Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

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

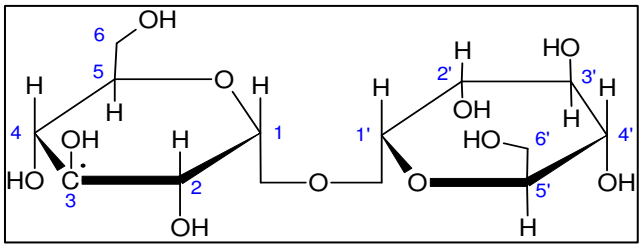
Mihaela Adeluta Tarpan, Hendrik De Cooman Einar Sagstuen, Michel Waroquier, and Freddy Callens

Table 1. DFT-calculated proton HF tensors (in MHz) for the C3, C4, C2' and C3'-centered radical models, labelled Model M1 to M4 (see below).

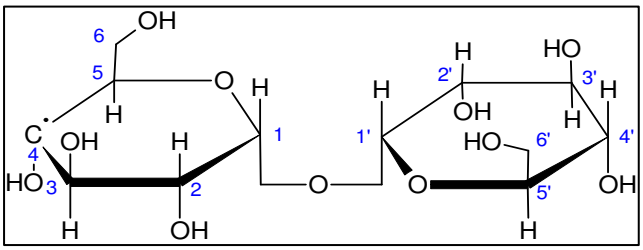
radical model	proton	isotropic values	anisotropic values	principal directions			δ(°)	δ'(°)
				a	b	c		
Model 1	H2	92.58	6.86	-0.804	0.360	-0.474	59	
			-2.13	0.249	0.927	0.282	64	
			-4.74	0.541	0.108	-0.834	13	
	H4	72.04	6.84	-0.062	-0.771	-0.634		75
			-1.97	0.276	-0.624	0.731		18
			-4.87	-0.959	-0.130	0.252		64
	HO3	4.49	20.90	0.206	-0.267	-0.942		
			-9.65	-0.181	-0.956	0.231		
			-11.25	-0.962	0.123	-0.245		
Model 2	H3	84.03	6.79	-0.121	0.717	0.686	25	
			-0.95	0.076	-0.682	0.727	64	
			-5.83	-0.990	-0.141	-0.028	61	
	H5	80.48	7.21	0.577	0.414	-0.704		44
			-2.97	0.779	-0.539	0.322		56
			-4.24	0.246	0.734	0.633		9
	HO4	-2.42	19.40	-0.927	0.040	0.372		
			-8.84	0.216	-0.755	0.619		
			-10.56	0.306	0.654	0.692		
Model 3	H1'	20.74	9.50	-0.454	0.835	0.310		
			-3.74	-0.495	-0.526	0.692		
			-5.76	0.741	0.161	0.652		
	H3'	92.24	7.24	-0.405	0.234	0.884	59	
			-1.86	0.544	0.839	0.027	53	
			-5.38	-0.735	0.492	-0.467	31	
	HO2'	75.45	16.83	0.970	-0.077	-0.230		9
			-6.40	-0.241	-0.425	-0.873		15
			-10.42	0.031	-0.902	0.431		12
Model 4	H2'	87.90	7.57	-0.278	0.201	0.939	60	
			-2.49	-0.855	-0.497	-0.147	27	
			-5.08	-0.437	0.844	-0.310	45	
	H4'	78.09	7.21	-0.839	-0.267	-0.474		23
			-1.85	-0.382	-0.331	0.863		25
			-5.36	0.387	-0.905	-0.175		23
	HO3'	0.58	20.41	-0.132	0.667	0.733		
			-9.12	-0.374	-0.718	0.587		
			-11.28	0.918	-0.196	0.344		

δ and δ' represent the angles between the DFT-calculated and experimental principal directions of A1(R1) and A2(R1), respectively.

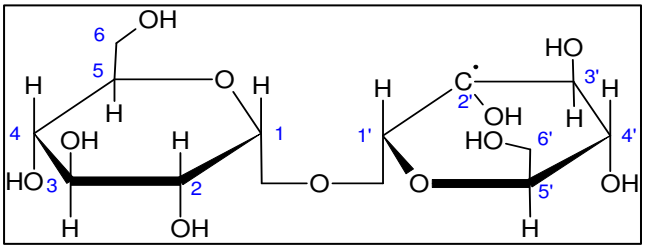
Model 1



Model 2



Model 3



Model 4