Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Identification of primary free radicals in trehalose dihydrate single crystals X-irradiated at 10 K

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Table 2. DFT-calculated proton HFC tensors and g tensors for the radical models: M5+(-I), M5+(-II) and M5+(-III)

δ represents the angle between the DFT-calculated and experimental principal directions of the corresponding tensors for radical R4 (Table 6). With respect to HFCs, only a comparison can be made for the Amax principal direction.

Supporting Information (Model M5+(-I))

g tensor

	Princ val	Princ dir			δ (°)
		a	b	c	
	2.0035	-0.538	0.806	-0.248	19
	2.0109	0.779	0.587	0.220	19
	2.0242	-0.323	0.075	0.944	6

HFC tensors	Iso	Aniso	Princ dir			δ (°)
			a	b	c	
H(C3')	**-1.17**	**-3.04**	0.252	-0.961	0.116	
		-1.38	-0.405	0.005	0.914	
		4.42	-0.879	-0.277	-0.388	39
H(C4')	**24.27**	**-4.80**	0.235	0.445	0.864	
		-3.89	0.613	-0.758	0.224	
		8.69	0.755	0.477	-0.451	40
H(C5')	**9.18**	**-7.79**	0.588	0.184	0.788	
		-0.74	-0.624	0.722	0.297	
		8.53	-0.515	-0.667	0.539	44
H(O6)(Treh2)	**-0.18**	**-6.13**	-0.714	-0.187	0.675	
		-5.10	0.441	-0.869	0.225	
		11.23	-0.544	-0.458	-0.702	28
H(O4') (transferred)	**-0.69**	**-5.65**	0.312	-0.020	0.950	
		-5.32	-0.455	0.874	0.168	
		10.97	-0.834	-0.485	0.264	50

Supporting Information (Model M5+(-II))

g tensor	Princ val		Princ dir			δ (°)
			a	b	c	
	2.0034		-0.528	0.803	-0.275	19
	2.0109		0.786	0.585	0.201	19
	2.0240		-0.322	0.110	0.940	4

HFC tensors	Iso	Aniso	Princ dir			δ (°)
			a	b	c	
H(C3')	**-1.50**	**-3.15**	0.240	-0.964	0.116	
		-1.45	-0.405	0.009	0.914	
		4.60	-0.882	-0.266	-0.389	39
H(C4')	**24.36**	**-4.94**	0.245	0.426	0.871	
		-3.89	0.593	-0.777	0.212	
		8.82	0.767	0.465	-0.443	40
H(C5')	**11.99**	**-8.03**	0.558	0.152	0.816	
		-0.62	-0.574	0.781	0.248	
		8.65	-0.599	-0.606	0.523	41
H(O6)(Treh2)	**-0.18**	**-6.19**	-0.729	-0.167	0.664	
		-5.13	0.423	-0.872	0.246	
		11.32	-0.538	-0.461	-0.706	28
H(O4') (transferred)	**-0.66**	**-5.59**	0.293	0.006	0.956	
		-5.29	-0.457	0.879	0.135	
		10.87	-0.840	-0.477	0.261	50

Supporting Information (Model M5+(-III))

g tensor	Princ val		Princ dir			δ (°)
			a	b	c	
	2.0043		-0.594	0.750	-0.290	14
	2.0104		0.731	0.654	0.196	14
	2.0241		-0.337	0.096	0.937	4

HFC tensors	Iso	Aniso	Princ dir			δ (°)
			a	b	c	
H(C3')	**-1.36**	**-3.12**	0.258	-0.963	0.084	
		-1.39	-0.381	-0.021	0.924	
		4.51	-0.888	-0.270	-0.372	40
H(C4')	**20.53**	**-4.82**	0.181	0.484	0.856	
		-3.71	0.623	-0.730	0.281	
		8.53	0.761	0.482	-0.434	41
H(C5')	**6.30**	**-7.78**	0.525	0.249	0.814	
		-0.87	-0.655	0.728	0.200	
		8.65	-0.543	-0.639	0.545	42
H(O6)(Treh2)	**-0.21**	**-5.98**	-0.700	-0.213	0.681	
		-4.89	0.472	-0.855	0.217	
		10.87	-0.536	-0.474	-0.699	29
H(O4') (transferred)	**-0.77**	**-5.63**	0.243	0.096	0.965	
		-5.31	-0.490	0.871	0.037	
		10.94	-0.837	-0.482	0.259	50