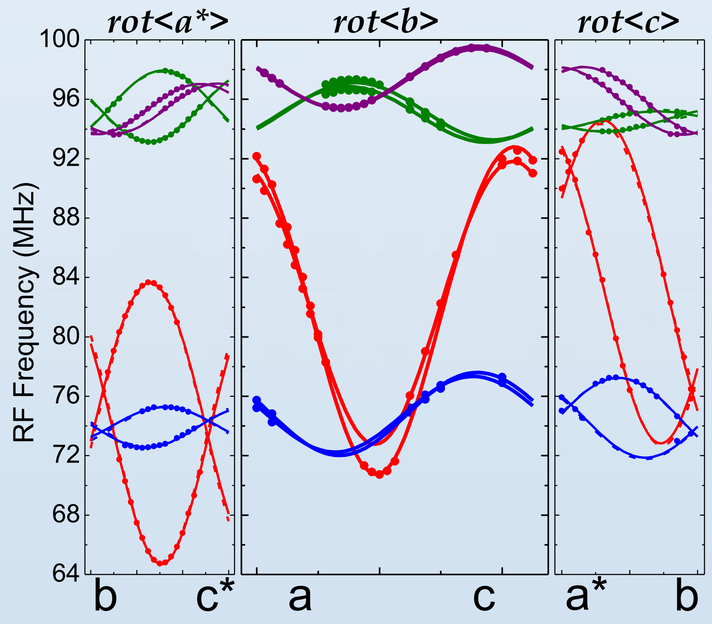


"Unstable" radicals (U1, U2)

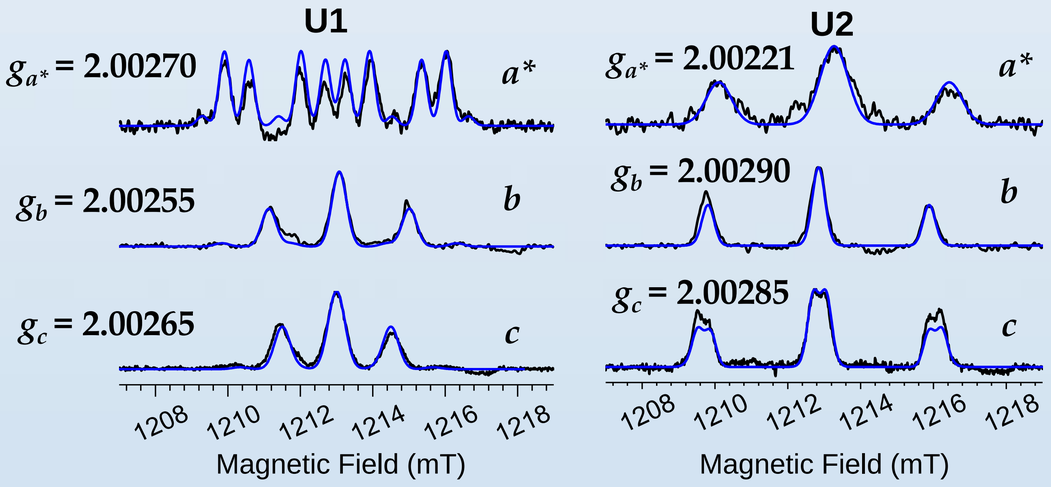
EPR



ENDOR



ENDOR-induced EPR

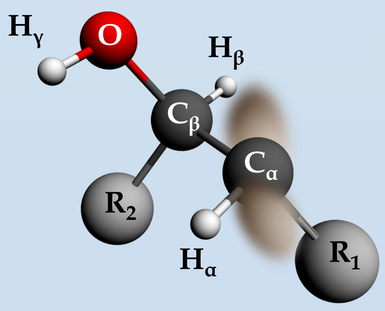


U1	a_{iso} (MHz)	b_{aniso} (MHz)	Eigenvectors a*	b	c
HF1 (H_α)	-55.6	-30.4	0.919	-0.383	0.094
		-6.7	-0.200	-0.658	-0.726
		37.1	0.340	0.649	-0.681
HF2 (H_β)	45.4	-5.7	0.706	-0.604	-0.370
		-3.4	0.171	0.653	-0.738
		9.1	-0.687	-0.458	-0.564

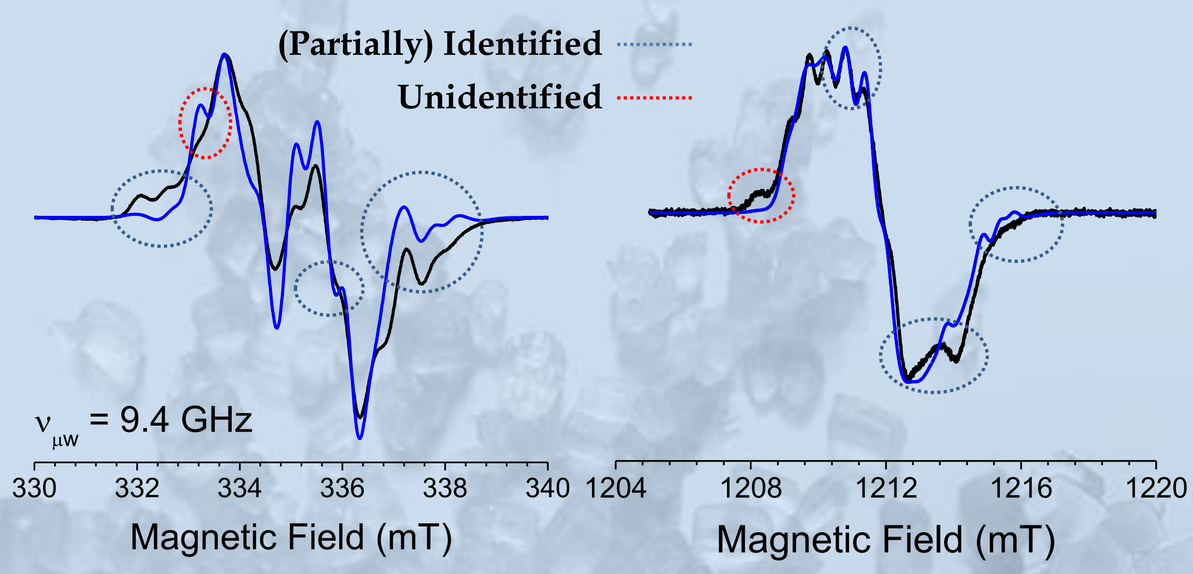
U2	a_{iso} (MHz)	b_{aniso} (MHz)	Eigenvectors a*	b	c
HF1 ($H_{\beta1}$)	86.7	-4.6	-0.517	-0.534	-0.670
		-2.3	0.767	-0.636	-0.086
		6.9	0.380	0.558	-0.738
HF2 ($H_{\beta2}$)	89.0	-5.2	0.124	-0.991	0.060
		-1.6	0.633	0.033	-0.773
		6.8	-0.764	-0.134	-0.631

Schonland Conj.	$\tilde{b}_{aniso}$ (MHz)	Eigenvectors a*	b	c
	-6.0	0.578	-0.549	0.604
	-0.3	-0.757	-0.637	0.145
	6.3	0.306	-0.541	-0.784
	-5.6	0.266	-0.932	-0.245
	-1.1	0.575	0.357	-0.736
	6.7	0.774	0.055	0.631

Radical fragment indicating α-, β- and γ-protons

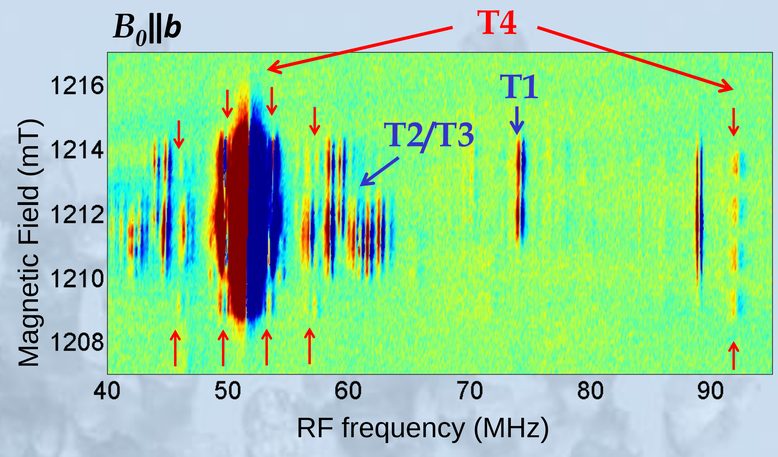


Powder simulations including U1 and U2



Evidence of T4

Q-band FF-ENDOR provides convincing evidence that one more species of stable radicals, is present in the RT irradiated single crystals of sucrose in smaller concentrations.



Conclusions

Even though subtle features of the dosimetric spectrum of irradiated sucrose can be explained by components of U1 and U2, broad lines still remain unidentified in the wings of the simulated spectrum. Recent experiments indicate that these are very likely to arise from the fourth stable radical species.