Supplementary Material (ESI) for *PCCP*

N-Methyl Stereochemistry in Tropinone: The conformational flexibility of the tropane motif

SUPPLEMENTARY INFORMATION

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Table S1. Rotational transitions and residuals (MHz) of equatorial tropinone (parent species).

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	F'	F''	obs.[a]	o.-c.[b]	J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	F'	F''	obs.	o.-c.
2	0	2	1	0	1	3	2	4557.984	0.001	5	3	2	4	3	1	6	5	11402.721	-0.001
						2	1	4558.074	0.003	6	0	6	5	0	5	7	6	13634.410	0.002
						2	2	4558.714	0.000							6	5	13634.548	0.000
3	0	3	2	0	2	4	3	6833.842	0.000							5	4	13634.419	-0.002
						3	2	6833.936	0.001	6	1	5	5	1	4	7	6	13805.177	0.001
						2	1	6833.957	-0.004							6	5	13805.227	-0.003
3	1	2	2	1	1	4	3	6907.187	0.000							5	4	13805.148	-0.002
						3	2	6907.350	0.000	6	1	6	5	1	5	7	6	13530.157	0.000
						2	1	6906.957	-0.008							6	5	13530.231	0.001
3	1	3	2	1	2	4	3	6769.017	0.001							5	4	13530.212	-0.001
						3	2	6769.261	-0.002	6	2	4	5	2	3	7	6	13715.539	0.000
						2	1	6769.242	0.006							6	5	13715.519	-0.001
4	0	4	3	0	3	5	4	9105.921	0.000							5	4	13715.550	0.002
						4	3	9106.027	0.000	6	2	5	5	2	4	7	6	13672.100	-0.001
						3	2	9105.969	-0.001							6	5	13672.214	0.000
4	1	3	3	1	2	5	4	9208.055	0.001	6	3	3	5	3	2	7	6	13685.385	0.000
						4	3	9208.138	0.003							6	5	13685.548	-0.005
						3	2	9207.974	0.000							5	4	13685.351	-0.006
						4	4	9207.496	0.002	6	3	4	5	3	3	7	6	13684.167	0.007
4	1	4	3	1	3	5	4	9023.987	-0.001							6	5	13684.343	0.006
						4	3	9024.122	0.001							5	4	13684.129	-0.002
						3	2	9024.110	-0.005	7	0	7	6	0	6	8	7	15889.295	0.003
4	2	2	3	2	1	5	4	9130.187	0.000							7	6	15889.446	0.001
						4	3	9130.399	0.000							6	5	15889.295	-0.004
4	2	3	3	2	2	5	4	9117.526	0.004	7	1	6	6	1	5	8	7	16100.517	0.000
						4	3	9117.827	0.002							7	6	16100.574	0.000
						3	2	9117.448	0.003							6	5	16100.499	0.001
5	0	5	4	0	4	6	5	11373.088	0.000	7	1	7	6	1	6	8	7	15780.991	0.001
						5	4	11373.210	-0.001							7	6	15781.055	0.001
						4	3	11373.112	0.000							6	5	15781.031	0.000
5	1	4	4	1	3	6	5	11507.527	0.001	7	2	5	6	2	4	8	7	16015.714	-0.001
						5	4	11507.583	-0.002							7	6	16015.655	0.002
						4	3	11507.487	0.002							6	5	16015.728	0.001
5	1	5	4	1	4	6	5	11277.769	0.000	7	2	6	6	2	5	8	7	15947.570	0.000
						5	4	11277.858	-0.003							7	6	15947.653	-0.002
5	2	3	4	2	2	6	5	11420.491	0.001	7	3	4	6	3	3	8	7	15969.366	0.002
						5	4	11420.546	-0.001							7	6	15969.460	0.000
						4	3	11420.480	-0.003							6	5	15969.352	-0.004
5	2	4	4	2	3	6	5	11395.354	0.001	7	3	5	6	3	4	7	6	15966.729	0.002
						5	4	11395.522	0.000							6	5	15966.609	0.000
						4	3	11395.331	-0.003										
						5	5	11395.825	0.000										
						4	4	11394.956	0.002										

[a]Observed. [b]Observed minus calculated.

Table S2. Rotational transitions and residuals (MHz) of the ^{13}C and ^{18}O monosubstituted isotopologues of equatorial tropinone.

								$^{13}C_1$-$^{13}C_5$		$^{13}C_2$-$^{13}C_4$		$^{13}C_3$		$^{13}C_6$-$^{13}C_7$		$^{13}C_9$		^{18}O	
J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	F'	F''	obs.[a]	o.-c.[b]	obs.	o.-c.	obs.	o.-c.	obs.	o.-c.	obs.	o.-c	obs.	o.-c
3	0	3	2	0	2	4	3	6818.494	0.000	6806.736	0.001	6791.671	0.000	6807.602	0.001	6726.311	-0.001	6601.753	-0.001
						3	2	6818.594	0.002	6806.832	-0.001	6791.761	-0.001	6807.690	0.001				
3	1	2	2	1	1	4	3	6897.202	0.000	6885.568	0.001	6863.657	-0.001	6874.818	0.001	6795.148	-0.001	6669.748	0.002
						3	2	6897.366	0.000	6885.729	-0.001	6863.822	0.002	6874.978	-0.001	6795.313	0.002	6669.906	-0.002
3	1	3	2	1	2	4	3	6749.608	0.000	6737.790	0.001	6727.868	-0.001	6747.733	0.003	6664.954	-0.001	6540.935	0.001
						3	2	6749.853	-0.003	6738.033	-0.004			6747.970	-0.006	6665.202	0.001		
4	0	4	3	0	3	5	4	9084.570	0.000	9068.848	0.000	9049.919	0.001	9071.732	0.000	8963.252	0.000	8797.386	0.000
						4	3	9084.684	0.001	9068.964	0.002	9050.022	0.000	9071.832	-0.001	8963.353	0.000	8797.484	0.000
						3	2	9084.617	-0.001	9068.895	-0.001								
4	1	4	3	1	3	5	4	8997.898	0.001	8982.130	0.002	8969.180	0.000	8995.804	0.003	8885.411	0.000	8720.101	0.001
						4	3	8998.032	0.001	8982.263	0.000	8969.312	0.000	8995.932	0.000	8885.542	0.000	8720.228	-0.002

[a]Observed. [b]Observed minus calculated.

Table S3. Rotational transitions and residuals (MHz) of the ^{15}N isotopologues of equatorial tropinone.

^{15}N							
J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	obs.[a]	o.-c.[b]
3	0	3	2	0	2	6808.968	0.000
3	1	2	2	1	1	6879.107	0.000
3	1	3	2	1	2	6746.706	0.000
4	0	4	3	0	3	9073.199	0.000
4	1	4	3	1	3	8994.280	0.000

[a]Observed. [b]Observed minus calculated.

Table S4. Rotational transitions and residuals (MHz) of axial tropinone (parent species).

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	F'	F''	obs.[a]	o.-c.[b]	J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	F'	F''	obs.	o.-c.
2	0	2	1	0	1	3	2	5110.184	0.001	4	2	2	3	2	1	5	4	10372.069	0.000
						2	1	5110.070	0.005							4	3	10371.778	0.000
						2	2	5109.233	-0.001							3	2	10372.156	-0.002
						1	1	5111.546	0.004	4	2	3	3	2	2	5	4	10238.222	0.000
2	1	2	1	1	1	3	2	5013.174	0.003							4	3	10237.829	0.000
						2	1	5012.281	-0.002							3	2	10238.322	0.000
						1	0	5013.704	-0.005	5	0	5	4	0	4	6	5	12572.698	-0.002
						1	1	5013.584	-0.004							5	4	12572.587	-0.001
3	0	3	2	0	2	4	3	7630.058	0.000							4	3	12572.659	0.000
						3	2	7629.937	-0.001	5	1	4	4	1	3	6	5	13013.978	0.000
						2	1	7629.908	0.003							5	4	13013.874	0.002
3	1	2	2	1	1	4	3	7845.169	0.000	5	1	5	4	1	4	6	5	12479.516	0.000
						3	2	7844.915	0.000							5	4	12479.422	0.002
						2	1	7845.248	0.001							4	3	12479.468	0.000
3	1	3	2	1	2	4	3	7510.893	0.000	5	2	3	4	2	2	6	5	13018.083	-0.003
						3	2	7510.613	-0.001							5	4	13017.961	-0.001
						2	1	7510.819	0.001							4	3	13018.105	0.000
3	2	1	2	2	0	3	2	7743.807	0.000	5	2	4	4	2	3	6	5	12779.420	-0.001
						2	1	7745.086	-0.001							5	4	12779.199	-0.001
3	2	2	2	2	1	3	2	7686.523	0.005							4	3	12779.445	0.001
						2	1	7687.904	0.000	6	0	6	5	0	5	7	6	15014.911	0.002
4	0	4	3	0	3	5	4	10115.714	0.000							6	5	15014.813	-0.005
						4	3	10115.591	-0.001							5	4	15014.877	-0.003
						3	2	10115.645	-0.002	6	1	5	5	1	4	7	6	15558.582	0.000
4	1	3	3	1	2	5	4	10439.994	0.000							6	5	15558.479	0.000
						4	3	10439.856	0.000	6	1	6	5	1	5	7	6	14950.477	0.001
						3	2	10440.001	0.001							6	5	14950.408	0.003
4	1	4	3	1	3	5	4	9999.888	0.001							5	4	14950.445	0.004
						4	3	9999.743	0.000	6	2	4	5	2	3	7	6	15665.556	-0.001
						3	2	9999.819	-0.001							6	5	15665.489	0.000
										6	2	5	5	2	4	7	6	15309.018	0.002
																6	5	15308.871	0.002

[a]Observed. [b]Observed minus calculated.

Table S5. Rotational transitions and residuals (MHz) of the ^{13}C monosubstituted isotopologues of axial tropinone.

								$^{13}C_1$-$^{13}C_5$		$^{13}C_2$-$^{13}C_4$		$^{13}C_3$		$^{13}C_6$-$^{13}C_7$		$^{13}C_9$	
J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	F'	F''	obs.[a]	o.-c.[b]	obs.	o.-c.	obs.	o.-c.	obs.	o.-c.	obs.	o.-c
3	0	3	2	0	2	4	3	7611.230	0.001	7605.869	-0.001	7588.123	-0.001	7587.250	-0.001	7530.551	0.002
						3	2	7611.112	0.000	7605.752	0.000	7588.005	0.000	7587.124	-0.001		
						2	1	7611.077	0.001	7605.717	0.000						
3	1	2	2	1	1	4	3	7815.910	0.000	7810.366	0.000	7801.501	0.001	7818.908	0.000	7757.287	0.000
3	1	3	2	1	2	4	3	7495.645	-0.001	7490.634	0.000	7468.940	0.000	7465.484	0.002	7408.330	-0.006
						3	2	7495.367	0.000	7490.355	0.000	7468.657	-0.004	7465.198	-0.004		
						2	1							7465.411	0.003		
4	0	4	3	0	3	5	4	10094.288	-0.001	10087.092	0.000	10060.657	-0.001	10051.767	0.000	9978.626	0.003
						4	3	10094.169	0.000	10086.972	0.001	10060.538	0.002	10051.643	0.001	9978.494	-0.005
4	1	4	3	1	3	5	4	9980.557	0.002	9973.853	0.001	9944.199	0.002	9937.363	0.001	9861.911	-0.001
						4	3	9980.410	-0.001	9973.710	0.001	9944.054	0.001	9937.215	-0.001	9861.772	0.005

[a]Observed. [b]Observed minus calculated.

Table S6. Substitution coordinates of tropinone.

Equatorial

	Substitution coordinates[a]			*Ab initio*[b]		
	$\|a\|$	$\|b\|$	$\|c\|$	*a*	*b*	*c*
C_1	0.568(5)[c]	1.145(3)	[0.000][d]	-0.568	-1.143	-0.080
C_2	0.882(4)	1.282(2)	0.535(7)	0.872	-1.279	-0.596
C_3	1.6511(17)	[0.000]	0.300(9)	1.641	0.000	-0.313
C_4	0.882(4)	1.282(2)	0.535(7)	0.873	1.280	-0.593
C_5	0.568(5)	1.145(3)	[0.000]	-0.567	1.143	-0.077
C_6	0.640(12)	0.769(9)	1.433(6)	-0.576	0.774	1.432
C_7	0.640(12)	0.769(9)	1.433(6)	-0.578	-0.778	1.430
N	1.1647(15)	[0.000]	0.776(2)	-1.185	0.001	-0.773
C_9	2.6236(11)	[0.000]	0.708(4)	-2.641	0.001	-0.628
O	2.8123(11)	[0.000]	[0.000]	2.778	0.000	0.137

Axial

	Substitution coordinates			*Ab initio*		
	$\|a\|$	$\|b\|$	$\|c\|$	*a*	*b*	*c*
C_1	0.666(2)	0.216(7)	1.1488(13)	0.658	0.248	-1.147
C_2	0.645(2)	0.571(3)	1.2791(12)	-0.614	-0.630	-1.276
C_3	1.4603(11)	0.451(3)	[0.000]	-1.430	-0.524	0.000
C_4	0.645(2)	0.571(3)	1.2791(12)	-0.614	-0.637	1.273
C_5	0.666(2)	0.216(7)	1.1488(13)	0.656	0.242	1.148
C_6	0.388(4)	1.6909(9)	0.775(2)	0.270	1.688	0.782
C_7	0.388(4)	1.6909(9)	0.775(2)	0.275	1.692	-0.775
C_9	1.9282(9)	1.5891(12)	[0.000]	2.021	-1.485	-0.002

[a]Principal inertial axis denoted as *a*, *b*, *c*. Coordinates in Angström. [b]MP2/6-311++G(d,p). [c]Errors in parenthesis in units of the last digit, calculated as the sum of the standard errors and the Costain's estimates: $\delta z = K/|z|$ (K=0.15 Å). [d]Values in square brackets constrained to zero because of small or imaginary coordinates.