

Electronic Supplementary Information

**Internal Motions and Sulfur Hydrogen Bonding
in Methyl 3-Mercaptopropionate**

Wesley G. D. P. Silva,^a Luca Evangelisti,^b Jennifer van Wijngaarden^{a*}

^aDepartment of Chemistry, University of Manitoba, Winnipeg, Manitoba R3T 2N2,
Canada

^bDepartment of Chemistry “G. Ciamician”, University of Bologna, Via Selmi 2, I-40126
Bologna, Italy

*Corresponding author: vanwijng@cc.umanitoba.ca

Table S1 Cartesian coordinates for the equilibrium structure of **I**.

Atom	Cartesian Coordinates (Angstroms)		
	X	Y	Z
S	-2.374325	-0.615735	-0.399142
C	-1.603708	0.810423	0.459181
C	-0.238369	1.199323	-0.083045
C	0.830239	0.173477	0.210066
O	0.719899	-0.750483	0.978419
O	1.951032	0.430162	-0.486370
C	3.049613	-0.470184	-0.261011
H	-1.536029	-1.546631	0.088374
H	-2.303683	1.631354	0.317994
H	-1.551979	0.589564	1.521944
H	0.090982	2.139234	0.371955
H	-0.273230	1.371023	-1.158386
H	3.854788	-0.110726	-0.893182
H	3.345338	-0.452938	0.786046
H	2.768912	-1.484780	-0.536000

Table S2 Cartesian coordinates for the equilibrium structure of **II**.

Atom	Cartesian Coordinates (Angstroms)		
	X	Y	Z
S	3.061327	-0.180163	-0.084097
C	1.389715	0.544478	0.103027
C	0.273830	-0.476140	-0.049833
C	-1.095880	0.161362	-0.013599
O	-1.315191	1.346969	-0.006502
O	-2.063035	-0.775290	-0.001608
C	-3.413315	-0.280570	0.006204
H	3.016746	-0.984079	0.994071
H	1.323748	1.300978	-0.675670
H	1.322513	1.062446	1.056067
H	0.371344	-1.014192	-0.994585
H	0.321608	-1.236133	0.731464
H	-4.046273	-1.161809	0.015056
H	-3.602256	0.319316	-0.881809
H	-3.588948	0.327874	0.891048

Table S3 Cartesian coordinates for the equilibrium structure of **III**.

Atom	Cartesian Coordinates (Angstroms)		
	X	Y	Z
S	-2.214019	-0.862274	0.021917
C	-1.626164	0.874351	0.100951
C	-0.285404	1.092970	-0.583316
C	0.841548	0.391871	0.140529
O	0.915568	0.268681	1.337058
O	1.779196	-0.050734	-0.715288
C	2.913190	-0.700054	-0.114284
H	-2.488076	-0.875163	-1.295435
H	-2.387650	1.526654	-0.318416
H	-1.541309	1.088105	1.163835
H	-0.307912	0.775807	-1.623914
H	-0.045351	2.161509	-0.576839
H	3.432172	-0.015184	0.553396
H	3.554059	-0.990723	-0.940184
H	2.591233	-1.573033	0.449444

Table S4 Cartesian coordinates for the equilibrium structure of **IV**.

Atom	Cartesian Coordinates (Angstroms)		
	X	Y	Z
S	-1.191215	-0.197430	0.472031
C	-0.892223	-1.234669	0.609783
C	-1.097236	0.307443	1.431045
C	-0.315184	0.474125	-0.588156
O	-0.628208	1.504692	-0.738601
O	-0.407476	-0.065149	-1.529448
C	1.130113	0.494752	-0.148993
H	1.706221	1.450249	0.306840
H	1.700446	-0.718359	-0.295692
H	3.066486	-0.824345	0.139862
H	3.353353	-1.854111	-0.046341
H	3.145686	-0.587966	1.199139
H	3.697536	-0.141283	-0.425030
H	-2.960637	-0.281840	0.008393
H	-3.195779	1.042747	0.027506

Table S5 Cartesian coordinates for the equilibrium structure of **V**.

Atom	Cartesian Coordinates (Angstroms)		
	X	Y	Z
S	3.001787	-0.310790	-0.000048
C	1.388678	0.570544	-0.000039
C	0.278901	-0.467199	0.000028
C	-1.091321	0.167463	0.000007
O	-1.314293	1.352143	-0.000039
O	-2.054263	-0.772815	-0.000001
C	-3.406523	-0.283845	0.000034
H	3.781655	0.784168	0.000809
H	1.318508	1.201206	-0.881732
H	1.318576	1.201243	0.881631
H	0.350498	-1.120672	0.871880
H	0.350443	-1.120764	-0.871756
H	-4.035648	-1.167843	0.001174
H	-3.590961	0.320398	0.885986
H	-3.591618	0.318504	-0.887089

Table S6 Cartesian coordinates for the equilibrium structure of **VI**.

Atom	Cartesian Coordinates (Angstroms)		
	X	Y	Z
S	-2.166398	-0.884463	0.000294
C	-1.627377	0.876972	-0.000267
C	-0.300628	0.991276	-0.737516
C	0.849719	0.442310	0.078018
O	0.985318	0.604003	1.264396
O	1.729190	-0.222374	-0.691181
C	2.876084	-0.755616	-0.006449
H	-3.006990	-0.802039	1.045307
H	-2.385001	1.483480	-0.489625
H	-1.504692	1.206020	1.027430
H	-0.082759	2.047862	-0.915427
H	-0.333956	0.502403	-1.709715
H	3.465820	-1.252791	-0.769515
H	2.561450	-1.462116	0.758707
H	3.445641	0.045915	0.459693

Table S7 Cartesian coordinates for the equilibrium structure of **VII**.

Atom	Cartesian Coordinates (Angstroms)		
	X	Y	Z
S	-2.035264	-0.768429	-0.438940
C	-1.438110	0.346113	0.890258
C	-0.342343	1.305773	0.442577
C	0.881904	0.630868	-0.132753
O	1.454803	0.979906	-1.132606
O	1.280893	-0.401267	0.634694
C	2.426271	-1.126615	0.158219
H	-2.518759	0.191369	-1.248567
H	-2.280801	0.897595	1.300494
H	-1.068863	-0.325829	1.660923
H	-0.709513	1.997359	-0.312604
H	-0.017877	1.899986	1.302746
H	2.597234	-1.913394	0.885750
H	3.290879	-0.469484	0.090918
H	2.220024	-1.548674	-0.823142

Table S8 Cartesian coordinates for the equilibrium structure of **VIII**.

Atom	Cartesian Coordinates (Angstroms)		
	X	Y	Z
S	-1.450974	0.441709	0.821620
C	-1.141213	-0.161737	1.669621
C	-2.291928	1.055765	1.138880
C	-0.322646	1.339816	0.333263
O	-0.025392	2.013616	1.144356
O	-0.648082	1.963541	-0.496426
C	0.938524	0.638040	-0.116317
H	1.705467	1.073146	-0.935801
H	1.134756	-0.526449	0.537283
H	2.335830	-1.238499	0.194141
H	3.211544	-0.632340	0.416249
H	2.336655	-1.489223	-0.864654
H	2.326210	-2.137112	0.802349
H	-2.149853	-0.661267	-0.466989
H	-1.096330	-1.492213	-0.546646

Table S9 Cartesian coordinates for the equilibrium structure of **IX**.

Atom	Cartesian Coordinates (Angstroms)		
	X	Y	Z
S	-2.076897	-0.610919	-0.537749
C	-1.416217	0.292535	0.924952
C	-0.336790	1.268070	0.469086
C	0.883995	0.608945	-0.134852
O	1.406500	0.941516	-1.167536
O	1.341931	-0.387753	0.646318
C	2.488157	-1.095449	0.145878
H	-2.812570	-1.502912	0.147886
H	-2.226197	0.838416	1.402581
H	-1.003368	-0.426466	1.625882
H	-0.004117	1.845945	1.335024
H	-0.722314	1.969382	-0.267996
H	2.709301	-1.855431	0.888221
H	3.330574	-0.417255	0.026108
H	2.256724	-1.551694	-0.814365

Table S10 Observed frequencies and residuals for the rotational transitions of the parent species of conformer **I**.

J'	K_a'	K_c'	J''	K_a''	K_c''	$\nu_{\text{obs}}/\text{GHz}$	$\nu_{\text{obs}} - \nu_{\text{calc}}/\text{MHz}$	Type
1	1	1	0	0	0	6.0610208	-0.0017	E
1	1	1	0	0	0	6.0623802	-0.0009	A
3	1	3	2	1	2	6.0742954	-0.0007	A
3	1	3	2	1	2	6.0744492	0.0019	E
3	2	1	2	2	0	6.1808901	0.0005	E
3	2	1	2	2	0	6.1825625	-0.0001	A
3	1	2	2	1	1	6.2821428	0.0000	E
3	1	2	2	1	1	6.2823467	-0.0007	A
5	0	5	4	1	4	6.5782720	-0.0006	A
5	0	5	4	1	4	6.5786582	0.0004	E
2	1	2	1	0	1	8.0519599	-0.0004	E
2	1	2	1	0	1	8.0526700	-0.0010	A
4	1	4	3	1	3	8.0979873	-0.0015	A
4	1	4	3	1	3	8.0980394	0.0026	E
4	0	4	3	0	3	8.2294527	0.0016	E
4	0	4	3	0	3	8.2294858	-0.0013	A
4	2	3	3	2	2	8.2379127	-0.0010	A
4	3	1	3	3	0	8.2406032	0.0042	E
4	2	2	3	2	1	8.2468366	-0.0009	A
4	1	3	3	1	2	8.3752408	0.0001	E
4	1	3	3	1	2	8.3753592	-0.0006	A
6	0	6	5	1	5	8.7838057	0.0002	A
6	0	6	5	1	5	8.7841291	-0.0002	E
3	1	3	2	0	2	10.0080756	0.0012	E
3	1	3	2	0	2	10.0086145	-0.0008	A
5	1	5	4	1	4	10.1207787	-0.0045	A
5	1	5	4	1	4	10.1207996	0.0056	E
5	0	5	4	0	4	10.2800754	0.0007	E
5	0	5	4	0	4	10.2801182	-0.0004	A
5	2	4	4	2	3	10.2962011	-0.0017	A
5	3	3	4	3	2	10.3014897	0.0014	A
5	3	2	4	3	1	10.3015111	-0.0016	E
5	3	3	4	3	2	10.3015258	0.0015	E
5	3	2	4	3	1	10.3016379	-0.0014	A
5	2	3	4	2	2	10.3140222	-0.0007	A
5	2	3	4	2	3	10.3456534	0.0028	E
3	1	2	2	0	2	10.4244588	-0.0013	E
3	1	2	2	0	2	10.4247230	-0.0002	A

5	1	4	4	1	3	10.4673052	0.0000	E
5	1	4	4	1	3	10.4674045	-0.0001	A
7	0	7	6	1	6	11.0086187	0.0005	A
7	0	7	6	1	6	11.0088917	-0.0009	E
8	2	6	8	1	7	11.0704261	-0.0002	A
8	2	6	8	1	7	11.0708453	0.0025	E
7	2	5	7	1	6	11.2658849	-0.0006	A
6	2	4	6	1	5	11.4535994	-0.0004	A
5	2	4	5	1	4	11.5875400	-0.0015	E
5	2	3	5	1	4	11.6270135	-0.0002	A
4	2	2	4	1	3	11.7803955	0.0000	A
3	2	1	3	1	2	11.9089178	0.0000	A
4	1	4	3	0	3	11.9308700	0.0021	E
4	1	4	3	0	3	11.9313313	-0.0019	A
2	2	0	2	1	1	12.0087014	-0.0012	A
6	1	6	5	1	5	12.1424795	-0.0019	A
6	2	5	5	2	3	12.3112016	0.0010	E
6	0	6	5	0	5	12.3262688	0.0032	E
6	0	6	5	0	5	12.3263141	-0.0022	A
6	2	5	5	2	4	12.3536972	-0.0018	A
6	4	3	5	4	2	12.3615919	0.0037	E
6	4	3	5	4	2	12.3616324	-0.0008	A
6	3	4	5	3	3	12.3627959	-0.0014	A
6	3	3	5	3	2	12.3629381	0.0007	E
6	3	4	5	3	3	12.3629523	0.0019	E
6	3	3	5	3	2	12.3631981	-0.0015	A
6	2	4	5	2	3	12.3847983	-0.0003	A
6	2	4	5	2	4	12.4271875	0.0022	E
4	2	3	4	1	4	12.4604880	0.0026	A
6	1	5	5	1	4	12.5581148	0.0006	E
6	1	5	5	1	4	12.5582124	-0.0002	A
4	1	3	3	0	3	12.6244560	-0.0016	E
5	2	4	5	1	5	12.6359068	0.0019	A
6	2	5	6	1	6	12.8471242	0.0018	A
7	2	6	7	1	7	13.0944662	0.0012	A
8	0	8	7	1	7	13.2480842	0.0009	A
8	0	8	7	1	7	13.2483129	-0.0017	E
8	2	7	8	1	8	13.3782646	0.0014	A
5	1	5	4	0	4	13.8222147	0.0038	E
5	1	5	4	0	4	13.8226269	-0.0023	A
7	1	7	6	1	6	14.1628867	0.0029	E
7	1	7	6	1	6	14.1629011	-0.0011	A
7	0	7	6	0	6	14.3672401	0.0028	E

7	0	7	6	0	6	14.3672928	-0.0011	A
7	2	6	6	2	5	14.4102421	-0.0026	A
7	4	3	6	4	2	14.4225894	0.0002	E
7	4	4	6	4	3	14.4226107	0.0021	E
7	4	3	6	4	2	14.4226606	-0.0040	A
7	3	5	6	3	4	14.4245925	-0.0018	A
7	3	5	6	3	4	14.4249842	0.0004	E
7	3	4	6	3	3	14.4254973	-0.0016	A
7	2	5	6	2	4	14.4597813	-0.0002	A
7	1	6	6	1	5	14.6473932	0.0015	E
7	1	6	6	1	5	14.6474955	-0.0004	A
9	0	9	8	1	8	15.4972021	0.0012	A
9	0	9	8	1	8	15.4973909	-0.0017	E
6	1	6	5	0	5	15.6846154	0.0052	E
6	1	6	5	0	5	15.6849884	-0.0037	A
2	2	1	1	1	0	16.1781928	-0.0016	E
8	1	8	7	1	7	16.1818629	0.0044	E
8	1	8	7	1	7	16.1818809	-0.0035	A
2	2	1	1	1	0	16.1964313	-0.0002	A
2	2	0	1	1	1	16.2666769	0.0002	A
2	2	0	1	1	1	16.2826131	-0.0058	E
8	0	8	7	0	7	16.4023084	0.0026	E
8	0	8	7	0	7	16.4023662	-0.0011	A
8	4	4	7	4	3	16.4839579	0.0034	E
8	4	5	7	4	4	16.4839761	-0.0018	E
8	4	5	7	4	4	16.4840277	-0.0026	A
8	4	4	7	4	3	16.4840443	-0.0019	A
8	3	6	7	3	5	16.4869068	-0.0021	A
8	3	5	7	3	4	16.4887144	-0.0017	A
8	2	6	7	2	5	16.5394858	0.0004	A
8	1	7	7	1	6	16.7348336	0.0021	E
8	1	7	7	1	6	16.7349447	0.0002	A
7	1	7	6	0	6	17.5212354	0.0069	E
7	1	7	6	0	6	17.5215734	-0.0046	A
10	0	10	9	1	9	17.7507780	0.0024	A
10	0	10	9	1	9	17.7509291	-0.0017	E

Table S11 Observed frequencies and residuals for the rotational transitions of the ^{34}S species of conformer **I**.

J'	K_a'	K_c'	J''	K_a''	K_c''	$\nu_{\text{obs}}/\text{GHz}$	$\nu_{\text{obs}} - \nu_{\text{calc}}/\text{MHz}$	Type
3	1	2	2	1	1	6.1407145	0.0000	E
3	1	2	2	1	1	6.1409190	-0.0002	A
4	1	4	3	1	3	7.9194733	0.0060	A
4	1	4	3	1	3	7.9195113	-0.0054	E
2	1	2	1	0	1	7.9460166	-0.0009	E
2	1	2	1	0	1	7.9467213	-0.0006	A
4	0	4	3	0	3	8.0464135	-0.0025	E
4	0	4	3	0	3	8.0464517	0.0008	A
4	2	3	3	2	2	8.0543299	-0.0014	A
4	2	3	3	2	2	8.0574465	0.0014	E
4	2	2	3	2	1	8.0594785	0.0005	E
4	2	2	3	2	1	8.0626620	-0.0004	A
4	1	3	3	1	2	8.1867414	-0.0011	E
4	1	3	3	1	2	8.1868611	0.0008	A
6	0	6	5	1	5	8.5112525	0.0012	A
6	0	6	5	1	5	8.5115706	0.0001	E
3	1	3	2	0	2	9.8599480	0.0016	E
5	1	5	4	1	4	9.8977395	-0.0006	A
5	1	5	4	1	4	9.8977533	0.0014	E
5	0	5	4	0	4	10.0517249	0.0010	E
5	0	5	4	0	4	10.0517658	-0.0004	A
5	2	4	4	2	3	10.0667989	-0.0012	A
5	2	4	4	2	3	10.0706843	0.0003	E
5	3	3	4	3	2	10.0717584	-0.0005	A
5	3	3	4	3	2	10.0717915	0.0024	E
5	3	2	4	3	1	10.0718936	-0.0018	A
5	2	3	4	2	2	10.0794675	0.0021	E
5	2	3	4	2	2	10.0834369	-0.0012	A
5	1	4	4	1	3	10.2318002	0.0001	E
5	1	4	4	1	3	10.2318967	-0.0007	A
8	2	6	8	1	7	11.0480939	-0.0017	A
8	2	6	8	1	7	11.0485986	0.0021	E
7	2	5	7	1	6	11.2389575	-0.0010	A
7	2	5	7	1	6	11.2403998	0.0012	E
6	2	4	6	1	5	11.4215632	-0.0011	A
6	2	4	6	1	5	11.4247481	-0.0009	E
5	2	3	5	1	4	11.5897757	-0.0002	A
5	2	3	5	1	4	11.5959686	-0.0025	E

4	2	2	4	1	3	11.7382353	0.0002	A
4	1	4	3	0	3	11.7417053	0.0012	E
4	1	4	3	0	3	11.7421591	-0.0022	A
4	2	2	4	1	3	11.7483088	0.0030	E
3	2	1	3	1	2	11.8624341	0.0010	A
6	0	6	5	0	5	12.0528894	0.0026	E
6	0	6	5	0	5	12.0529331	-0.0026	A
6	2	5	5	2	4	12.0785253	-0.0011	A
6	2	5	5	2	4	12.0815251	0.0002	E
6	3	4	5	3	3	12.0870504	-0.0023	A
6	3	3	5	3	2	12.0871756	-0.0002	E
6	3	4	5	3	3	12.0871911	0.0027	E
6	3	3	5	3	2	12.0874146	-0.0019	A
6	2	4	5	2	3	12.1044630	0.0013	E
6	2	4	5	2	3	12.1075672	-0.0006	A
6	1	5	5	1	4	12.2756841	0.0002	E
6	1	5	5	1	4	12.2757795	0.0000	A
8	0	8	7	1	7	12.8744179	0.0013	A
8	0	8	7	1	7	12.8746428	-0.0021	E
5	1	5	4	0	4	13.5930435	0.0034	E
5	1	5	4	0	4	13.5934478	-0.0027	A
7	1	7	6	1	6	13.8510163	0.0017	E
7	1	7	6	1	6	13.8510302	-0.0015	A
7	0	7	6	0	6	14.0491653	0.0015	E
7	0	7	6	0	6	14.0492171	-0.0015	A
7	2	6	6	2	5	14.0893609	-0.0014	A
7	2	6	6	2	5	14.0910831	0.0021	E
7	3	5	6	3	4	14.1028021	-0.0006	A
7	3	4	6	3	3	14.1031508	0.0028	E
7	3	5	6	3	4	14.1031523	0.0000	E
7	3	4	6	3	3	14.1036195	-0.0011	A
7	2	5	6	2	4	14.1337888	0.0010	E
7	2	5	6	2	4	14.1356325	-0.0008	A
7	1	6	6	1	5	14.3181385	0.0003	E
7	1	6	6	1	5	14.3182391	0.0000	A
9	0	9	8	1	8	15.0733410	-0.0010	A
9	0	9	8	1	8	15.0735293	-0.0022	E
6	1	6	5	0	5	15.4162986	0.0035	E
6	1	6	5	0	5	15.4166647	-0.0049	A
8	1	8	7	1	7	15.8257075	0.0052	E
8	1	8	7	1	7	15.8257216	-0.0052	A
8	0	8	7	0	7	16.0399066	0.0025	E
8	0	8	7	0	7	16.0399619	-0.0018	A

8	2	7	7	2	6	16.0991590	-0.0016	A
8	2	7	7	2	6	16.1000644	0.0020	E
8	3	6	7	3	5	16.1190370	-0.0011	A
8	3	6	7	3	5	16.1197614	0.0001	E
8	3	5	7	3	4	16.1198095	0.0018	E
8	3	5	7	3	4	16.1206706	-0.0017	A
8	2	6	7	2	5	16.1670792	0.0018	E
8	2	6	7	2	5	16.1681249	-0.0010	A
8	1	7	7	1	6	16.3588805	0.0010	E
8	1	7	7	1	6	16.3589887	-0.0001	A
7	1	7	6	0	6	17.2144279	0.0049	E
7	1	7	6	0	6	17.2147596	-0.0060	A
9	1	9	8	1	8	17.7989132	0.0053	E
9	1	9	8	1	8	17.7989141	0.0062	E
9	1	9	8	1	8	17.7989324	-0.0057	A
9	1	9	8	1	8	17.7989329	-0.0052	A
9	0	9	8	0	8	18.0245923	0.0034	E
9	0	9	8	0	8	18.0246489	-0.0034	A
9	1	8	8	1	7	18.3976103	0.0121	E
9	1	8	8	1	7	18.3977064	-0.0108	A

Table S12 Observed frequencies and residuals for the rotational transitions of the $^{13}\text{C}_2$ species of conformer **I**.

J'	K_a'	K_c'	J''	K_a''	K_c''	$\nu_{\text{obs}}/\text{GHz}$	$\nu_{\text{obs}} - \nu_{\text{calc}}/\text{MHz}$	Type
4	1	4	3	1	3	8.0505832	0.0055	A
4	1	4	3	1	3	8.0506231	-0.0029	E
4	0	4	3	0	3	8.1821470	-0.0006	E
4	0	4	3	0	3	8.1821796	-0.0011	A
4	2	3	3	2	2	8.1907060	-0.0022	A
4	2	3	3	2	2	8.1940104	-0.0003	E
4	2	2	3	2	1	8.1963775	-0.0018	E
4	2	2	3	2	1	8.1997497	0.0009	A
4	1	3	3	1	2	8.3282258	-0.0020	E
4	1	3	3	1	2	8.3283417	0.0003	A
3	1	3	2	0	2	9.9314380	0.0000	E
3	1	3	2	0	2	9.9314385	0.0005	E
5	1	5	4	1	4	10.0614989	-0.0015	A
5	1	5	4	1	4	10.0615158	0.0034	E
5	0	5	4	0	4	10.2208570	-0.0031	E
5	0	5	4	0	4	10.2208992	-0.0011	A
5	2	4	4	2	3	10.2371805	-0.0022	A
5	2	4	4	2	3	10.2411511	0.0044	E
5	2	3	4	2	2	10.2552393	0.0038	A
5	1	4	4	1	3	10.4085142	-0.0020	E
5	1	4	4	1	3	10.4086098	0.0003	A
6	1	6	5	1	5	12.0713141	-0.0011	A
6	1	6	5	1	5	12.0713141	0.0045	E
6	0	6	5	0	5	12.2550836	-0.0014	E
6	0	6	5	0	5	12.2551290	-0.0027	A
6	2	5	5	2	4	12.2828561	0.0006	A
6	2	5	5	2	4	12.2857814	0.0028	E
6	3	4	5	3	3	12.2920512	-0.0019	A
6	3	3	5	3	2	12.2924609	-0.0046	A
6	2	4	5	2	3	12.3113361	0.0023	E
6	2	4	5	2	3	12.3143656	0.0065	A
6	1	5	5	1	4	12.4875315	-0.0020	E
6	1	5	5	1	4	12.4876258	0.0009	A
7	1	7	6	1	6	14.0798264	0.0029	E
7	1	7	6	1	6	14.0798421	0.0024	A
7	0	7	6	0	6	14.2840237	-0.0054	E
7	0	7	6	0	6	14.2840761	-0.0053	A
7	2	6	6	2	5	14.3275661	-0.0014	A

7	2	6	6	2	5	14.3291972	0.0016	E
7	3	5	6	3	4	14.3420782	-0.0011	A
7	3	4	6	3	3	14.3424822	-0.0020	E
7	3	5	6	3	4	14.3424823	-0.0023	E
7	3	4	6	3	3	14.3430051	-0.0013	A
7	2	5	6	2	4	14.3760013	0.0078	E
7	1	6	6	1	5	14.5649983	-0.0013	E
7	1	6	6	1	5	14.5650983	0.0023	A
8	1	8	7	1	7	16.0868948	0.0066	E
8	1	8	7	1	7	16.0869125	0.0010	A
8	0	8	7	0	7	16.3069979	-0.0065	E
8	0	8	7	0	7	16.3070541	-0.0071	A
8	2	7	7	2	6	16.3711606	0.0013	A
8	1	7	7	1	6	16.6406048	0.0013	E
8	1	7	7	1	6	16.6407116	0.0039	A

Table S13 Observed frequencies and residuals for the rotational transitions of the $^{13}\text{C}_3$ species of conformer **I**.

J'	K_a'	K_c'	J''	K_a''	K_c''	$\nu_{\text{obs}}/\text{GHz}$	$\nu_{\text{obs}} - \nu_{\text{calc}}/\text{MHz}$	Type
4	1	4	3	1	3	8.0802409	-0.0023	A
4	1	4	3	1	3	8.0802894	0.0019	E
4	0	4	3	0	3	8.2167624	0.0013	E
4	0	4	3	0	3	8.2167954	-0.0002	A
4	2	3	3	2	2	8.2260856	0.0000	A
4	2	2	3	2	1	8.2323914	0.0000	E
4	2	2	3	2	1	8.2359495	-0.0012	A
4	1	3	3	1	2	8.3691120	-0.0009	E
4	1	3	3	1	2	8.3692263	0.0010	A
5	1	5	4	1	4	10.0984314	-0.0027	A
5	1	5	4	1	4	10.0984467	0.0031	E
5	0	5	4	0	4	10.2635137	0.0000	E
5	2	4	4	2	3	10.2812989	-0.0016	A
5	2	3	4	2	2	10.2969241	-0.0011	E
5	1	4	4	1	3	10.4594562	-0.0012	E
5	1	4	4	1	3	10.4595530	0.0015	A
6	1	6	5	1	5	12.1154173	0.0009	E
6	0	6	5	0	5	12.3053813	-0.0012	E
6	0	6	5	0	5	12.3054322	0.0012	A
6	2	5	5	2	4	12.3356430	-0.0020	A
6	3	4	5	3	3	12.3456439	0.0004	A

6	3	3	5	3	2	12.3458212	-0.0001	E
6	3	4	5	3	3	12.3458363	0.0030	E
6	3	3	5	3	2	12.3461155	0.0000	A
6	2	4	5	2	3	12.3671257	0.0004	E
6	2	4	5	2	3	12.3700074	0.0004	A
6	1	5	5	1	4	12.5484158	-0.0015	E
6	1	5	5	1	4	12.5485125	0.0017	A
7	1	7	6	1	6	14.1310000	0.0006	E
7	1	7	6	1	6	14.1310170	-0.0003	A
7	0	7	6	0	6	14.3415164	0.0012	E
7	0	7	6	0	6	14.3415691	-0.0001	A
7	2	6	6	2	5	14.3889429	-0.0026	A
7	2	6	6	2	5	14.3904375	-0.0009	E
7	3	5	6	3	4	14.4047255	0.0000	A
7	3	5	6	3	4	14.4051913	-0.0012	E
7	3	4	6	3	3	14.4051997	0.0023	E
7	3	4	6	3	3	14.4057869	0.0002	A
7	2	5	6	2	4	14.4420288	-0.0005	E
7	2	5	6	2	4	14.4436481	-0.0002	A
7	1	6	6	1	5	14.6356821	-0.0007	E
7	1	6	6	1	5	14.6357840	0.0017	A
8	1	8	7	1	7	16.1450184	0.0015	E
8	0	8	7	0	7	16.3711849	0.0000	E
8	0	8	7	0	7	16.3712430	-0.0006	A
8	2	7	7	2	6	16.4410278	-0.0020	A
8	2	7	7	2	6	16.4417888	-0.0009	E
8	2	6	7	2	5	16.5215555	0.0003	E
8	2	6	7	2	5	16.5224612	0.0002	A
8	1	7	7	1	6	16.7209106	-0.0001	E
8	1	7	7	1	6	16.7210200	0.0012	A

Table S14 Observed frequencies and residuals for the rotational transitions of the $^{13}\text{C}_4$ species of conformer **I**.

J'	K_a'	K_c'	J''	K_a''	K_c''	$\nu_{\text{obs}}/\text{GHz}$	$\nu_{\text{obs}} - \nu_{\text{calc}}/\text{MHz}$	Type
4	1	4	3	1	3	8.0858042	-0.0039	A
4	1	4	3	1	3	8.0858572	0.0008	E
4	0	4	3	0	3	8.2168246	0.0001	E
4	0	4	3	0	3	8.2168610	0.0019	A
4	2	2	3	2	1	8.2307650	0.0009	E
4	2	2	3	2	1	8.2340948	0.0002	A
4	1	3	3	1	2	8.3620716	-0.0007	E
4	1	3	3	1	2	8.3621886	-0.0002	A
5	0	5	4	0	4	10.2643773	-0.0008	A
5	2	3	4	2	2	10.2980587	0.0012	A
5	1	4	4	1	3	10.4508545	-0.0021	E
5	1	4	4	1	3	10.4509535	0.0006	A
6	0	6	5	0	5	12.3074452	0.0016	E
6	0	6	5	0	5	12.3074921	-0.0002	A
6	2	5	5	2	4	12.3346939	-0.0008	A
6	2	5	5	2	4	12.3376556	0.0006	E
6	3	4	5	3	3	12.3437379	0.0027	A
6	3	3	5	3	2	12.3438759	0.0000	E
6	3	4	5	3	3	12.3438917	0.0032	E
6	3	3	5	3	2	12.3441340	0.0004	A
6	2	4	5	2	3	12.3655860	-0.0011	A
6	1	5	5	1	4	12.5383927	-0.0009	E
6	1	5	5	1	4	12.5384890	0.0005	A
7	1	7	6	1	6	14.1416233	0.0009	E
7	1	7	6	1	6	14.1416394	-0.0002	A
7	0	7	6	0	6	14.3453661	0.0006	E
7	0	7	6	0	6	14.3454189	-0.0010	A
7	2	6	6	2	5	14.3880874	-0.0011	A
7	2	6	6	2	5	14.3897498	-0.0008	E
7	3	5	6	3	4	14.4023448	-0.0015	A
7	3	5	6	3	4	14.4027308	-0.0032	E
7	3	4	6	3	3	14.4027336	0.0016	E
7	3	4	6	3	3	14.4032409	-0.0011	A
7	2	5	6	2	4	14.4355083	-0.0001	E
7	2	5	6	2	4	14.4372964	-0.0001	A
7	1	6	6	1	5	14.6244090	-0.0007	E
7	1	6	6	1	5	14.6245110	0.0010	A
8	1	8	7	1	7	16.1575895	0.0036	E

8	1	8	7	1	7	16.1576073	-0.0032	A
8	0	8	7	0	7	16.3774213	0.0008	E
8	0	8	7	0	7	16.3774799	0.0001	A
8	2	7	7	2	6	16.4403798	-0.0018	A
8	2	7	7	2	6	16.4412450	-0.0003	E
8	2	6	7	2	5	16.5126878	-0.0004	E
8	2	6	7	2	5	16.5136995	0.0018	A
8	1	7	7	1	6	16.7086005	-0.0004	E
8	1	7	7	1	6	16.7087109	0.0014	A

Table S15 Observed frequencies and residuals for the rotational transitions of the $^{13}\text{C}7$ species of conformer **I**.

J'	K_a'	K_c'	J''	K_a''	K_c''	$\nu_{\text{obs}}/\text{GHz}$	$\nu_{\text{obs}} - \nu_{\text{calc}}/\text{MHz}$	Type
4	1	4	3	1	3	7.9464120	-0.0022	A
4	1	4	3	1	3	7.9464668	0.0010	E
4	0	4	3	0	3	8.0738261	-0.0005	E
4	0	4	3	0	3	8.0738610	0.0022	A
4	2	3	3	2	2	8.0817517	0.0002	A
4	2	3	3	2	2	8.0848794	-0.0005	E
4	2	2	3	2	1	8.0869054	0.0000	E
4	2	2	3	2	1	8.0900993	0.0002	A
4	1	3	3	1	2	8.2146385	-0.0015	E
4	1	3	3	1	2	8.2147549	0.0000	A
5	0	5	4	0	4	10.0859747	-0.0005	E
5	0	5	4	0	4	10.0860145	0.0001	A
5	1	4	4	1	3	10.2666689	-0.0022	E
5	1	4	4	1	3	10.2667650	0.0011	A
6	0	6	5	0	5	12.0939714	0.0005	E
6	0	6	5	0	5	12.0940137	-0.0027	A
6	2	5	5	2	4	12.1196557	0.0008	A
6	2	5	5	2	4	12.1226902	0.0009	E
6	3	3	5	3	2	12.1285523	-0.0013	A
6	2	4	5	2	3	12.1456227	0.0016	E
6	2	4	5	2	3	12.1487568	0.0020	A
6	1	5	5	1	4	12.3175264	-0.0004	E
6	1	5	5	1	4	12.3176177	0.0007	A
7	1	7	6	1	6	13.8981624	0.0000	E
7	1	7	6	1	6	13.8981765	-0.0007	A
7	0	7	6	0	6	14.0970726	0.0017	E
7	0	7	6	0	6	14.0971214	-0.0006	A

7	2	6	6	2	5	14.1373433	-0.0010	A
7	2	6	6	2	5	14.1390906	0.0003	E
7	3	5	6	3	4	14.1508019	0.0002	A
7	3	5	6	3	4	14.1511544	-0.0015	E
7	3	4	6	3	3	14.1511545	0.0024	E
7	3	4	6	3	3	14.1516203	0.0004	A
7	2	5	6	2	4	14.1818449	-0.0014	E
7	2	5	6	2	4	14.1837109	0.0016	A
8	0	8	7	0	7	16.0946245	0.0019	E
8	0	8	7	0	7	16.0946788	0.0005	A
8	2	7	7	2	6	16.1539927	-0.0026	A
8	2	7	7	2	6	16.1549145	-0.0011	E
8	1	7	7	1	6	16.4146623	0.0002	E
8	1	7	7	1	6	16.4147639	-0.0001	A

Table S16 Observed frequencies and residuals for the rotational transitions of the parent species of conformer **II+**. XIAM fit.

J'	K_a'	K_c'	J''	K_a''	K_c''	$\nu_{\text{obs}}/\text{GHz}$	$\nu_{\text{obs}} - \nu_{\text{calc}}/\text{MHz}$	Type
4	0	4	3	0	3	6.1801263	-0.0086	A
4	0	4	3	0	3	6.1801332	0.0034	E
5	1	5	4	1	4	7.5838545	0.0009	A
5	1	5	4	1	4	7.5840688	-0.0003	E
3	1	2	3	0	3	7.6455312	0.0005	A
5	0	5	4	0	4	7.7226556	-0.0051	E
5	0	5	4	0	4	7.7226651	-0.0026	A
5	2	4	4	2	3	7.7285888	0.0098	A
5	2	4	4	2	3	7.7315594	0.0070	E
5	2	3	4	2	2	7.7322672	0.0106	E
5	2	3	4	2	2	7.7352458	0.0065	A
4	1	3	4	0	4	7.7634070	-0.0051	A
5	1	4	4	1	3	7.8716559	0.0000	E
5	1	4	4	1	3	7.8718808	-0.0018	A
6	1	6	5	1	5	9.0997178	-0.0024	A
6	1	6	5	1	5	9.0998404	-0.0012	E
6	0	6	5	0	5	9.2635217	-0.0071	E
6	0	6	5	0	5	9.2635343	-0.0036	A
6	1	5	5	1	4	9.4451803	-0.0014	E
6	1	5	5	1	4	9.4453149	-0.0020	A
2	1	2	1	0	1	10.4765595	-0.0008	A
7	1	7	6	1	6	10.6151029	-0.0018	A

7	1	7	6	1	6	10.6151791	0.0007	E
7	0	7	6	0	6	10.8024016	-0.0072	E
7	0	7	6	0	6	10.8024162	-0.0044	A
7	2	6	6	2	5	10.8184513	0.0128	A
7	2	6	6	2	5	10.8241506	0.0025	E
7	1	6	6	1	5	11.0181346	-0.0012	E
7	1	6	6	1	5	11.0182254	-0.0009	A
3	1	3	2	0	2	11.9361366	0.0025	A
3	1	3	2	0	2	11.9361366	0.0025	A
8	1	8	7	1	7	12.1299337	-0.0017	A
8	1	8	7	1	7	12.1299850	0.0029	E
8	0	8	7	0	7	12.3389777	-0.0068	E
8	0	8	7	0	7	12.3389936	-0.0057	A
8	2	7	7	2	6	12.3686354	-0.0014	E
8	2	6	7	2	5	12.3907069	0.0073	A
8	1	7	7	1	6	12.5904459	-0.0014	E
8	1	7	7	1	6	12.5905157	0.0018	A
4	1	4	3	0	3	13.3648378	0.0001	E
4	1	4	3	0	3	13.3674452	0.0005	A
9	1	9	8	1	8	13.6441450	0.0001	A
9	1	9	8	1	8	13.6441777	0.0027	E
9	0	9	8	0	8	13.8729478	-0.0043	E
9	0	9	8	0	8	13.8729635	-0.0071	A
9	1	8	8	1	7	14.1620262	0.0008	E
9	1	8	8	1	7	14.1620798	0.0010	A
10	1	10	9	1	9	15.1576727	0.0021	A
10	1	10	9	1	9	15.1576934	0.0039	E
10	0	10	9	0	9	15.4040247	-0.0019	E
10	0	10	9	0	9	15.4040452	-0.0042	A
10	1	9	9	1	8	15.7327736	0.0048	E
10	1	9	9	1	8	15.7328195	0.0047	A
11	1	11	10	1	10	16.6704527	-0.0018	A
11	1	11	10	1	10	16.6704712	0.0059	E
11	0	11	10	0	10	16.9319477	-0.0011	E
11	0	11	10	0	10	16.9319725	-0.0039	A

Table S17 Observed frequencies and residuals for the rotational transitions of the parent species of conformer **II-**. XIAM fit.

J'	K_a'	K_c'	J''	K_a''	K_c''	$\nu_{\text{obs}}/\text{GHz}$	$\nu_{\text{obs}} - \text{calc}/\text{MHz}$	Type
4	0	4	3	0	3	6.1801332	-0.0002	E
4	0	4	3	0	3	6.1801396	0.0014	A
5	1	5	4	1	4	7.5838545	0.0016	A
5	1	5	4	1	4	7.5840688	0.0023	E
3	1	2	3	0	3	7.6455312	-0.0061	A
5	0	5	4	0	4	7.7226651	0.0000	E
5	0	5	4	0	4	7.7226744	0.0028	A
5	2	4	4	2	3	7.7285888	0.0054	A
5	2	4	4	2	3	7.7315594	0.0038	E
5	2	3	4	2	2	7.7322672	0.0039	E
5	2	3	4	2	2	7.7352458	0.0017	A
4	1	3	4	0	4	7.7634232	0.0002	A
5	1	4	4	1	3	7.8716562	-0.0117	E
5	1	4	4	1	3	7.8718806	-0.0113	A
5	1	4	5	0	5	7.9126362	-0.0070	A
6	1	6	5	1	5	9.0997178	-0.0015	A
6	1	6	5	1	5	9.0998404	0.0006	E
6	0	6	5	0	5	9.2635343	0.0006	E
6	0	6	5	0	5	9.2635468	0.0045	A
6	1	5	5	1	4	9.4451803	-0.0145	E
6	1	5	5	1	4	9.4453149	-0.0132	A
2	1	2	1	0	1	10.4765595	0.0001	A
7	1	7	6	1	6	10.6151029	-0.0006	A
7	1	7	6	1	6	10.6151791	0.0023	E
7	0	7	6	0	6	10.8024162	0.0019	E
7	0	7	6	0	6	10.8024303	0.0048	A
7	2	6	6	2	5	10.8184383	-0.0064	A
7	2	6	6	2	5	10.8241362	-0.0044	E
7	1	6	6	1	5	11.0181474	-0.0030	E
7	1	6	6	1	5	11.0182388	-0.0005	A
3	1	3	2	0	2	11.9361366	0.0056	A
8	1	8	7	1	7	12.1299278	-0.0062	A
8	1	8	7	1	7	12.1299779	-0.0026	E
8	0	8	7	0	7	12.3389936	0.0034	E
8	0	8	7	0	7	12.3390105	0.0059	A
8	2	7	7	2	6	12.3686206	0.0011	E
8	3	6	7	3	5	12.3707237	0.0068	A
8	3	6	7	3	5	12.3708744	0.0078	E

8	2	6	7	2	5	12.3907069	-0.0015	A
8	1	7	7	1	6	12.5904638	0.0003	E
8	1	7	7	1	6	12.5905331	0.0043	A
4	1	4	3	0	3	13.3648378	0.0003	E
4	1	4	3	0	3	13.3674452	0.0067	A
9	1	9	8	1	8	13.6441356	-0.0077	A
9	1	9	8	1	8	13.6441684	-0.0049	E
9	0	9	8	0	8	13.8729635	0.0054	E
9	0	9	8	0	8	13.8729800	0.0040	A
9	1	8	8	1	7	14.1620464	0.0030	E
9	1	8	8	1	7	14.1621007	0.0053	A
10	1	10	9	1	9	15.1576598	-0.0088	A
10	1	10	9	1	9	15.1576817	-0.0060	E
10	0	10	9	0	9	15.4040365	0.0039	E
10	0	10	9	0	9	15.4040562	0.0015	A
10	1	9	9	1	8	15.7327918	0.0033	E
10	1	9	9	1	8	15.7328381	0.0051	A
11	1	11	10	1	10	16.6704423	-0.0099	A
11	1	11	10	1	10	16.6704609	-0.0024	E
11	0	11	10	0	10	16.9319596	0.0050	E
11	0	11	10	0	10	16.9319843	0.0028	A

Table S18 Observed frequencies and residuals for the rotational transitions of the parent species of conformer **II** (A state fit using SPFIT).

J'	K_a'	K_c'	J''	K_a''	K_c''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \nu_{\text{calc}}/\text{MHz}$	Type
4	0	4	3	0	3	6180.1263	-0.0112	A-
4	0	4	3	0	3	6180.1396	0.0020	A+
5	1	5	4	1	4	7583.8545	0.0007	A-
5	1	5	4	1	4	7583.8545	0.0007	A+
3	1	2	3	0	3	7645.5312	-0.0033	A-
3	1	2	3	0	3	7645.5312	-0.0033	A+
5	0	5	4	0	4	7722.6651	-0.0056	A-
5	0	5	4	0	4	7722.6744	0.0036	A+
5	2	4	4	2	3	7728.5887	0.0063	A-
5	2	4	4	2	3	7728.5887	0.0063	A+
5	2	3	4	2	2	7735.2458	0.0028	A-
5	2	3	4	2	2	7735.2458	0.0028	A+
4	1	3	4	0	4	7763.4070	-0.0115	A-
4	1	3	4	0	4	7763.4218	0.0031	A+
5	1	4	4	1	3	7871.8806	-0.0084	A-
5	1	4	5	0	5	7912.6362	-0.0005	A+

6	1	6	5	1	5	9099.7178	-0.0023	A-
6	1	6	5	1	5	9099.7178	-0.0023	A+
6	0	6	5	0	5	9263.5343	-0.0068	A-
6	0	6	5	0	5	9263.5468	0.0057	A+
6	1	5	5	1	4	9445.3149	-0.0095	A-
2	1	2	1	0	1	10476.5595	-0.0003	A-
2	1	2	1	0	1	10476.5595	-0.0003	A+
7	1	7	6	1	6	10615.1028	-0.0013	A-
7	1	7	6	1	6	10615.1028	-0.0013	A+
7	0	7	6	0	6	10802.4162	-0.0076	A-
7	0	7	6	0	6	10802.4302	0.0064	A+
7	2	6	6	2	5	10818.4382	-0.0044	A+
7	2	6	6	2	5	10818.4513	0.0086	A-
7	1	6	6	1	5	11018.2254	-0.0092	A-
7	1	6	6	1	5	11018.2388	0.0041	A+
3	1	3	2	0	2	11936.1366	0.0041	A-
3	1	3	2	0	2	11936.1366	0.0041	A+
8	1	8	7	1	7	12129.9278	-0.0064	A+
8	1	8	7	1	7	12129.9337	-0.0005	A-
8	0	8	7	0	7	12338.9936	-0.0087	A-
8	0	8	7	0	7	12339.0105	0.0081	A+
8	3	6	7	3	5	12370.7237	0.0095	A+
8	2	6	7	2	5	12390.7069	0.0019	A-
8	2	6	7	2	5	12390.7069	0.0019	A+
8	1	7	7	1	6	12590.5157	-0.0072	A-
8	1	7	7	1	6	12590.5331	0.0101	A+
4	1	4	3	0	3	13367.4452	0.0040	A-
4	1	4	3	0	3	13367.4452	0.0040	A+
9	1	9	8	1	8	13644.1356	-0.0074	A+
9	1	9	8	1	8	13644.1450	0.0020	A-
9	0	9	8	0	8	13872.9635	-0.0095	A-
9	0	9	8	0	8	13872.9800	0.0069	A+
9	1	8	8	1	7	14162.0798	-0.0084	A-
9	1	8	8	1	7	14162.1007	0.0123	A+
10	1	10	9	1	9	15157.6598	-0.0078	A+
10	1	10	9	1	9	15157.6727	0.0050	A-
10	0	10	9	0	9	15404.0452	-0.0057	A-
10	0	10	9	0	9	15404.0562	0.0052	A+
10	1	9	9	1	8	15732.8195	-0.0049	A-
10	1	9	9	1	8	15732.8381	0.0136	A+
11	1	11	10	1	10	16670.4423	-0.0079	A+
11	1	11	10	1	10	16670.4527	0.0023	A-
11	0	11	10	0	10	16931.9725	-0.0042	A-

11	0	11	10	0	10	16931.9843	0.0075	A+
----	---	----	----	---	----	------------	--------	----

Table S19 Observed frequencies and residuals for the rotational transitions of the parent species of conformer II (E state fit using SPFIT).

J'	K_a'	K_c'	J''	K_a''	K_c''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \nu_{\text{calc}}/\text{MHz}$	Type
4	0	4	3	0	3	6180.1332	0.0014	E+
4	0	4	3	0	3	6180.1332	0.0014	E-
5	1	5	4	1	4	7584.0688	-0.0002	E+
5	1	5	4	1	4	7584.0688	-0.0002	E-
5	0	5	4	0	4	7722.6556	-0.0071	E+
5	0	5	4	0	4	7722.6651	0.0023	E-
5	2	4	4	2	3	7731.5594	-0.0052	E+
5	2	4	4	2	3	7731.5594	-0.0052	E-
5	2	3	4	2	2	7732.2672	0.0162	E+
5	2	3	4	2	2	7732.2672	0.0162	E-
5	1	4	4	1	3	7871.6559	-0.0053	E+
5	1	4	4	1	3	7871.6562	-0.0050	E-
6	1	6	5	1	5	9099.8404	0.0049	E+
6	1	6	5	1	5	9099.8404	0.0049	E-
6	0	6	5	0	5	9263.5217	-0.0087	E+
6	0	6	5	0	5	9263.5343	0.0038	E-
6	1	5	5	1	4	9445.1803	-0.0134	E+
6	1	5	5	1	4	9445.1803	-0.0134	E-
7	1	7	6	1	6	10615.1791	0.0110	E+
7	1	7	6	1	6	10615.1791	0.0110	E-
7	0	7	6	0	6	10802.4016	-0.0083	E+
7	0	7	6	0	6	10802.4162	0.0062	E-
7	2	6	6	2	5	10824.1362	-0.0993	E-
7	2	6	6	2	5	10824.1506	-0.0849	E+
7	1	6	6	1	5	11018.1346	-0.0179	E+
7	1	6	6	1	5	11018.1474	-0.0051	E-
8	1	8	7	1	7	12129.9779	0.0096	E-
8	1	8	7	1	7	12129.9850	0.0167	E+
8	0	8	7	0	7	12338.9777	-0.0068	E+
8	0	8	7	0	7	12338.9936	0.0091	E-
8	2	7	7	2	6	12368.6206	-0.1675	E-
8	2	7	7	2	6	12368.6354	-0.1527	E+
8	3	6	7	3	5	12370.8744	0.0125	E-
8	1	7	7	1	6	12590.4459	-0.0217	E+
8	1	7	7	1	6	12590.4638	-0.0038	E-
4	1	4	3	0	3	13364.8378	0.0001	E+

4	1	4	3	0	3	13364.8378	0.0001	E-
9	1	9	8	1	8	13644.1684	0.0104	E-
9	1	9	8	1	8	13644.1777	0.0196	E+
9	0	9	8	0	8	13872.9478	-0.0028	E+
9	0	9	8	0	8	13872.9635	0.0128	E-
9	1	8	8	1	7	14162.0262	-0.0225	E+
9	1	8	8	1	7	14162.0464	-0.0023	E-
10	1	10	9	1	9	15157.6817	0.0122	E-
10	1	10	9	1	9	15157.6934	0.0239	E+
10	0	10	9	0	9	15404.0247	0.0016	E+
10	0	10	9	0	9	15404.0365	0.0133	E-
10	1	9	9	1	8	15732.7736	-0.0210	E+
10	1	9	9	1	8	15732.7918	-0.0028	E-
11	1	11	10	1	10	16670.4609	0.0187	E-
11	1	11	10	1	10	16670.4712	0.0290	E+
11	0	11	10	0	10	16931.9477	0.0049	E+
11	0	11	10	0	10	16931.9596	0.0168	E-

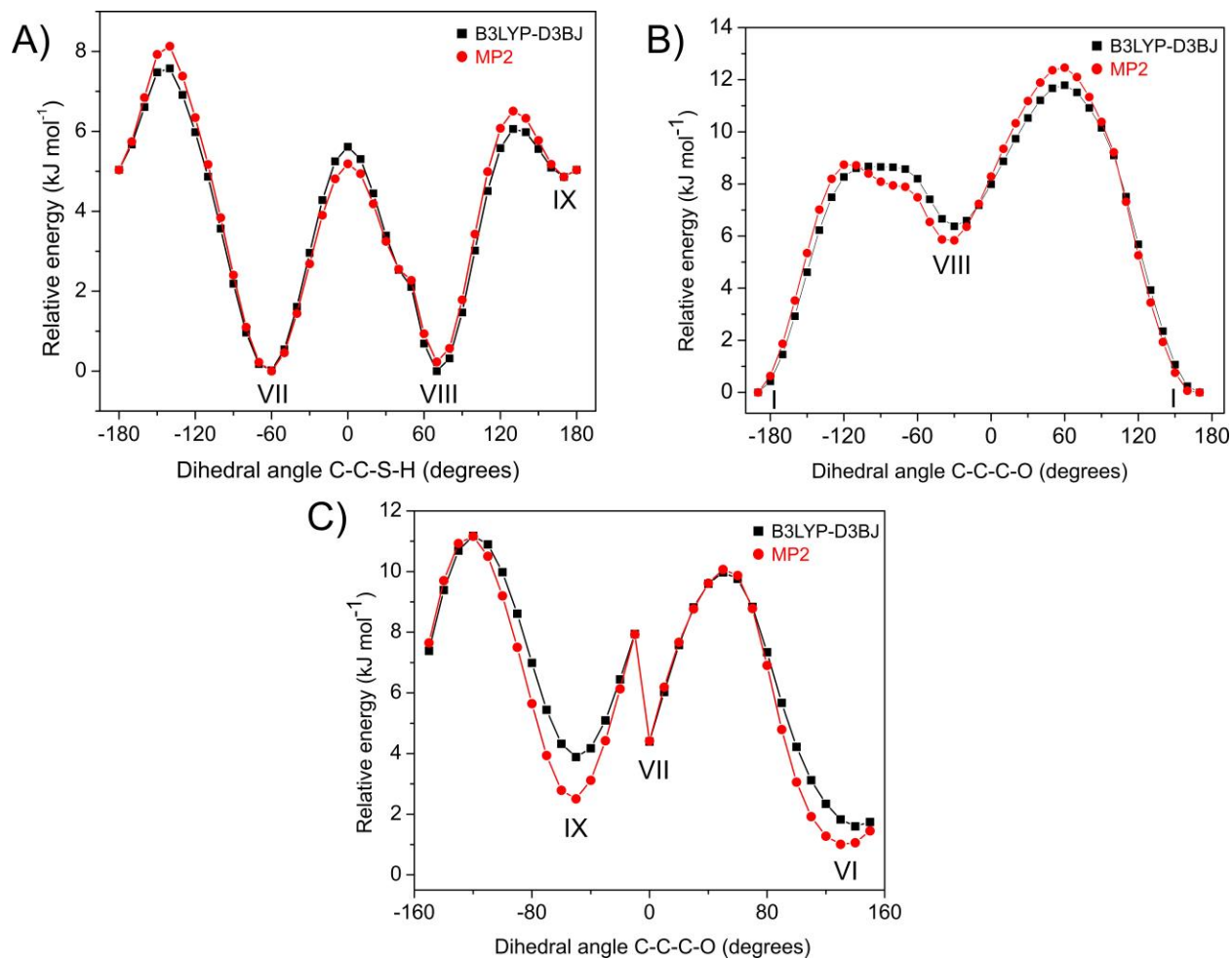


Figure S1. Conversion pathway between conformers A) **VII**, **VIII**, and **IX** B) **I** and **VIII**, C) **VI**, **VII**, and **IX**. The potential energy curves were calculated using the B3LYP-D3BJ and MP2 methods with the aug-cc-pVTZ basis set.