Electronic Supplementary Information

Synthesis and structural elucidation of a trifluoromethylated cyclopentene hydrazone: A combined X-ray and computational studies

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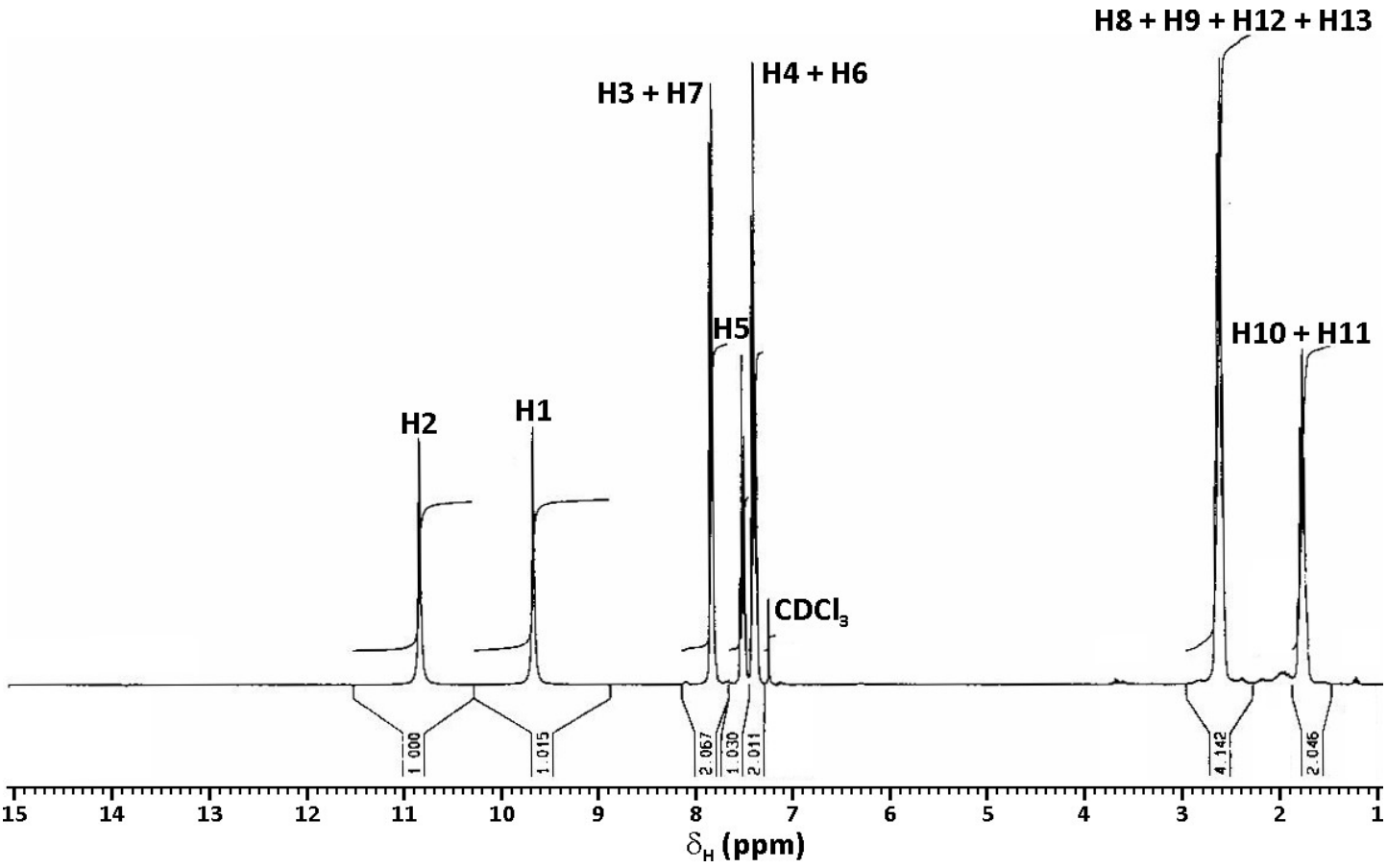

Fig. S1 The ^{1}H NMR spectrum of **1** recorded in $CDCl_3$.

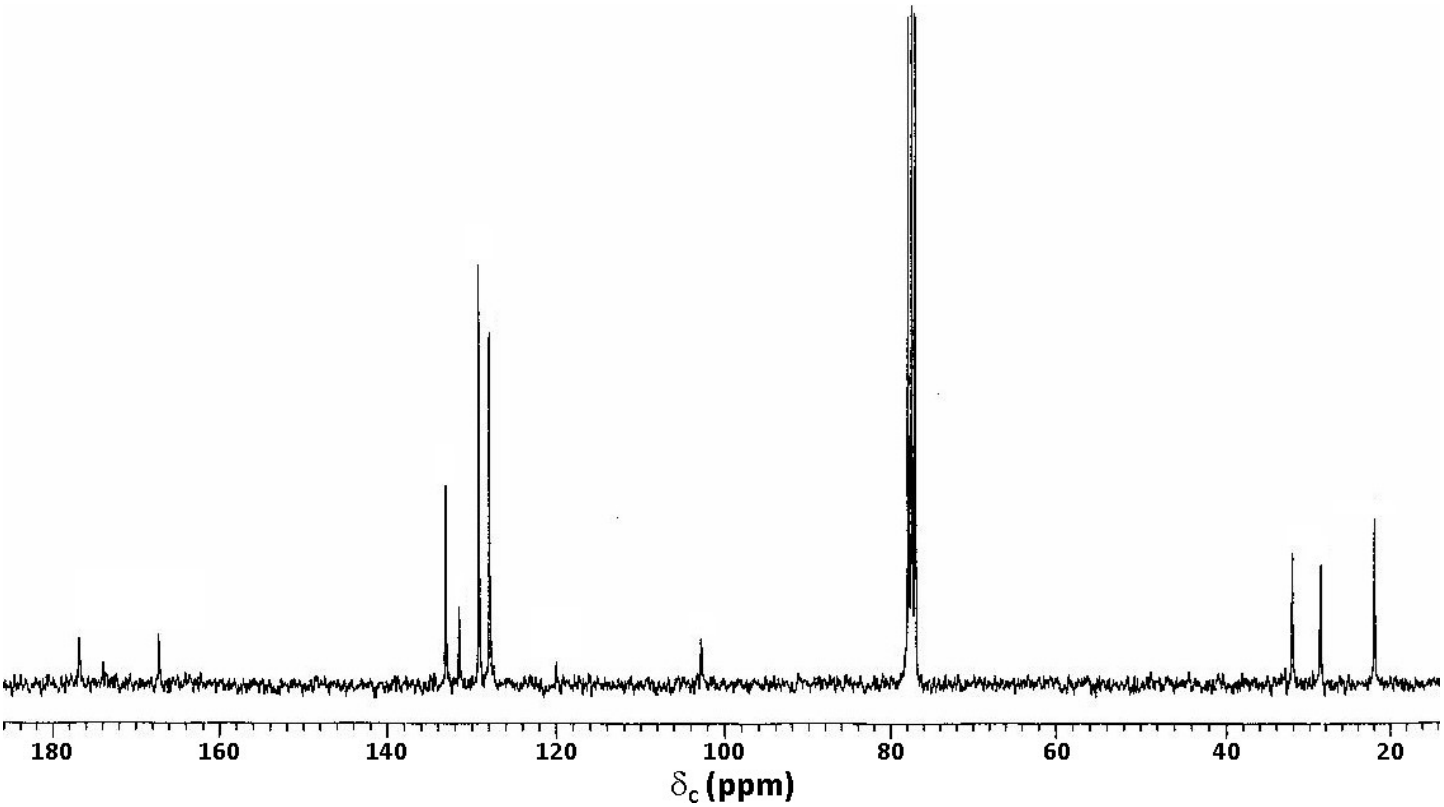

Fig. S2 The ^{1}H NMR spectrum of **1** recorded in $CDCl_3$.

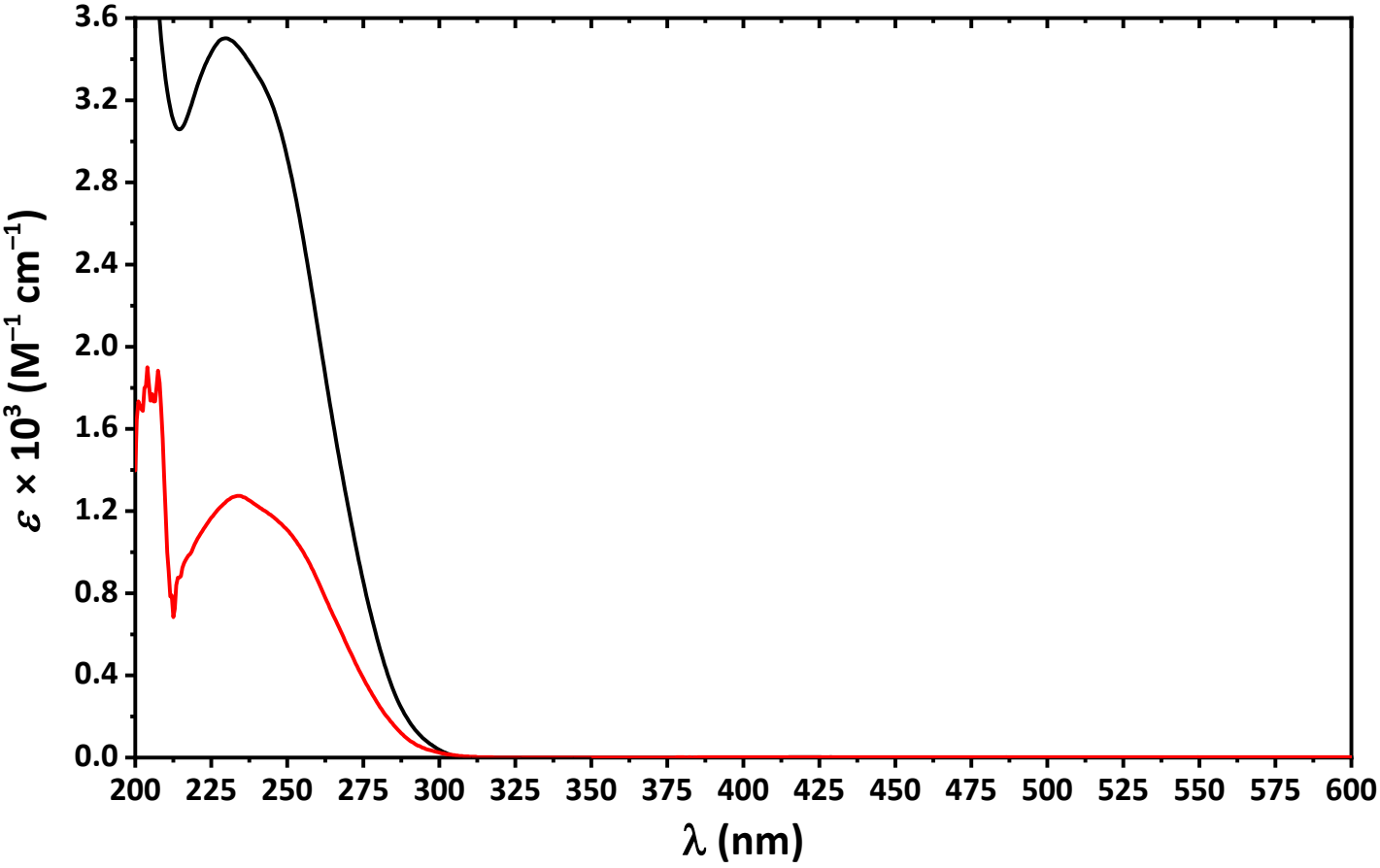

Fig. S3 The UV-vis spectra of **1** recorded in MeOH (black) and *n*-heptane (red).

Table S1. Cartesian coordinates of the optimized structure of tautomers **1**, **1'** and **1''**.

Atom	Tautomer **1**			Tautomer **1'**			Tautomer **1''**		
	x	*y*	*z*	*x*	*y*	*z*	*x*	*y*	*z*
H1	1.8011050	–0.0554460	–1.7255390	–0.4857580	2.0555810	1.5682260	1.5394580	1.1930430	–0.1344160
H2	–0.3689080	–1.1365950	–0.8156670	–2.2872390	–0.6041230	1.8857960	–2.7298660	0.5818990	–1.3849370
H3	3.6464060	1.1430030	–1.5325820	1.8670850	–1.1956220	–1.4729240	3.1853490	1.2393850	1.3119090
H4	6.0987920	1.1541110	–1.7684530	4.1294980	–2.0461890	–1.9882660	5.5858490	1.7375910	1.5587570
H5	7.5088820	–0.2246630	–0.2556290	6.0856290	–1.2847010	–0.6566620	7.2822580	0.3245420	0.4157060
H6	6.4409370	–1.6170920	1.5073120	5.7696210	0.3808360	1.1659740	6.5521860	–1.6053100	–0.9741300
H7	3.9577050	–1.6297160	1.7425200	3.4982350	1.2874550	1.6308880	4.1210800	–2.1071910	–1.2203840
H8	–3.3306690	2.3908500	–0.4648580	–4.3581360	–0.5240740	0.5781520	–3.9758560	2.4970920	–0.5463090
H9	–3.5159860	1.7908170	1.1791250	–3.4793960	–0.7387590	–0.9413300	–3.0755800	2.4792480	0.9805580
H10	–1.3820910	2.5928000	1.8662390	–4.1208720	–3.0422760	–0.3981800	–1.9614370	4.2707100	–0.2867380
H11	–1.7065160	3.8174210	0.6349500	–3.8008000	–2.7883570	1.3153090	–1.9998500	3.3143190	–1.7706220
H12	–0.2230480	2.7103230	–0.9533160	–1.6721360	–3.7471380	0.8460630	0.2303920	2.7732870	–1.0243080
H13	0.5724600	2.2128440	0.5395490	–1.7555910	–3.3482440	–0.8682430	–0.2329430	2.8570010	0.6815290
C1	2.1539690	–0.3494840	0.3076290	1.2260340	0.7417940	0.4474690	2.0499550	–0.8229790	–0.2097960
C2	–2.7987210	–0.6725600	–0.3045820	–1.3071990	0.6861380	0.5220420	–2.9701940	–0.1144440	0.6391450
C3	–4.3219550	–0.7907130	–0.0211240	–1.7456570	1.4773260	–0.7445150	–3.6887710	–1.3648950	0.0574790
C4	3.6377260	–0.2798420	0.1057360	2.5339760	0.0913270	0.1287070	3.4929190	–0.4485100	–0.0148390
C5	4.2450820	0.5110430	–0.8830160	2.7159250	–0.8473610	–0.8989670	3.9108880	0.6330960	0.7767190
C6	5.6355180	0.5308640	–1.0095100	3.9941420	–1.3298290	–1.1833410	5.2716580	0.9080520	0.9322100
C7	6.4276880	–0.2397430	–0.1543530	5.0944030	–0.8980730	–0.4374140	6.2245690	0.1088650	0.2957260
C8	5.8274040	–1.0219630	0.8376590	4.9176800	0.0372510	0.5867950	5.8138900	–0.9767000	–0.4851550
C9	4.4399680	–1.0376760	0.9719400	3.6466360	0.5402220	0.8589140	4.4567040	–1.2589680	–0.6330800
C10	–0.8148130	0.7652030	–0.2994820	–1.2293650	–1.6769110	0.3607170	–0.9369920	1.0717450	–0.2981820
C11	–2.1721100	0.5926450	–0.0815740	–2.1561280	–0.5731730	0.7951910	–2.4570990	0.9015390	–0.3719720
C12	–2.7964240	1.9078600	0.3645500	–3.4812750	–0.9898060	0.1227050	–2.9910860	2.3313880	–0.1016240
C13	–1.5678170	2.7451390	0.7978620	–3.4571240	–2.5340960	0.3062290	–1.9006500	3.2523190	–0.6805040
C14	–0.3751560	2.1756470	–0.0041730	–1.9666780	–2.9666310	0.1363410	–0.5776420	2.5488540	–0.3168740
N1	1.3866660	–0.0078270	–0.8042200	0.0429770	0.0653410	0.2498330	1.1670060	0.2496390	–0.1409450
N2	0.0130590	–0.1886010	–0.7797550	–0.0343060	–1.3303220	0.0666260	–0.1776360	0.0462920	–0.2278590
O1	1.6371650	–0.6592100	1.3700600	1.1900350	1.9019730	0.8878870	1.6917180	–1.9679590	–0.4265900
O2	–2.2180770	–1.6960920	–0.6979060	–1.3161090	1.5282980	1.6251110	–2.8932530	0.0219140	1.8360940
F1	–5.0242890	0.1380150	–0.7247610	–3.0180040	1.9131420	–0.6124580	–2.9269710	–1.9841990	–0.8653220
F2	–4.8018250	–1.9956310	–0.3484130	–0.9696830	2.5509730	–0.9737500	–4.0218500	–2.2469270	1.0022440
F3	–4.5929980	–0.5812470	1.2944590	–1.6961420	0.6980230	–1.8570400	–4.8315390	–0.9549790	–0.5632030