Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Fourth stable radical species in X-irradiated solid-state sucrose

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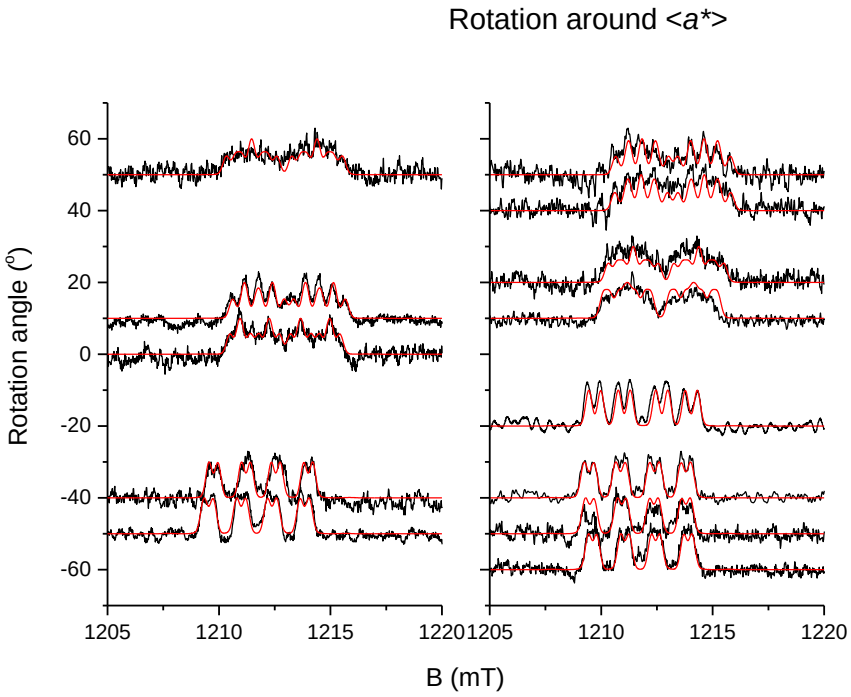
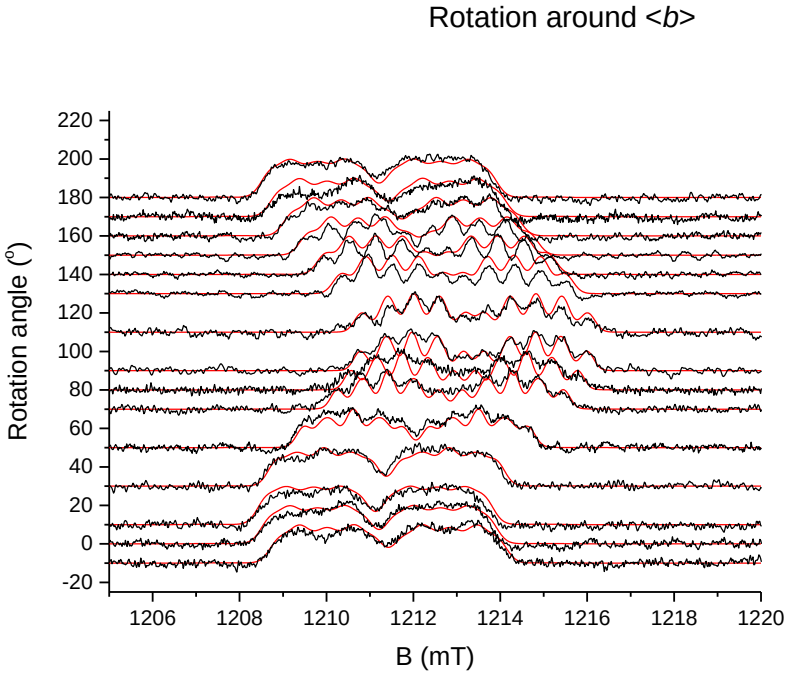
Supporting information

Figure S1. Angular dependence of the Q-band EIE spectra of the fourth radical species recorded at 110 K: experiment (black) and simulation (red) of the absorption EPR spectra using the experimental tables from Table 1 and Figure 1.





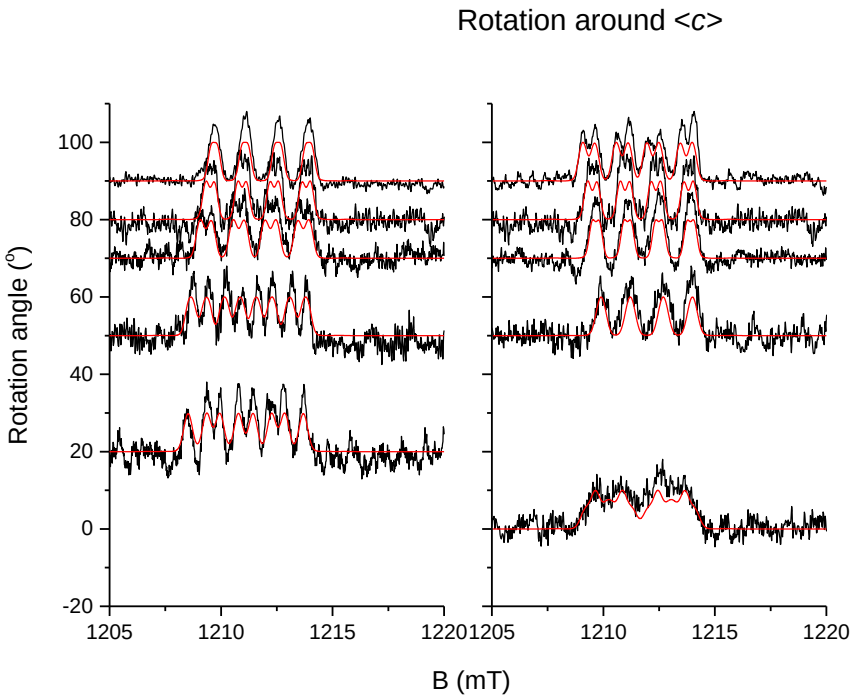

Rotation around <c>
Rotation angle (°)
100
80
60
40
20
0
-20
1205
1210
1215
1220
1205
1210
1215
1220
B (mT)

Table S1. Schonland conjugates of the experimental tensors (Table 1) of the fourth radical species in X-irradiated sucrose. Principal values of the g tensor are also presented as shifts δg_i (i = {1,2,3}) from the free electron g-value g_e = 2.002319 and expressed in ppt. HF tensors are expressed in MHz.

				Eigenvectors		
Tensor	g-value	Iso	δg_i /Aniso	a^*	b	c
g	2.00173		-0.59	0.397	0.223	0.890
	2.00484		2.52	-0.313	-0.879	0.360
	2.00596		3.64	0.863	-0.422	-0.278
β1-HF		80.23	-5.48	0.505	0.640	0.579
			0.82	-0.839	0.204	0.505
			4.66	0.205	-0.740	0.640
β2-HF		36.22	-3.84	0.432	-0.279	0.858
			-2.42	-0.794	0.334	0.508
			6.26	-0.428	-0.901	-0.077
β3-HF		-15.78	-7.96	0.799	-0.593	0.098
			-3.36	-0.123	-0.001	0.992
			11.32	-0.588	-0.805	-0.074
hydroxy-HF		-6.11	-11.27	0.645	-0.341	0.684
			-5.48	0.650	-0.227	-0.725
			16.75	0.402	0.912	0.075

Table S2. Comparison of the experimental HF tensors, (expressed in MHz,) in the reference frame of the **g** tensor to the calculated tensors, using the structure in Figure 5B.

						β1-HF			β2-HF			β3-HF			hydroxy-HF		
					Iso→		80.12			36.22			-15.78			-7.07	
					Aniso→	-4.31	-1.45	5.76	-3.84	-2.42	6.26	-8.09	-3.07	11.17	-7.96	-6.56	14.52
					*a**	0.600	-0.686	0.412	0.931	0.204	-0.302	0.053	0.998	0.045	0.996	-0.077	0.040
					b	-0.800	-0.505	0.324	0.346	-0.754	0.558	-0.071	-0.041	0.997	0.086	0.835	-0.543
	Iso	Aniso	*a**	*b*	*c*	-0.014	-0.524	-0.852	-0.114	-0.624	-0.773	0.996	-0.056	0.068	0.009	0.545	0.839
H1	-13.02	-6.71	0.003	-0.142	0.990							5					
		-3.52	1.000	-0.002	-0.003								4				
		10.23	0.002	0.990	0.142									5			
H3b	38.03	-3.56	0.964	0.006	-0.265				22								
		-2.38	-0.111	-0.899	-0.424					23							
		5.94	-0.241	0.438	-0.866						9						
H3a	67.35	-3.50	0.591	-0.806	0.027	2											
		-2.71	-0.701	-0.530	-0.476		3										
		6.21	0.399	0.262	-0.879			4									
H2	-9.61	-10.74	1.000	-0.008	-0.006										5		
		-3.00	0.010	0.834	0.552											5	
		13.74	0.001	-0.552	0.834												2