

Properties of the only thorium fullerene, Th@C₈₄, uncovered.

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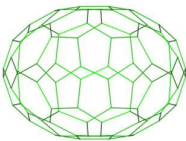
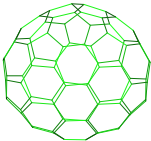
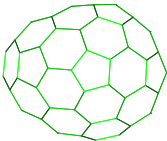
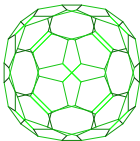
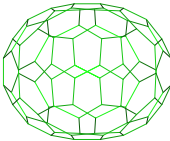
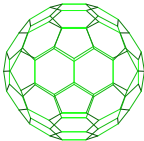
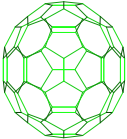
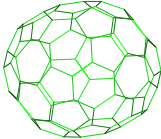
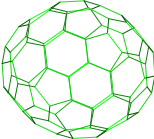
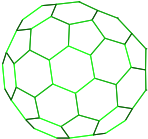
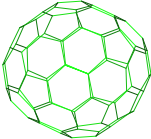
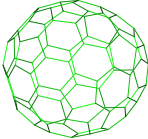
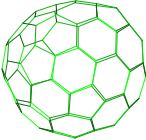
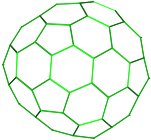
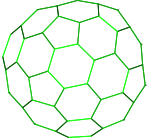
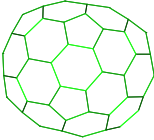
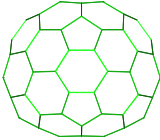
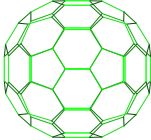
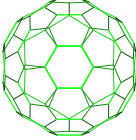
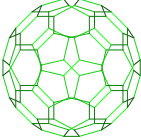
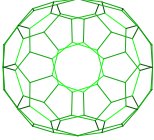
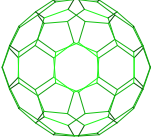
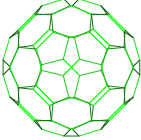
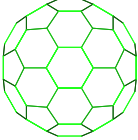
					
No.1-D2	No.2-C2	No.3-Cs	No.4-D2d	No.5-D2	No.6-C2v
213.7	136.0	109.9	58.1	65.0	73.1
					
No.7-C2v	No.8-C2	No.9-C2	No.10-Cs	No.11-C2	No.12-C1
106.8	96.3	114.1	122.8	35.6	53.1
					
No.13-C2	No.14-Cs	No.15-Cs	No.16-Cs	No.17-C2v	No.18-C2v
106.9	63.9	49.4	33.9	92.3	65.7
					
No.19-D3d	No.20-Td	No.21-D2	No.22-D2	No.23-D2d	No.24-D6h
43.7	129.1	71.2	1.2	0.0	29.0

Figure S1. The 24 IPR isomers of C₈₄ and their relative energies in kJ/mol. Optimized at the PBE0/def2-TZVPP level.

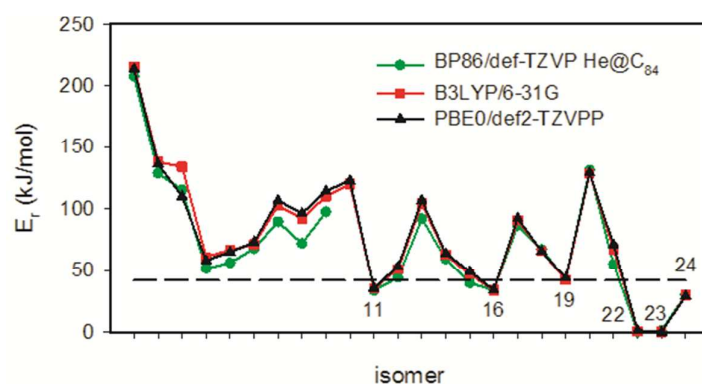


Figure S2. Relative energies of the 24 isomers of C_{84} as obtained at the PBE0/def2-TZVPP level (this work, black triangles) and B3LYP/6-31G level (Ref. ^[1], red squares). Relative energies of $He@C_{84}$ obtained at the BP86/def-TZVP/Th-ECP level taken from Ref. ^[2] are displayed for comparison. The 40 kJ/mol limit is defined by the dashed line. Numbers designate isomers below or close that limit.

Supporting Information

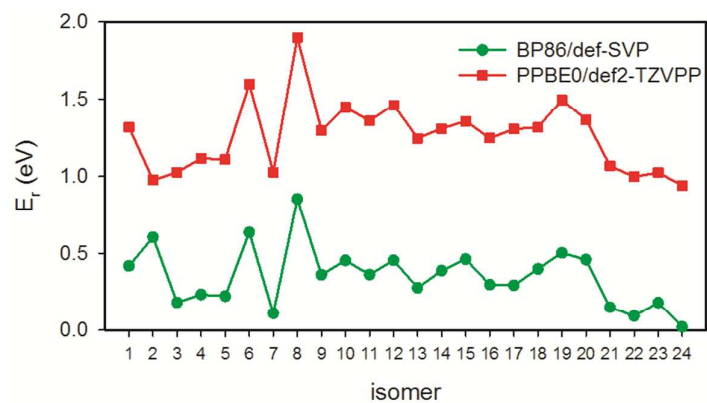


Figure S3. HOMO-LUMO gap of 24 IPR Th@C₈₄ isomers as obtained at the BP86/def-SVP (green circles) and PBE0/def2-TZVPP (red squares) levels.

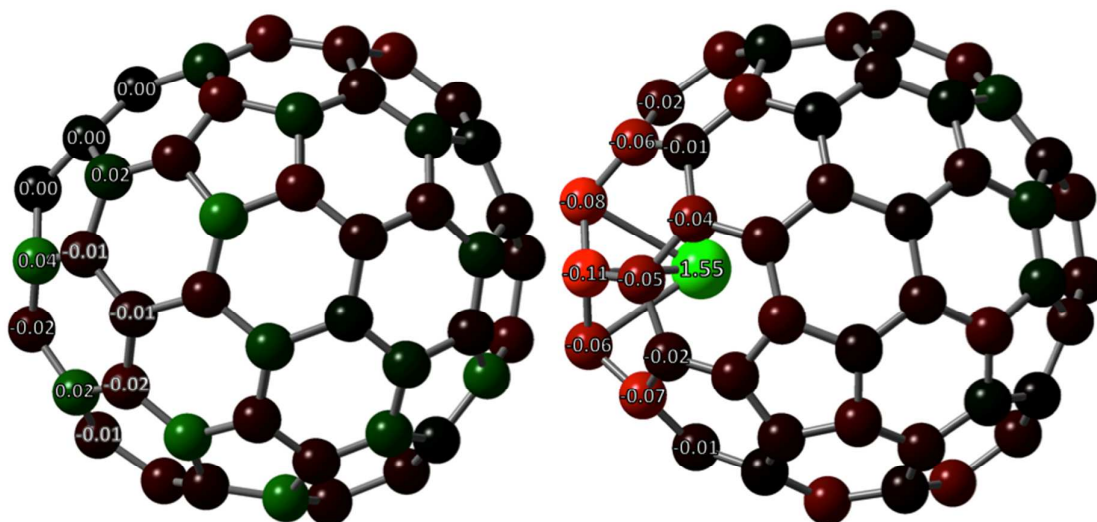


Figure S4. The NPA charge distribution (green – red color scale) for empty C₈₄-C₅(10) cage on the left and Th@C₈₄-C₅(10) isomer on the right. NPA charges for several selected atoms are displayed as well.

Supporting Information

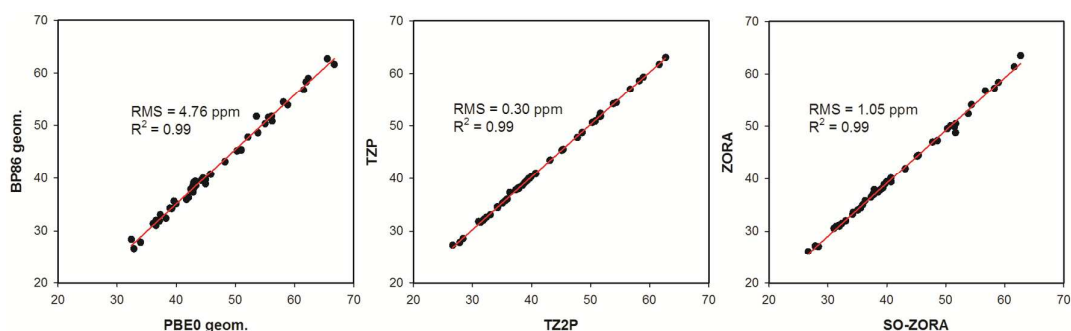


Figure S5. Comparison of calculated ^{13}C NMR shieldings in $\text{Th@C}_{84}\text{-C}_{5(10)}$ (ppm) at various computational levels against the benchmark data obtained at SO ZORA PBE40/TZP level using PBE0/def2-TZVPP/Th-ECP structure (red line) (a) The effect of optimized geometry using low-level BP86/def-SVP/Th-ECP-optimized structures. (b) The basis set effect on ^{13}C NMR shielding comparing TZP and TZ2P basis sets. (c) The effect of spin-orbital interaction comparing SO ZORA and SO approach.

Table S1. Calculated ^{13}C chemical shifts

Carbon	δ (ppm)	δ (ppm)
	PBE40/TZ2P/ZORA	PBE40/TZ2P/SO
C(1)	131.0	130.0
C(2)	132.7	130.6
C(3)	137.7	135.8
C(4)	148.1	146.7
C(5)	121.5	121.7
C(6)	134.6	132.7
C(7)	128.2	127.7
C(8)	135.1	132.9
C(9)	138.0	136.7
C(10)	126.6	125.5
C(11)	153.5	152.1
C(12)	135.0	133.7
C(13)	143.1	141.4
C(14)	147.6	146.0
C(15)	147.1	146.6
C(16)	121.5	121.8
C(17)	136.2	132.8
C(18)	148.0	146.7
C(19)	136.3	132.9
C(20)	123.6	122.9
C(21)	123.6	122.9
C(22)	127.8	126.3
C(23)	127.8	126.3
C(24)	140.7	139.4
C(25)	140.6	139.3
C(26)	145.7	143.9
C(27)	126.6	125.7
C(28)	135.1	133.1
C(29)	153.5	152.3
C(30)	145.6	143.9
C(31)	140.7	139.5
C(32)	140.5	139.3
C(33)	138.0	136.9
C(34)	134.5	133.0
C(35)	128.3	128.0
C(36)	132.7	130.9
C(37)	137.8	136.2
C(38)	131.0	130.4
C(39)	143.1	141.6
C(40)	134.9	133.9
C(41)	147.6	146.3
C(42)	147.1	146.9
C(43)	146.8	145.4
C(44)	145.6	144.8
C(45)	153.0	151.8
C(46)	151.8	150.6

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C(47)	144.9	144.1
C(48)	154.0	152.9
C(49)	146.0	145.2
C(50)	157.8	157.0
C(51)	157.9	156.4
C(52)	147.6	146.3
C(53)	135.5	134.6
C(54)	154.4	153.9
C(55)	147.6	146.4
C(56)	148.0	147.3
C(57)	149.2	148.6
C(58)	148.1	147.3
C(59)	154.1	153.6
C(60)	147.3	146.1
C(61)	154.1	153.6
C(62)	146.8	145.7
C(63)	145.6	145.0
C(64)	151.0	149.9
C(65)	148.6	147.7
C(66)	151.0	149.9
C(67)	147.0	145.9
C(68)	146.2	145.5
C(69)	150.6	149.5
C(70)	147.0	146.0
C(71)	150.0	149.2
C(72)	158.9	158.4
C(73)	151.5	150.8
C(74)	153.9	153.3
C(75)	151.5	150.8
C(76)	157.8	157.3
C(77)	157.9	156.7
C(78)	146.1	145.5
C(79)	154.0	153.2
C(80)	150.6	148.7
C(81)	146.2	144.7
C(82)	151.8	150.1
C(83)	144.9	143.6
C(84)	153.0	151.2

References

- [1] G. Sun. M. Kerstes. *J. Phys. Chem. A* **2001**, 105, 5212-5220.
- [2] P. Stepanek. P. Bour. M. Straka. *Chem. Phys. Lett.* **2010**, 500, 54.

PBE0/def2-TZVPP/Th-ECP optimized structures of 24 Th@C₈₄ IPR isomersTh@C₈₄-D₂(1)

C	2.124635	-0.715522	-4.181096
C	0.855476	-1.403570	-4.149602
C	2.165288	0.695446	-4.356932
C	-0.327434	-0.720701	-4.434180
C	-1.556647	-1.108585	-3.793887
C	4.042842	0.859807	-2.745797
C	3.933370	-0.576729	-2.504263
C	3.099111	1.485683	-3.579873
C	2.961630	-1.324246	-3.166822
C	2.157126	-2.278008	-2.416220
C	1.298400	-3.031918	1.195264
C	0.139062	-3.401925	1.934247
C	1.182374	-2.963504	-0.260457
C	2.328090	-2.470648	-1.017044
C	3.433972	-1.770808	-0.342559
C	4.220972	-0.842144	-1.109260
C	-0.311031	-2.630440	-2.277564
C	0.859841	-2.344446	-3.034197
C	-3.680057	-2.430547	0.472620
C	-2.651966	-2.745057	-0.532961
C	-1.340974	-3.223793	-0.074603
C	-0.136364	-3.047240	-0.893409
C	-1.149822	-3.516635	1.309133
C	-1.596247	-2.073892	-2.722729
C	-3.721632	-0.985423	-1.933041
C	-2.734132	-2.063312	-1.814107
C	4.495289	0.630612	0.833432
C	4.440910	1.472511	-1.490929
C	4.679007	0.403708	-0.532049
C	3.390414	-1.604736	1.105111
C	2.366646	-2.305405	1.881570
C	3.992388	-0.427632	1.668376
C	3.911455	1.880648	1.298472
C	3.463736	2.812076	0.355036
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C	2.686753	3.178641	-1.817354
C	2.374428	2.652519	-3.075219
C	2.462013	-0.488096	3.568668
C	3.360998	0.209343	2.800579
C	3.103335	1.592596	2.455033
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C	0.253405	3.295897	-1.222384
C	-0.077942	2.856724	-2.587084

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C	-2.984619	2.460586	0.623025
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C	1.239700	2.924198	1.517713
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C	0.854839	-2.118933	3.884936
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C	-3.340156	-2.550296	1.873865
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C	-3.130159	-0.904556	3.715723
C	-4.545555	-0.498266	-0.842761
C	-4.612576	-0.591104	1.662728
C	-4.596297	-1.283909	0.372680
Th	-2.424095	-0.120255	0.396702

Th@C₈₄-C₂(2)

C	3.710681	1.677560	1.899063
C	3.581612	0.369891	2.476486
C	4.252448	1.817810	0.624706
C	4.097031	-0.727513	1.835015
C	3.373418	-1.969484	1.867447
C	0.646113	3.730557	1.630952
C	2.023134	3.392945	1.425994
C	2.574480	2.435784	2.277113
C	1.725704	1.561973	3.071750
C	-0.505291	0.575306	3.222431
C	0.352427	1.722838	3.095574

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C	-0.150504	2.914863	2.491209
C	-2.736813	-0.362108	2.901146
C	-1.917527	0.772201	2.987312
C	1.509887	-0.886804	3.068571
C	2.310570	0.278855	3.121603
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C	3.576732	1.953457	-1.585086
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C	0.163417	2.955632	-2.558567
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C	-2.297054	0.251356	-3.080243
C	-1.494349	-0.911157	-3.043063
C	-4.107489	-0.752780	-1.826663
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C	-4.751520	-0.603057	-0.572068
C	-4.079960	-1.662729	1.534372
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C	-4.305812	0.767908	1.402616
C	-4.449803	-1.766458	0.196160
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C	-2.471663	-3.484110	1.301091
C	-3.030762	-2.483733	2.058550
C	-3.708570	-2.678197	-0.646122
C	0.651955	-4.266479	-0.134646
C	-1.619961	-3.873447	-0.815067
C	-0.657483	-4.259147	0.168326
Th	-0.353390	2.031408	-0.154217

Th@C₈₄-C₅(3)

C	-1.596938	0.717137	3.569134
C	-2.525668	1.449093	2.826040
C	-3.619402	0.713752	2.312166
C	-4.317738	1.144169	1.126612
C	-3.873601	2.280823	0.490915
C	-0.661294	3.033155	2.273876
C	-2.059878	2.652631	2.165466
C	-2.802592	3.065396	1.033720
C	-0.105668	3.804304	1.238730
C	-0.839418	4.057222	0.046026
C	-2.142711	3.664015	-0.071317
C	0.277332	2.254516	3.061805
C	1.714379	2.255917	2.756708
C	-0.243293	1.160976	3.756794
C	2.493448	1.164243	3.181416
C	-4.572936	-0.002172	-1.015194
C	-4.029534	1.140152	-1.662430
C	-4.731876	0.001136	0.384278
C	-3.743900	2.282606	-0.944837
C	-2.626722	3.089908	-1.294804
C	-3.091598	0.705478	-2.671224
C	-1.937659	1.437959	-2.978063
C	-1.712701	2.705075	-2.289518
C	0.661229	2.528703	-2.897801

Supporting Information

C	-0.370302	3.208359	-2.191612
C	0.037176	3.936474	-1.062554
C	-3.873837	-2.278130	0.501696
C	-3.744137	-2.286705	-0.934024
C	-4.317848	-1.138413	1.132034
C	-4.029627	-1.147627	-1.656990
C	-3.091655	-0.717790	-2.667839
C	-2.627042	-3.095754	-1.280176
C	-1.712960	-2.715714	-2.276687
C	-1.937807	-1.451830	-2.971195
C	0.447145	1.360128	-3.671005
C	-0.840505	0.703380	-3.553222
C	-0.840557	-0.720107	-3.549836
C	0.447011	-1.377488	-3.664471
C	-0.839822	-4.056941	0.065228
C	-2.802861	-3.060213	1.048189
C	-2.143064	-3.664152	-0.053996
C	0.036808	-3.941534	-1.043917
C	0.660992	-2.542408	-2.885727
C	-0.370595	-3.218629	-2.176354
C	-0.106037	-3.798498	1.256729
C	-0.661565	-3.022332	2.288124
C	-2.060130	-2.642181	2.177964
C	-2.525798	-1.435465	2.832823
C	-3.619491	-0.702481	2.315536
C	-1.597008	-0.700137	3.572458
C	1.714151	-2.243022	2.767306
C	0.277138	-2.240009	3.072349
C	-0.243396	-1.143161	3.762155
C	2.493332	-1.149445	3.186928
C	1.886336	0.008749	3.743288
C	0.542785	0.009459	4.005939
C	1.274824	-3.744747	0.900613
C	3.369187	-2.552085	0.929522
C	2.202325	-2.996596	1.626201
C	2.012938	-2.557005	-2.468480
C	2.360102	-3.176839	-1.229814
C	1.364084	-3.856444	-0.530339
C	3.387721	-2.570222	-0.502341
C	4.485769	-0.688392	0.171434
C	4.081583	-1.406284	1.340489
C	3.665989	-0.699732	2.469467
C	4.485860	0.688831	0.168196
C	2.691390	-1.418193	-3.029313
C	3.684331	-0.728838	-2.208712
C	4.029927	-1.390239	-0.991182
C	2.691541	1.403625	-3.036015
C	1.720669	0.705773	-3.852262
C	1.720588	-0.724137	-3.848841
C	4.029990	1.385175	-0.997743

Supporting Information

C	3.684384	0.718035	-2.212145
C	1.364428	3.853780	-0.548616
C	3.387893	2.567452	-0.514516
C	2.360369	3.170807	-1.244882
C	2.013181	2.545161	-2.480604
C	3.666053	0.711075	2.466114
C	4.081755	1.412268	1.333829
C	3.369411	2.556117	0.917432
C	2.202585	3.003984	1.611996
C	1.275169	3.748743	0.882875
Th	1.237864	-0.003651	-1.610007

Th@C₈₄-D_{2d}(4)

C	-1.411248	-3.525443	-1.312824
C	-2.405147	-2.713736	-1.927107
C	-3.547012	-2.406130	-1.124502
C	-4.338900	-1.217285	-1.369271
C	-3.941684	-0.342351	-2.394031
C	-0.547453	-1.745314	-3.382912
C	-1.977559	-1.807313	-3.000789
C	-2.799536	-0.661335	-3.230007
C	-0.055086	-0.533441	-3.944010
C	-0.866307	0.659229	-3.963816
C	-2.202842	0.601233	-3.612121
C	0.445621	-2.627536	-2.752121
C	1.865229	-2.250936	-2.704859
C	-0.045551	-3.554322	-1.779514
C	2.727280	-2.827592	-1.677665
C	-4.811231	0.698737	0.126089
C	-4.339555	1.594113	-0.909510
C	-4.813469	-0.700625	-0.102350
C	-3.939533	1.093913	-2.155366
C	-1.412498	3.768765	-0.118165
C	-3.544185	2.645049	-0.295362
C	-2.402551	3.198873	-0.960017
C	-1.975806	2.686733	-2.267690
C	-0.549157	2.753214	-2.646882
C	-2.797140	1.670780	-2.849825
C	-0.057234	1.780994	-3.562207
C	-3.916522	-1.088330	2.174705
C	-3.914812	0.349239	2.405483
C	-4.326179	-1.592573	0.929328
C	-4.327273	1.219069	1.387570
C	-3.536317	2.412025	1.130936
C	-2.386783	2.727685	1.925115
C	-1.404791	3.537453	1.297683
C	-0.823252	-0.632733	3.948991
C	-2.766357	-1.654595	2.853652
C	-2.163518	-0.578087	3.611273
C	-1.947140	1.827041	2.997633

Supporting Information

C	-2.764167	0.677349	3.235407
C	-0.016579	0.559909	3.916486
C	-0.516517	1.771918	3.363068
C	-0.014322	-1.755808	3.542397
C	-0.514767	-2.727275	2.630277
C	-1.948896	-2.666816	2.263339
C	-2.389356	-3.185394	0.961811
C	-3.539134	-2.640396	0.310810
C	-1.403393	-3.757791	0.110876
C	1.889905	-2.986954	1.801389
C	0.470057	-3.361361	1.741317
C	-0.032887	-3.931527	0.529735
C	2.740309	-3.205728	0.635190
C	2.109318	-3.554148	-0.605696
C	0.768562	-3.930501	-0.659816
C	1.355374	-1.299888	3.507736
C	3.502398	-1.138900	2.342751
C	2.327397	-1.929175	2.692083
C	2.320570	0.972650	3.141214
C	1.353992	0.135610	3.736070
C	3.465318	0.297125	2.550442
C	1.899303	2.276861	2.645675
C	-0.022700	3.570814	1.750267
C	0.471092	2.654624	2.718574
C	2.729550	2.869172	1.629858
C	4.871141	-0.139566	0.691272
C	4.392082	-1.420065	1.222893
C	3.957499	-2.473464	0.307897
C	4.862764	0.100307	-0.778280
C	3.863866	2.414468	-0.369515
C	3.871384	2.182458	1.049974
C	4.280431	0.900241	1.532903
C	4.265499	1.353169	-1.239489
C	0.782402	3.973426	0.630317
C	2.717117	3.248465	-0.689179
C	2.132572	3.637198	0.567989
C	1.314521	1.323583	-3.540419
C	3.438321	1.103551	-2.387142
C	2.289013	1.930106	-2.720823
C	1.875205	3.008440	-1.831952
C	0.446863	3.387068	-1.765753
C	-0.035193	3.946416	-0.551098
C	3.949021	-2.235375	-1.147397
C	4.375212	-0.945187	-1.684060
C	3.474595	-0.323950	-2.646717
C	2.294912	-0.964121	-3.217169
C	1.315654	-0.109795	-3.780380
Th	2.541190	-0.434210	-0.096669

Th@C₈₄-D₂(5)

Supporting Information

C	1.381119	-3.066522	2.280450
C	2.269269	-2.028272	2.587154
C	3.437180	-1.950535	1.792488
C	4.159371	-0.742467	1.661729
C	3.739210	0.389832	2.330695
C	0.020511	-2.998841	2.628321
C	-1.911837	-1.665946	3.061362
C	-0.526424	-1.836846	3.202584
C	0.318105	-0.680271	3.405033
C	1.743245	-0.821652	3.202302
C	2.530271	0.341569	3.099815
C	4.662944	0.587806	-0.327048
C	4.243180	1.763651	0.371485
C	4.654497	-0.645939	0.305133
C	3.813956	1.669679	1.698217
C	2.707300	2.443818	2.127341
C	2.102032	3.401637	1.304135
C	0.747402	3.778825	1.625461
C	-2.504778	-0.384818	3.102817
C	-1.717233	0.770385	3.162968
C	-0.289127	0.625388	3.367042
C	0.551775	1.769235	3.137206
C	1.927297	1.612642	3.026144
C	0.008301	2.945169	2.533959
C	3.798378	-1.731154	-1.710838
C	3.720364	-0.451439	-2.330759
C	4.237863	-1.824377	-0.382620
C	4.162203	0.684334	-1.674237
C	3.440372	1.890888	-1.804236
C	2.249238	1.933798	-2.541512
C	1.351777	2.981316	-2.207862
C	2.509309	3.459725	-0.088840
C	3.515194	2.592986	-0.529549
C	1.488925	3.814236	-1.047390
C	0.730017	-3.775567	-1.635270
C	2.054583	-3.429551	-1.305891
C	2.692788	-2.503847	-2.151902
C	1.910551	-1.692917	-3.047330
C	-0.318667	-0.708446	-3.399213
C	0.524976	-1.863921	-3.187118
C	-0.022823	-3.020655	-2.603141
C	-2.530029	0.317599	-3.102516
C	-1.743901	-0.847038	-3.195298
C	1.717798	0.742631	-3.169346
C	2.504475	-0.412649	-3.099510
C	-0.006092	2.923958	-2.558523
C	-0.550462	1.743409	-3.151887
C	0.289562	0.597033	-3.372178
C	-1.926106	1.588770	-3.039473
C	2.464066	-3.477960	0.095580

Supporting Information

C	3.514538	-2.644381	0.527868
C	-0.188372	-4.225737	-0.657511
C	0.185143	-4.220259	0.692815
C	1.491909	-3.814645	1.057597
C	-1.494833	-3.822195	-1.025657
C	-2.466699	-3.476728	-0.066508
C	-3.516540	-2.646020	-0.505749
C	-2.270821	-2.048060	-2.570084
C	-1.383482	-3.084380	-2.254706
C	-3.438656	-1.962787	-1.776099
C	-2.057177	-3.416939	1.334490
C	-0.732901	-3.761210	1.666756
C	-2.694655	-2.483694	2.172697
C	-4.654964	-0.644908	-0.299722
C	-4.239227	-1.817879	0.397827
C	-3.799650	-1.713882	1.725203
C	-4.662486	0.594071	0.322126
C	-3.812672	1.658342	-1.712068
C	-3.738908	0.373218	-2.333838
C	-4.159924	-0.753134	-1.655443
C	-4.241809	1.763717	-0.386199
C	-0.744550	3.765722	-1.657015
C	-2.099429	3.392212	-1.332511
C	-2.705422	2.428003	-2.147644
C	-1.486012	3.823927	1.015424
C	-0.188781	4.346965	0.684252
C	0.192082	4.340980	-0.720588
C	-3.513202	2.599999	0.507843
C	-2.506661	3.462223	0.059891
C	-3.720687	-0.429098	2.334412
C	-4.161673	0.701469	1.668444
C	-3.438921	1.908505	1.788334
C	-2.247764	1.956654	2.525236
C	-1.349513	3.000617	2.182785
Th	0.000796	2.040624	-0.008597

Th@C₈₄-C_{2v}(6)

C	2.073081	-1.479291	2.913811
C	3.213431	-0.710433	2.472352
C	4.083579	-1.142447	1.398648
C	1.804333	-2.755391	2.272969
C	2.660679	-3.149581	1.170504
C	3.742854	-2.341311	0.725497
C	-0.518103	-2.648527	3.111234
C	0.446492	-3.293295	2.301140
C	-0.063892	-4.011311	1.162701
C	0.752063	-4.169771	-0.016891
C	2.077795	-3.758363	-0.015584
C	-1.414152	-3.829920	0.713720
C	-2.361002	-3.066115	1.453135

Supporting Information

C	-1.921757	-2.610291	2.745721
C	4.681333	0.021733	-0.753801
C	4.084083	-1.134430	-1.413941
C	4.681104	0.017484	0.745547
C	3.743333	-2.337339	-0.748077
C	2.661348	-3.143172	-1.198109
C	3.214332	-0.696209	-2.485496
C	2.074214	-1.462599	-2.932001
C	1.805282	-2.742426	-2.298532
C	-0.517070	-2.630340	-3.136472
C	0.447307	-3.279874	-2.329894
C	-0.063525	-4.004438	-1.195761
C	3.815354	2.376114	0.748278
C	3.815593	2.380375	-0.742922
C	4.187986	1.182723	1.469528
C	4.188348	1.191191	-1.471058
C	3.253666	0.743118	-2.512990
C	2.643348	3.110531	-1.164936
C	1.778743	2.733749	-2.279181
C	2.074523	1.479173	-2.941700
C	-0.206086	-1.413503	-3.863441
C	1.022873	-0.733851	-3.644454
C	1.023008	0.742644	-3.641100
C	-0.217510	1.417300	-3.847718
C	2.073645	1.462268	2.941218
C	1.778175	2.720806	2.286242
C	3.252780	0.728647	2.508323
C	2.643015	3.103755	1.174277
C	2.039826	3.700487	0.006338
C	0.715108	4.146893	0.007443
C	-0.095236	3.981444	1.179740
C	0.419487	3.255723	2.311555
C	-0.540027	2.606501	3.124365
C	-0.094936	3.988129	-1.165983
C	-0.539068	2.624480	-3.118885
C	0.420098	3.268817	-2.301745
C	-0.218735	1.395013	3.846099
C	1.021865	0.721642	3.635779
C	1.021624	-0.754784	3.630232
C	-1.453690	0.674820	4.046101
C	-1.449022	-0.722975	4.044021
C	-0.207247	-1.435817	3.845129
C	-2.519061	1.399610	3.373888
C	-2.506057	-1.451486	3.369175
C	-3.531211	-0.755220	2.708351
C	-3.542424	0.697328	2.713714
C	-1.452191	3.799453	0.730794
C	-2.391309	3.023475	1.472056
C	-1.950878	2.568142	2.762835
C	-3.417999	2.270417	-0.739521

Supporting Information

C	-3.418136	2.266160	0.741863
C	-4.006392	1.153144	1.419190
C	-4.006190	1.161407	-1.423621
C	-2.518068	1.419216	-3.376226
C	-1.950008	2.584099	-2.758043
C	-2.390819	3.031857	-1.464763
C	-1.452015	3.803554	-0.718549
C	-3.541804	0.713119	-2.720627
C	-2.505043	-1.431869	-3.388025
C	-1.447823	-0.699438	-4.058352
C	-1.452490	0.698325	-4.052336
C	-3.530656	-0.739510	-2.723750
C	-1.413918	-3.825701	-0.746130
C	-2.360620	-3.057725	-1.481456
C	-1.920831	-2.594264	-2.771154
C	-4.408569	-0.029350	0.685476
C	-3.992085	-1.210994	1.410276
C	-3.396029	-2.315124	0.727753
C	-4.408582	-0.025363	-0.696932
C	-3.992016	-1.202897	-1.428497
C	-3.395953	-2.310904	-0.752191
Th	2.331526	0.455785	-0.003170

Th@C₈₄-C_{2v}(7)

C	-1.344593	-4.054273	-0.734924
C	-2.329334	-3.309375	-1.459228
C	-3.393253	-2.690827	-0.726270
C	-1.899087	-2.678978	-2.672857
C	-0.504540	-2.688478	-3.059768
C	0.493066	-3.356298	-2.292797
C	0.026114	-4.140442	-1.187277
C	-2.501753	-1.439353	-3.124659
C	-3.492690	-0.752385	-2.334808
C	-3.983332	-1.443381	-1.175791
C	-4.390887	-0.719868	0.002301
C	-4.404304	0.688301	0.006214
C	-1.476973	-0.710653	-3.813148
C	-1.466791	0.687426	-3.809257
C	-2.502986	1.418485	-3.105030
C	-3.497069	0.724168	-2.330899
C	-3.992854	1.414119	-1.167373
C	1.023952	-0.756382	-3.542276
C	-0.223074	-1.427572	-3.703643
C	-0.228482	1.391509	-3.701536
C	1.016292	0.714652	-3.523488
C	2.114590	-1.498039	-2.907907
C	2.710688	-3.195244	-1.188954
C	1.852241	-2.798884	-2.267675
C	3.260730	-0.749768	-2.515653
C	-2.495702	1.399623	3.118090

Supporting Information

C	-3.491604	0.709928	2.342251
C	-3.989345	1.406874	1.183582
C	-3.394638	2.651674	0.737700
C	-1.315721	3.981158	0.731393
C	-2.330990	3.253389	1.463880
C	-1.909465	2.632363	2.676159
C	-1.915509	2.648739	-2.656614
C	-2.335291	3.262890	-1.439861
C	-3.396936	2.656793	-0.715251
C	-1.317637	3.986245	-0.706098
C	-3.487380	-0.766427	2.337364
C	-3.980620	-1.450332	1.175314
C	-1.457349	0.663992	3.815293
C	-1.467558	-0.733453	3.810428
C	-2.494527	-1.458278	3.120786
C	-0.218908	1.368830	3.709156
C	-0.213357	-1.450223	3.694073
C	1.033481	-0.778230	3.533944
C	1.025739	0.692786	3.524187
C	0.044469	4.188676	1.197686
C	0.510842	3.358630	2.334753
C	-0.491082	2.622096	3.026214
C	1.857338	2.773714	2.283411
C	2.102573	1.441937	2.884300
C	3.258281	0.687176	2.489742
C	-1.892692	-2.694612	2.660148
C	-2.325886	-3.318153	1.444059
C	-3.391653	-2.695176	0.717284
C	-1.343013	-4.059044	0.713412
C	-0.496663	-2.706450	3.043647
C	0.499388	-3.369994	2.270281
C	0.028963	-4.147020	1.161291
C	2.165296	-3.850224	-0.014872
C	0.847894	-4.293911	-0.014634
C	3.267863	-0.765434	2.501179
C	2.122500	-1.516181	2.892116
C	1.858301	-2.812930	2.245068
C	2.714019	-3.202927	1.160964
C	3.762134	2.310986	0.723413
C	4.104652	1.132659	1.420277
C	4.591697	-0.026423	0.698922
C	4.126771	-1.200677	1.416928
C	3.801564	-2.366072	0.716862
C	0.866666	4.437184	0.011301
C	2.203156	3.906422	0.007916
C	2.717001	3.191869	1.185407
C	-0.498807	2.641513	-3.010064
C	0.505709	3.376109	-2.319261
C	0.041323	4.198575	-1.175232
C	4.101806	1.141828	-1.426501

Supporting Information

C	3.251533	0.703289	-2.495772
C	2.095249	1.460543	-2.882481
C	3.760683	2.315926	-0.721507
C	2.714978	3.200553	-1.175603
C	1.852398	2.790768	-2.275005
C	3.799950	-2.361570	-0.743235
C	4.590106	-0.021772	-0.713577
C	4.122908	-1.191810	-1.437129
Th	0.574429	2.046126	-0.001778

Th@C₈₄-C₂(8)

C	-1.632586	-3.243621	1.881755
C	-2.454204	-3.193341	0.744773
C	-3.571304	-2.316765	0.808126
C	-4.123867	-1.746321	-0.373519
C	-3.591073	-2.080910	-1.599200
C	-0.417282	-3.815201	-0.612230
C	-1.851908	-3.518600	-0.537994
C	-2.490556	-2.999081	-1.684657
C	0.240096	-3.588814	-1.828151
C	-0.410397	-2.939973	-2.912859
C	-1.748027	-2.627922	-2.835612
C	0.411700	-3.820205	0.584174
C	1.846754	-3.525144	0.512051
C	-0.245293	-3.601857	1.801688
C	2.486128	-3.014950	1.662563
C	-4.325530	0.587879	-1.056294
C	-3.728890	0.245763	-2.314515
C	-4.515799	-0.391736	-0.097923
C	-3.402020	-1.064111	-2.593605
C	-2.210780	-1.354794	-3.314976
C	-2.824573	1.285150	-2.687711
C	-1.614155	1.024975	-3.344267
C	-1.301626	-0.359121	-3.703427
C	1.079831	0.246618	-3.886463
C	0.088783	-0.758044	-3.902985
C	0.495501	-2.053514	-3.545787
C	-2.553975	3.148280	0.874780
C	-3.564387	2.149224	0.667045
C	-3.835515	1.859470	-0.672514
C	-2.943399	2.333866	-1.717029
C	-1.919090	3.257611	-1.506968
C	-1.814132	3.802885	-0.157579
C	0.595575	4.311584	-0.394191
C	-0.589107	4.308934	0.425830
C	0.757750	1.592945	-3.575622
C	-0.544396	2.004290	-3.185012
C	-0.708020	3.145138	-2.301895
C	0.495559	3.764795	-1.740356
C	-3.753813	1.130182	1.679343

Supporting Information

C	-4.227306	-0.130305	1.267715
C	-1.749408	3.138381	2.037336
C	-1.911959	2.138881	2.982920
C	-2.912630	1.158659	2.834275
C	-0.489919	3.752366	1.767837
C	-0.755527	1.567728	3.587504
C	0.547292	1.980087	3.199648
C	0.712649	3.127133	2.325103
C	2.946618	2.316918	1.734010
C	1.923901	3.244063	1.530923
C	1.820052	3.799769	0.185504
C	-2.405309	-0.033871	3.424337
C	-2.759049	-1.298596	2.896461
C	-3.684352	-1.341807	1.834721
C	-1.788234	-2.316093	2.949099
C	-1.079539	0.219495	3.888343
C	-0.090049	-0.786552	3.897466
C	-0.498517	-2.078897	3.530640
C	1.744130	-2.651261	2.816231
C	0.406054	-2.961893	2.891140
C	2.826303	1.261231	2.696917
C	1.615416	0.997948	3.351777
C	1.301096	-0.388333	3.700793
C	2.208651	-1.382317	3.305027
C	4.326157	0.573925	1.060608
C	3.729061	0.223255	2.316175
C	3.400402	-1.088026	2.585688
C	4.515192	-0.399084	0.094850
C	2.558765	3.151316	-0.851749
C	3.567417	2.149050	-0.651293
C	3.838008	1.848880	0.686090
C	2.914259	1.175256	-2.825640
C	1.915040	2.157848	-2.967122
C	1.754057	3.151344	-2.014166
C	4.227029	-0.127021	-1.268732
C	3.755459	1.137021	-1.671047
C	1.784775	-2.296928	-2.966021
C	3.682367	-1.333535	-1.844536
C	2.757158	-1.281151	-2.906009
C	2.405303	-0.012191	-3.424420
C	3.588053	-2.097782	1.583653
C	4.121233	-1.755025	0.360792
C	3.567914	-2.315938	-0.825174
C	2.449574	-3.191331	-0.768223
C	1.627823	-3.232055	-1.905600
Th	0.002611	2.043875	0.007364

Th@C₈₄-C₂(9)

C	-0.912602	-3.208566	-2.316274
C	-2.062846	-3.163224	-1.511265

Supporting Information

C	-3.093748	-2.287559	-1.927006
C	-4.025161	-1.749783	-0.998789
C	-3.939704	-2.112893	0.331347
C	-0.591166	-3.788954	0.433031
C	-1.918221	-3.500571	-0.106784
C	-2.910103	-3.009446	0.766568
C	-0.373443	-3.573518	1.800814
C	-1.357365	-2.944129	2.616298
C	-2.592317	-2.650351	2.110599
C	0.580763	-3.791871	-0.421488
C	1.908605	-3.505520	0.117451
C	0.363613	-3.579982	-1.789916
C	2.901839	-3.019816	-0.757383
C	-4.457532	0.569293	-0.386375
C	-4.376050	0.185446	1.005203
C	-4.288931	-0.390270	-1.363167
C	-4.124546	-1.123245	1.349517
C	-3.228437	-1.413455	2.434772
C	-3.730372	1.232449	1.722175
C	-2.784744	0.973871	2.752633
C	-2.531134	-0.409944	3.129345
C	-0.313259	0.261675	4.007579
C	-1.252461	-0.765987	3.733230
C	-0.718158	-2.048938	3.509955
C	-2.501259	3.181856	0.970851
C	-3.876643	1.856860	-0.533769
C	-3.527335	2.282984	0.794514
C	-1.634725	3.062488	2.081548
C	-0.557747	1.579719	3.591818
C	-1.754299	1.943745	2.955100
C	-1.811195	3.796633	-0.118652
C	-1.992355	3.201651	-1.439482
C	-3.029442	2.184092	-1.614502
C	-2.882341	1.179892	-2.653825
C	-3.511709	-0.077880	-2.513034
C	-1.708445	1.207312	-3.442746
C	-0.576894	4.294152	0.409217
C	0.588670	4.291300	-0.422286
C	0.424448	3.738249	-1.776759
C	-0.818216	3.197816	-2.274655
C	-0.689403	2.173067	-3.229782
C	0.695388	2.180901	3.223219
C	0.826952	3.202163	2.264787
C	-0.414148	3.744544	1.765219
C	-1.095677	0.030683	-3.937184
C	-1.619838	-1.238384	-3.599751
C	-2.838090	-1.279699	-2.909521
C	-0.698832	-2.274594	-3.364107
C	0.313976	0.248652	-4.008264
C	1.250363	-0.780763	-3.730840

Supporting Information

C	0.712526	-2.061554	-3.503674
C	2.585026	-2.663891	-2.102492
C	1.349266	-2.955779	-2.607306
C	3.733799	1.216922	-1.725921
C	2.787446	0.957868	-2.755593
C	2.530009	-0.426395	-3.128052
C	3.224557	-1.429728	-2.430430
C	0.562098	1.567296	-3.596564
C	1.643156	3.051764	-2.090948
C	1.759691	1.930004	-2.961037
C	4.459113	0.558175	0.384663
C	4.376584	0.170334	-1.005744
C	4.121499	-1.138723	-1.346081
C	4.287856	-0.397937	1.364388
C	2.509975	3.171986	-0.980558
C	3.881709	1.847786	0.528144
C	3.533609	2.270846	-0.801420
C	1.711795	1.213047	3.439152
C	3.511526	-0.079922	2.513343
C	2.885595	1.180013	2.650310
C	3.035429	2.180607	1.607915
C	2.001086	3.200300	1.429660
C	1.821497	3.791724	0.107092
C	0.692603	-2.266294	3.371060
C	2.834584	-1.278673	2.913452
C	1.616452	-1.231906	3.603584
C	1.095781	0.039609	3.937183
C	3.933914	-2.124757	-0.324890
C	4.020370	-1.757844	1.004152
C	3.087477	-2.290238	1.934000
C	2.054158	-3.164319	1.520902
C	0.903795	-3.204015	2.326048
Th	0.002296	2.011543	-0.003519

Th@C₈₄-C₅(10)

C	1.480564	-3.046194	-2.359163
C	2.592139	-2.174844	-2.317132
C	3.487166	-2.280382	-1.167356
C	4.411989	-1.247891	-0.728283
C	4.391627	0.017174	-1.462644
C	1.224840	-0.487731	-3.620745
C	2.488714	-0.882450	-2.991506
C	3.423171	0.149114	-2.547321
C	0.961095	0.908668	-3.811409
C	1.812701	1.895584	-3.225700
C	2.989930	1.520854	-2.571672
C	0.065209	-1.386207	-3.607176
C	-1.307064	-0.843673	-3.653990
C	0.260536	-2.679468	-3.040084
C	-2.362398	-1.634422	-3.099232

Supporting Information

C	4.389227	0.011852	1.469444
C	4.374569	1.289412	0.727911
C	4.410777	-1.250504	0.730564
C	4.375792	1.292082	-0.716394
C	3.438688	2.188963	-1.378695
C	3.436372	2.183787	1.392089
C	2.520402	3.118100	0.727195
C	2.521586	3.120798	-0.711632
C	0.226760	4.106361	-0.711432
C	1.325716	3.575461	-1.450932
C	1.019338	2.989259	-2.725026
C	1.807591	1.883637	3.235524
C	3.419067	0.139752	2.553069
C	2.985671	1.511283	2.581803
C	1.014943	2.978932	2.737578
C	0.225584	4.103543	0.727194
C	1.323398	3.569992	1.466389
C	0.955060	0.894588	3.816012
C	1.219113	-0.500927	3.620662
C	2.483926	-0.893351	2.991957
C	2.588550	-2.183318	2.313290
C	3.485316	-2.284564	1.164491
C	1.476987	-3.054879	2.350590
C	-1.312760	-0.856995	3.648457
C	0.059537	-1.399273	3.601931
C	0.255819	-2.690472	3.030711
C	-2.367181	-1.645599	3.089158
C	-2.102940	-2.876142	2.396655
C	-0.820782	-3.408523	2.386283
C	-0.385245	1.436975	3.797560
C	-2.698764	1.171388	3.101736
C	-1.527433	0.595307	3.705028
C	-1.144352	3.936062	1.170336
C	-1.448030	3.199620	2.364478
C	-0.343656	2.732924	3.150316
C	-2.644662	2.425092	2.396382
C	1.113040	-3.904165	1.214669
C	1.837786	-3.803017	-0.005388
C	3.022253	-2.991023	-0.003048
C	1.114866	-3.899620	-1.226897
C	-0.307264	-4.083598	-1.228371
C	-1.067312	-4.111256	-0.008271
C	-0.309128	-4.088002	1.213097
C	-2.936650	-2.951603	1.201893
C	-2.419373	-3.521304	-0.008385
C	-2.934793	-2.947267	-1.217458
C	-2.099263	-2.867533	-2.410670
C	-0.817081	-3.399921	-2.399991
C	-3.803764	-1.805739	1.205679
C	-4.202966	-1.147336	-0.005468

Supporting Information

C	-3.801783	-1.801293	-1.218407
C	-4.123193	1.035846	1.213349
C	-3.652571	0.341687	2.402466
C	-3.494544	-1.034620	2.402256
C	-4.121101	1.040275	-1.215925
C	-4.368576	0.315789	-0.002831
C	-1.987585	3.841210	0.005674
C	-3.510164	2.338197	-1.217782
C	-3.157934	3.002003	0.003182
C	-3.512230	2.333701	1.221075
C	-0.338690	2.744753	-3.140830
C	-2.640850	2.434080	-2.391473
C	-1.444272	3.208550	-2.354779
C	-1.142535	3.940588	-1.157334
C	-3.490697	-1.025832	-2.411690
C	-3.648634	0.350551	-2.406907
C	-2.693843	1.182921	-3.101708
C	-1.521623	0.608949	-3.705419
C	-0.379244	1.451083	-3.793020
Th	2.375516	-0.025806	0.001440

Th@C₈₄-C₂(11)

C	-3.609876	-1.257980	-1.474855
C	-4.258151	-0.653475	-0.383722
C	-4.394952	0.755616	-0.267871
C	-3.138735	-0.404711	-2.552891
C	-3.362265	0.982056	-2.446958
C	-3.960855	1.566728	-1.294742
C	-1.453170	-2.105781	-3.152280
C	-2.012517	-0.840066	-3.367967
C	-1.140344	0.116369	-3.934523
C	-1.327570	1.505152	-3.674802
C	-2.401640	1.933364	-2.942495
C	0.260611	-0.109710	-4.031339
C	0.838016	-1.336321	-3.677075
C	-0.077599	-2.364478	-3.350857
C	-3.478373	2.291894	1.381985
C	-3.007000	3.125522	0.309509
C	-4.167859	1.129479	1.104956
C	-3.259085	2.783554	-0.994342
C	-2.247821	2.982485	-1.984237
C	-1.728365	3.643769	0.680112
C	-0.690584	3.813060	-0.256688
C	-0.971669	3.469978	-1.646423
C	1.440613	3.155318	-1.980281
C	0.123465	3.062021	-2.488100
C	-0.065200	2.119880	-3.501241
C	-0.959954	1.107950	3.778777
C	-2.232181	1.152904	3.175125
C	-2.516086	2.310714	2.418894

Supporting Information

C	-1.463130	3.203725	2.004496
C	-0.157602	3.064269	2.476768
C	0.034711	2.088778	3.490809
C	2.356821	1.875003	2.852191
C	1.287944	1.466569	3.632561
C	1.742431	3.634500	-0.683292
C	0.658300	3.804462	0.251039
C	0.926481	3.451733	1.612258
C	2.247129	2.947165	1.921625
C	-2.902150	-0.095352	2.856829
C	-3.892773	-0.052872	1.852711
C	-4.080749	-1.152836	0.956976
C	-2.213460	-1.357581	3.096983
C	-2.561856	-2.467783	2.299420
C	-3.429374	-2.322726	1.178400
C	-0.300498	-0.122831	4.031100
C	-0.885244	-1.354937	3.671502
C	0.018738	-2.391918	3.353129
C	-0.344118	-3.424688	2.454738
C	-1.612821	-3.463475	1.934079
C	1.417041	-2.138573	3.149247
C	1.970714	-0.873737	3.351867
C	1.104164	0.094154	3.916541
C	-1.931322	-2.961015	-2.092807
C	-2.960792	-2.540678	-1.236079
C	-2.911984	-3.072140	0.071001
C	-0.855628	-3.755885	-1.640449
C	-0.704242	-4.112873	-0.280104
C	-1.799273	-3.811579	0.549204
C	0.786908	-3.769800	1.643028
C	0.632646	-4.119670	0.290795
C	1.739485	-3.831126	-0.544576
C	1.542482	-3.460438	-1.929036
C	0.281606	-3.411572	-2.441796
C	1.881797	-2.981658	2.098862
C	2.907067	-2.565535	1.232407
C	2.842625	-3.096112	-0.077550
C	4.039298	1.604208	1.300878
C	3.345497	0.966434	2.394282
C	3.091942	-0.455016	2.520782
C	4.484290	0.755610	0.242594
C	4.227672	-0.642967	0.363636
C	3.552673	-1.290742	1.474682
C	3.544008	2.377633	-1.424201
C	3.083527	3.222892	-0.361833
C	3.349703	2.851821	1.009233
C	4.252824	1.146172	-1.139364
C	0.939197	1.124196	-3.787637
C	2.193918	1.149678	-3.202497
C	2.499325	2.299481	-2.399115

Supporting Information

C	3.342797	-2.319946	-1.188015
C	2.512721	-2.474346	-2.303143
C	2.168427	-1.345371	-3.103605
C	3.990810	-1.131896	-0.950056
C	3.846483	-0.032230	-1.845522
C	2.849547	-0.106586	-2.872608
Th	2.032412	1.046717	0.019964

Th@C₈₄-C₁(12)

C	-3.641322	0.156807	2.352610
C	-4.091940	-0.616283	1.229997
C	-4.386064	0.135515	0.044850
C	-3.349921	1.562496	2.249942
C	-3.491769	2.275654	1.011918
C	-4.091923	1.540651	-0.057056
C	-3.644995	-2.013475	1.095860
C	-3.532268	-2.576297	-0.216440
C	-2.698252	-0.403440	3.306817
C	-2.250796	-1.706870	3.159694
C	-2.753143	-2.547821	2.091545
C	-1.783720	0.627957	3.750706
C	-0.858739	-2.029672	3.413224
C	0.101373	-1.017271	3.730357
C	-0.388244	0.362770	3.906464
C	-1.350747	2.882472	2.848476
C	-2.250803	1.860405	3.156675
C	0.043065	2.708847	3.144401
C	0.525314	1.471993	3.651040
C	1.895559	1.173032	3.359838
C	-2.227357	3.619939	-0.682765
C	-2.526553	3.345566	0.688026
C	-1.479847	3.639284	1.618625
C	-1.703343	-3.461384	1.753305
C	-1.543891	-3.956511	0.418904
C	-2.490392	-3.504927	-0.558362
C	-0.215921	-4.277312	-0.014190
C	-0.533332	-3.148379	2.581154
C	0.789124	-3.361468	2.106611
C	0.921623	-4.048776	0.844460
C	3.070915	-2.930112	0.445115
C	2.030769	-3.752543	-0.007813
C	2.427171	-0.159337	3.336539
C	1.489247	-1.280695	3.358578
C	1.836350	-2.442627	2.559613
C	3.074161	-2.367935	1.774258
C	0.195841	-4.043015	-1.382818
C	-0.713093	-3.452505	-2.324469
C	-2.067091	-3.242172	-1.930895
C	-0.163752	-2.539084	-3.283927
C	1.243734	-2.170892	-3.254783

Supporting Information

C	2.122318	-2.663938	-2.246180
C	1.590475	-3.679233	-1.375122
C	-0.912847	-1.405687	-3.749493
C	-2.234605	-1.121804	-3.271963
C	-2.828443	-2.124723	-2.433320
C	-3.768715	-1.762099	-1.397069
C	-4.192586	-0.445492	-1.276524
C	-1.686709	1.358108	-3.441643
C	-2.640550	0.280770	-3.124067
C	-3.679948	0.566477	-2.176232
C	-1.852024	2.623341	-2.795457
C	-2.821336	2.819985	-1.745633
C	-3.718521	1.806327	-1.441582
C	0.022403	-0.346857	-4.043373
C	0.762180	1.927206	-3.662569
C	-0.329286	1.023431	-3.907430
C	3.782696	-2.047499	-0.438672
C	3.214903	-1.791255	-1.771744
C	3.351677	-0.452726	-2.289945
C	2.384330	0.047978	-3.283346
C	1.359458	-0.828967	-3.743638
C	2.080546	1.444505	-3.350351
C	3.591581	1.888948	-1.455560
C	2.661779	2.362084	-2.385997
C	1.706079	3.350970	-2.014131
C	0.561063	3.131019	-2.876523
C	-0.714894	3.454026	-2.445658
C	4.478938	-1.068981	0.392140
C	4.617197	0.267933	-0.137278
C	4.059508	0.527573	-1.459494
C	3.868731	1.224334	2.092078
C	3.698661	-0.124180	2.620590
C	4.029289	-1.274209	1.790324
C	4.330450	1.429570	0.714169
C	0.800045	3.450068	2.137881
C	2.099296	3.069592	1.746374
C	2.721952	2.003873	2.514830
C	-0.909272	4.003062	-1.114451
C	1.543888	3.734655	-0.631582
C	0.190705	4.107665	-0.196058
C	-0.148796	3.986731	1.184915
C	3.603121	2.392850	-0.102559
C	2.507013	3.235525	0.343191
Th	2.253227	-0.001540	0.611069

Th@C₈₄-C₂(13)

C	-3.047803	3.125075	-1.180023
C	-2.774652	3.607031	0.167494
C	-3.886856	1.961167	-1.384259
C	-3.305648	2.882901	1.331740

Supporting Information

C	0.886608	3.896108	1.115926
C	-1.374403	3.980461	0.210716
C	-0.496497	3.807967	1.356296
C	-0.968149	2.976397	2.464328
C	-0.006216	2.168340	3.215110
C	-2.366590	2.573832	2.411417
C	-0.483561	1.000284	3.897616
C	-2.216285	1.063533	-3.155514
C	-1.356544	2.213603	-2.926030
C	-3.431513	0.971497	-2.335362
C	-1.797771	3.188445	-1.937877
C	1.055438	2.962083	-2.494310
C	0.071088	2.159931	-3.248156
C	0.533840	0.983473	-3.912284
C	2.424212	2.538292	-2.468584
C	2.807183	1.253183	-3.016090
C	1.896349	0.507353	-3.738563
C	-0.814330	3.824456	-1.111434
C	1.435672	3.986716	-0.239108
C	0.594385	3.760913	-1.365071
C	-3.838188	-0.323211	-1.847506
C	-0.290422	-0.174028	-4.084523
C	-1.657518	-0.175250	-3.690822
C	-2.212103	-1.449980	-3.303421
C	-3.247507	-1.501524	-2.318597
C	0.551636	-1.357842	-3.914904
C	0.031212	-2.561454	-3.344647
C	-1.375990	-2.603977	-3.078309
C	0.909148	-3.321753	-2.506978
C	2.224271	-2.832252	-2.167174
C	2.722482	-1.598439	-2.671210
C	1.896438	-0.928787	-3.645966
C	-2.490435	-3.260489	0.848971
C	-3.296152	-2.476357	-0.026129
C	-3.035953	-2.619589	-1.432141
C	-1.888738	-3.330837	-1.929691
C	0.397526	-4.053751	-1.368200
C	-0.991950	-4.009166	-1.036813
C	-1.352247	-4.019156	0.358738
C	-3.884223	-1.224342	0.485840
C	-4.286982	-0.193874	-0.486671
C	-4.425696	1.224192	-0.208745
C	-3.569471	-0.768969	1.814430
C	-3.700744	0.666543	2.088939
C	-4.126834	1.681894	1.125095
C	-2.184725	-2.816490	2.180306
C	-2.663869	-1.567275	2.673679
C	-1.837337	-0.897087	3.636930
C	-1.824048	0.542321	3.707390
C	-2.732037	1.291021	2.951334

Supporting Information

C	-0.861979	-3.310582	2.520498
C	1.416462	-2.604508	3.091493
C	0.011123	-2.553759	3.362702
C	-0.500680	-1.346131	3.938610
C	1.410011	-4.038317	-0.333959
C	1.049659	-4.021360	1.055218
C	-0.352417	-4.048659	1.389081
C	1.937110	-3.343858	1.942615
C	3.325812	-1.537404	2.349027
C	2.251967	-1.458975	3.315204
C	1.706579	-0.183223	3.695322
C	0.339784	-0.173007	4.083961
C	3.931388	-0.382611	1.894663
C	2.532027	-3.277396	-0.823139
C	3.361836	-2.505212	0.045813
C	3.096775	-2.646663	1.450905
C	4.075751	1.568081	-1.102985
C	3.744478	0.593696	-2.113277
C	3.637526	-0.804082	-1.828986
C	4.363697	1.133048	0.196177
C	4.343686	-0.271386	0.501297
C	3.957198	-1.261511	-0.462883
C	3.040424	3.000001	1.144379
C	2.772964	3.471463	-0.206172
C	3.265275	2.763253	-1.315032
C	3.831146	1.865382	1.346180
C	2.289378	1.052713	3.151010
C	1.428435	2.224929	2.907108
C	1.846740	3.183677	1.934900
C	3.483674	0.920987	2.370067
Th	-1.933327	1.258282	0.033024

Th@C₈₄-C₅(14)

C	-2.666892	3.423674	1.081223
C	-1.534156	4.141930	0.559151
C	-3.577736	2.730023	0.195906
C	-1.323046	4.178959	-0.876599
C	0.019748	3.949152	-1.329906
C	-0.396428	3.812154	1.374142
C	0.961838	3.638685	0.917139
C	1.175954	3.728841	-0.498265
C	3.267358	2.502290	-0.254658
C	2.318656	3.092336	-1.099731
C	2.250567	2.564604	-2.419504
C	-1.915991	0.692465	3.516923
C	-2.720605	1.407353	2.642787
C	-2.223396	2.693875	2.229170
C	-0.851472	3.013334	2.451372
C	0.010706	2.219408	3.247140
C	-0.590625	1.132104	3.883014

Supporting Information

C	1.520929	-0.032549	3.962058
C	0.168527	-0.025481	4.175668
C	3.083052	2.475733	1.162373
C	1.881744	2.912625	1.750866
C	1.421269	2.214581	2.950225
C	2.170050	1.125851	3.431601
C	-3.603103	0.692733	1.746498
C	-3.970048	1.405738	0.553789
C	-1.911226	-0.733271	3.509762
C	-2.723278	-1.461927	2.627694
C	-3.610661	-0.740434	1.735035
C	-2.223531	-2.731322	2.250859
C	-0.873953	-3.097977	2.497823
C	-0.014939	-2.295926	3.254108
C	-0.610619	-1.178939	3.876800
C	-2.621337	-3.353673	1.025124
C	-3.492386	-2.694884	0.188368
C	-4.014308	-1.419392	0.546753
C	-4.128258	-0.695400	-0.659887
C	-4.102796	0.671555	-0.658323
C	-1.498123	-4.064680	0.498716
C	-3.239831	-2.698173	-1.241525
C	-2.166415	-3.390218	-1.749394
C	-1.286018	-4.108878	-0.867801
C	2.160376	-1.202200	3.418980
C	1.399659	-2.286269	2.937013
C	0.919689	-3.706894	0.901717
C	-0.393690	-3.853641	1.369948
C	-2.206118	3.453551	-1.758269
C	-3.328668	2.730909	-1.242476
C	-3.537689	1.408359	-1.733062
C	-3.551307	-1.418548	-1.755975
C	-1.584241	-1.469900	-3.226400
C	-2.717143	-0.742670	-2.681467
C	-2.707973	0.699394	-2.689350
C	0.804493	-1.408370	-3.808345
C	-0.446767	-0.744542	-3.755786
C	-0.442781	0.698333	-3.743946
C	-1.580373	1.411175	-3.205637
C	-1.388405	2.764877	-2.737740
C	-1.381428	-2.795435	-2.778800
C	-0.063012	3.237941	-2.558327
C	1.015986	2.589539	-3.116312
C	0.815977	1.360505	-3.779825
C	2.905627	-1.441749	-2.774060
C	2.034185	-0.712047	-3.657452
C	2.053105	0.654874	-3.655750
C	4.003439	-1.450513	-0.656260
C	3.749484	-0.767626	-1.864307
C	-0.060348	-3.331396	-2.635695

Supporting Information

C	3.252955	-2.593973	-0.272525
C	2.305242	-3.174793	-1.120210
C	2.237367	-2.635517	-2.424003
C	0.993694	-2.652550	-3.141955
C	3.342618	-0.762739	2.764930
C	3.800072	-1.450821	1.656685
C	3.060802	-2.557449	1.157169
C	1.860451	-2.980095	1.742049
C	1.144723	-3.814381	-0.531368
C	0.032467	-4.016070	-1.369819
C	4.344900	0.635749	0.534718
C	3.799725	1.351324	1.659120
C	3.349663	0.669131	2.763066
C	4.348723	-0.742056	0.542211
C	2.931542	1.371927	-2.783904
C	3.758681	0.689517	-1.864058
C	4.029587	1.357674	-0.653892
Th	-1.276513	1.829587	-0.193123

Th@C₈₄-C₅(15)

C	-3.495012	0.287930	-2.345319
C	-4.188465	-0.186564	-1.167786
C	-1.176611	1.020078	-3.859432
C	-1.571668	-0.292576	-3.803236
C	-2.734507	-0.662563	-3.068428
C	0.198777	1.339724	-3.891838
C	-0.600482	-1.326785	-3.718323
C	0.778619	-1.040024	-3.608609
C	1.192460	0.341262	-3.714912
C	3.261097	-0.211820	-2.534779
C	2.435841	0.761456	-3.109334
C	2.573490	2.071674	-2.584065
C	-2.517420	-2.004795	-2.628868
C	-3.078694	-2.448187	-1.423172
C	-3.887494	-1.511469	-0.702591
C	-2.385857	-3.428406	-0.703287
C	-1.209366	-2.410397	-3.027301
C	-0.452549	-3.302338	-2.247740
C	-1.111966	-3.898446	-1.146898
C	0.988419	-4.193150	0.013955
C	-0.380345	-4.256839	0.013997
C	2.879516	-1.599339	-2.502391
C	1.601556	-2.011527	-2.917209
C	0.988893	-3.146874	-2.232139
C	1.682285	-3.726752	-1.147495
C	-2.387302	-3.424306	0.724857
C	-3.080376	-2.439765	1.437411
C	-3.890860	-1.507182	0.712448
C	-2.517725	-1.985772	2.638736
C	-1.210271	-2.389177	3.041374

Supporting Information

C	-0.453051	-3.287425	2.268259
C	-1.112206	-3.890714	1.171916
C	-2.735728	-0.640603	3.067777
C	-3.504169	0.305916	2.344209
C	-4.199089	-0.179441	1.170372
C	-4.475573	0.629271	-0.002756
C	-3.979729	1.987782	-0.006824
C	-1.572556	-0.267004	3.800978
C	-1.177395	1.045544	3.849902
C	-1.910109	2.028443	3.106445
C	-3.042508	1.685158	2.350491
C	-3.256311	2.458819	1.151676
C	1.681916	-3.719689	1.171711
C	0.988297	-3.132311	2.252311
C	0.778089	-1.015969	3.614555
C	-0.602149	-1.302093	3.725374
C	-1.908153	2.008302	-3.122741
C	-3.034743	1.666263	-2.360040
C	-3.249319	2.444868	-1.165751
C	-2.186291	3.292338	-0.711891
C	-1.002861	3.592855	-1.451636
C	-0.938963	2.994229	-2.713188
C	1.466328	2.988965	-2.615537
C	0.318992	2.619607	-3.265611
C	1.426892	3.733322	1.381762
C	0.198285	3.953322	0.709990
C	0.198897	3.947962	-0.735470
C	1.427266	3.724553	-1.405484
C	-2.188455	3.298899	0.691574
C	-0.939849	3.011934	2.692666
C	-1.003528	3.604090	1.428254
C	3.316362	2.342222	1.398335
C	2.612902	3.365283	0.671724
C	2.613149	3.361338	-0.693009
C	4.076463	0.079831	1.401006
C	4.008980	1.309494	0.723987
C	0.317703	2.640504	3.247903
C	3.260640	-0.195881	2.535605
C	2.435315	0.781383	3.104168
C	2.572928	2.088163	2.570360
C	1.465752	3.006116	2.596077
C	2.943461	-3.222330	0.725011
C	3.536091	-2.183889	1.408634
C	2.879238	-1.582946	2.512531
C	1.600889	-1.992160	2.929946
C	1.191832	0.365137	3.712145
C	0.197388	1.365563	3.882588
C	4.236961	-1.160345	-0.683559
C	3.536853	-2.193114	-1.395319
C	2.943653	-3.227264	-0.704642

Supporting Information

C	4.236204	-1.155545	0.689913
C	3.315966	2.332841	-1.412892
C	4.008988	1.304854	-0.732204
C	4.076402	0.070902	-1.402060
Th	-2.100326	0.495578	0.022832

Th@C₈₄-C_s(16)

C	4.187612	-1.445780	-0.680252
C	3.925635	-0.724093	-1.894707
C	4.404812	-0.743791	0.489055
C	3.928790	0.646930	-1.896116
C	2.931842	1.346672	-2.627984
C	1.539449	-3.328300	-2.114047
C	3.365515	-2.604212	-0.666344
C	2.722106	-2.661842	-1.955372
C	0.523634	2.683878	-2.873248
C	0.618552	1.367831	-3.449968
C	1.866433	0.674197	-3.299265
C	1.874462	-0.776133	-3.313906
C	2.930456	-1.432026	-2.644113
C	0.533623	-2.804309	-2.969725
C	0.618188	-1.499207	-3.497549
C	0.929721	-3.984948	-0.996369
C	1.463496	-3.807146	0.301699
C	2.698767	-3.048924	0.486924
C	2.904805	-2.294676	1.720729
C	3.775383	-1.191915	1.690176
C	0.514874	-3.851439	1.340905
C	-1.867652	-2.683416	-2.711977
C	-0.694879	-3.350776	-2.489872
C	-0.467826	-4.035778	-1.246313
C	-1.413423	-3.961121	-0.210197
C	-0.876918	-3.964544	1.096555
C	-1.844134	-1.434419	-3.385952
C	-1.830884	1.340758	-3.352091
C	-0.624283	-0.779105	-3.703937
C	-0.615926	0.666018	-3.674373
C	0.709910	-3.088552	2.548961
C	1.853196	-2.298406	2.735560
C	1.673213	-1.162819	3.557007
C	2.481861	-0.005722	3.373791
C	3.511577	-0.009407	2.472603
C	-2.734033	-2.640458	1.959665
C	-1.541562	-3.278002	2.163158
C	-0.567427	-2.699950	3.036479
C	-0.789880	-1.442801	3.641445
C	0.376338	-0.714547	3.947517
C	-2.900166	-2.670408	-1.700576
C	-2.679408	-3.269685	-0.448553
C	-3.335488	-2.647108	0.639555

Supporting Information

C	4.198664	1.379846	-0.676643
C	4.428361	0.685801	0.486672
C	3.796412	1.151994	1.687397
C	1.680962	1.156713	3.528394
C	0.725277	3.059919	2.449466
C	1.881085	2.263124	2.691122
C	2.939464	2.266807	1.705751
C	2.722014	3.039724	0.470725
C	3.430375	2.568309	-0.684217
C	-3.018668	-1.402168	2.609328
C	-2.031993	-0.731590	3.383621
C	-2.022321	0.707513	3.359106
C	-0.775463	1.408273	3.588120
C	0.374859	0.710318	3.936748
C	-0.549370	2.647118	2.918492
C	0.563731	3.955991	1.345980
C	1.569021	3.900292	0.305633
C	0.970843	4.078970	-1.031682
C	1.532655	3.240720	-2.058071
C	2.732038	2.568166	-1.927108
C	-2.738399	2.616699	1.922539
C	-1.512915	3.258324	2.085557
C	-0.879504	4.080763	1.096658
C	-1.489279	4.091145	-0.246930
C	-0.464250	4.148639	-1.298768
C	-3.881595	-0.699546	1.738178
C	-3.889648	0.673272	1.714862
C	-2.992706	1.384694	2.569852
C	-3.609175	-1.453855	-1.844042
C	-4.151300	-0.760366	-0.735179
C	-4.045850	-1.441486	0.499807
C	-3.620969	1.374722	-1.844504
C	-2.987438	0.642621	-2.903252
C	-2.988967	-0.727738	-2.918541
C	-4.061087	1.392458	0.490079
C	-4.163199	0.694487	-0.743661
C	-0.685644	3.287697	-2.449104
C	-3.343518	2.606201	0.623653
C	-2.671305	3.256766	-0.464565
C	-2.919044	2.610364	-1.718124
C	-1.862432	2.587687	-2.674329
Th	-0.125085	2.096099	-0.093995

Th@C₈₄-C_{2v}(17)

C	-4.007895	-1.419363	-1.413528
C	-3.532844	-2.583030	-0.685716
C	-4.428113	-0.325938	-0.735616
C	-3.540631	-2.593785	0.661593
C	-2.428141	-3.153917	1.372268
C	-1.152161	-2.357144	-3.272998

Supporting Information

C	-3.194221	-1.265087	-2.573058
C	-2.337436	-2.427250	-2.632437
C	-0.005260	-3.054126	2.724987
C	-0.004964	-3.607108	1.450874
C	-1.288346	-3.638268	0.721796
C	-1.286647	-3.639428	-0.745491
C	-2.423412	-3.145943	-1.398060
C	-0.011249	-3.043746	-2.748765
C	-0.009147	-3.607110	-1.472021
C	-0.741644	-1.149345	-3.921318
C	-1.476696	0.024286	-3.745472
C	-2.764280	-0.015964	-3.017483
C	-3.216627	1.170825	-2.280524
C	-4.058281	0.978172	-1.181603
C	-0.745496	1.229547	-3.759418
C	2.311835	-2.404547	-2.632888
C	1.123623	-2.365432	-3.283728
C	0.692317	-1.146811	-3.897202
C	1.437963	0.025874	-3.755135
C	0.679788	1.227496	-3.748957
C	2.411311	-3.139327	-1.391216
C	2.414424	-3.165312	1.375406
C	1.269144	-3.642857	-0.747761
C	1.275666	-3.643334	0.717113
C	-1.186385	2.377867	-3.040811
C	-2.381651	2.388155	-2.280941
C	-2.408612	3.244686	-1.171393
C	-3.151485	2.895117	-0.002035
C	-3.965874	1.812208	-0.003396
C	-0.037090	3.094346	-2.624799
C	1.179001	3.935036	-0.694849
C	-0.053330	3.864459	-1.441038
C	-1.243816	3.947465	-0.733530
C	3.177300	-1.274379	-2.600671
C	2.705924	-0.016467	-3.024903
C	3.136038	1.173853	-2.300462
C	2.293621	2.328691	-2.286944
C	1.123675	2.378301	-3.067540
C	2.307207	3.192772	-1.132343
C	-3.999774	-1.420409	1.383107
C	-4.433172	-0.330776	0.714574
C	-4.042024	0.977495	1.155565
C	-2.409822	3.245578	1.161544
C	-1.131036	2.371050	2.983757
C	-2.363935	2.374475	2.239593
C	-3.194742	1.166823	2.256733
C	-2.742914	-0.030293	2.980338
C	-3.196322	-1.279392	2.559193
C	1.240179	4.075716	0.739971
C	-0.025157	4.027627	1.464065

Supporting Information

C	-1.205880	3.948383	0.721499
C	0.026083	3.184060	2.670813
C	-0.693707	1.208795	3.618684
C	-1.463918	-0.000615	3.682882
C	-0.723305	-1.149980	3.855824
C	-1.148175	-2.376683	3.259329
C	-2.331995	-2.423444	2.607715
C	0.723335	1.226885	3.665356
C	4.081050	0.949201	1.177597
C	3.208986	1.178372	2.276628
C	2.758358	-0.038577	2.992724
C	1.470157	-0.001880	3.687605
C	0.729826	-1.152491	3.882670
C	3.934031	1.791762	-0.028414
C	3.086669	2.894743	0.007429
C	2.449307	3.374469	1.194038
C	2.477377	2.436134	2.379159
C	1.196330	2.451336	3.105112
C	3.953500	-1.409189	-1.398968
C	4.398200	-0.320174	-0.718657
C	4.002039	0.992994	-1.158518
C	4.038471	-1.480468	1.419662
C	3.529463	-2.587280	0.673711
C	3.522642	-2.594585	-0.687381
C	4.397077	-0.328301	0.723132
C	1.140686	-2.365955	3.248390
C	3.190909	-1.292293	2.531080
C	2.322051	-2.443997	2.606890
Th	0.772047	1.686747	0.787586

Th@C₈₄-C_{2v}(18)

C	4.138737	1.420011	0.689291
C	3.374934	2.377702	1.405331
C	4.136902	1.423093	-0.704259
C	2.630196	3.317418	0.712115
C	1.380400	3.810676	1.182222
C	2.645503	-0.534571	3.242427
C	4.047360	0.181893	1.383101
C	3.325381	0.455325	2.604631
C	0.686147	-1.481236	3.889265
C	1.385246	-0.246037	3.853124
C	-0.680725	-1.482487	3.891060
C	-1.390953	3.806719	1.185566
C	-0.723800	3.114508	2.298130
C	0.717098	3.116427	2.296578
C	1.448528	2.041604	2.939300
C	2.793217	1.769690	2.557204
C	-1.451848	2.038738	2.943111
C	-0.722526	0.980992	3.626320
C	0.722808	0.982403	3.624361

Supporting Information

C	-1.382129	-0.248638	3.856904
C	2.631288	-1.850016	2.709683
C	3.195126	-2.107293	1.434073
C	3.888487	-1.046492	0.718580
C	3.886553	-1.043256	-0.743762
C	4.043693	0.188036	-1.403257
C	2.587446	-3.138031	0.705774
C	0.732775	-3.385644	2.325671
C	1.409457	-3.788589	1.151268
C	1.412813	-2.459764	3.130141
C	2.585554	-3.134856	-0.736759
C	3.191309	-2.100899	-1.462105
C	2.624148	-1.838037	-2.735086
C	2.636969	-0.520216	-3.262047
C	3.318491	0.466833	-2.621664
C	-0.686199	-4.194181	-0.013524
C	0.686477	-4.192857	-0.015331
C	1.406387	-3.783439	-1.182024
C	0.726655	-3.375326	-2.352856
C	1.404577	-2.445915	-3.155015
C	-1.407592	-2.462451	3.133812
C	-0.727903	-3.387028	2.327574
C	-1.406887	-3.791232	1.154931
C	2.628338	3.320584	-0.714793
C	3.371289	2.383959	-1.414075
C	2.786473	1.780994	-2.567041
C	1.375114	-0.229015	-3.868165
C	-0.732024	0.996996	-3.630378
C	0.713294	0.998388	-3.632205
C	1.440816	2.054595	-2.944419
C	-2.803723	1.775770	-2.559572
C	-1.459535	2.051753	-2.940637
C	-0.729802	3.124869	-2.293016
C	0.711085	3.126766	-2.295225
C	1.377359	3.816035	-1.179458
C	-0.690931	-1.465307	-3.906129
C	0.675914	-1.464060	-3.907905
C	-1.392263	-0.231605	-3.864675
C	-1.409929	-3.786078	-1.178310
C	-0.734023	-3.376718	-2.350946
C	-1.415822	-2.448594	-3.151319
C	0.698679	4.307593	0.003403
C	-0.713123	4.304945	0.005263
C	-1.394103	3.812087	-1.175555
C	-4.148565	1.415163	-0.693315
C	-3.386475	2.377572	-1.405299
C	-2.643222	3.315148	-0.707850
C	-4.146766	1.412061	0.700032
C	-2.651902	-0.525150	-3.255030
C	-4.055093	0.180352	-1.392634

Supporting Information

C	-3.333603	0.460539	-2.612914
C	-2.589216	-3.139828	-0.730016
C	-4.051492	0.174203	1.393639
C	-3.892252	-1.053938	0.728722
C	-3.894146	-1.050677	-0.733551
C	-3.198765	-2.107034	-1.453768
C	-2.635369	-1.843042	-2.728179
C	-3.326804	0.449002	2.613290
C	-2.643410	-0.539492	3.249224
C	-2.628257	-1.855074	2.716550
C	-3.195004	-2.113448	1.442455
C	-2.587336	-3.143022	0.712565
C	-2.641347	3.311960	0.718970
C	-3.382723	2.371303	1.414255
C	-2.797058	1.764477	2.564368
Th	-0.001380	2.030393	-0.001215

Th@C₈₄-D_{3d}(19)

C	2.582089	0.088858	-3.147204
C	3.443405	-0.798761	-2.462979
C	4.252355	-0.374075	-1.369492
C	2.577813	1.476678	-2.739350
C	3.438912	1.878063	-1.680469
C	4.262641	0.947235	-0.988439
C	0.286071	1.725441	-3.612209
C	1.379618	2.255515	-2.932180
C	1.049261	3.266207	-1.978949
C	1.869559	3.551928	-0.869879
C	3.061361	2.858318	-0.722479
C	-0.276509	3.611636	-1.611638
C	-1.383806	2.964868	-2.232226
C	-1.061047	2.115522	-3.303979
C	4.269306	-1.071597	0.966423
C	4.293272	0.308125	1.368647
C	4.263044	-1.412729	-0.367507
C	4.271453	1.300600	0.412678
C	3.491154	2.467526	0.588260
C	3.462288	0.457139	2.511874
C	2.605219	1.568837	2.689603
C	2.594928	2.645665	1.689464
C	0.303627	3.387785	2.408983
C	1.472065	3.567258	1.566865
C	1.092742	4.061365	0.221014
C	2.567728	-3.176661	0.035725
C	2.572666	-2.815015	1.449159
C	3.433270	-2.472068	-0.821035
C	3.442469	-1.796697	1.873412
C	3.052199	-0.858661	2.893041
C	1.881822	-1.052140	3.585034
C	1.060803	-2.180720	3.315180

Supporting Information

C	1.369043	-3.049631	2.245907
C	0.268716	-3.692303	1.659357
C	1.067732	0.061066	3.920200
C	0.294383	2.227948	3.267993
C	1.397074	1.345019	3.454468
C	3.041372	-2.138516	-2.170353
C	0.265816	-4.042261	0.267684
C	1.366800	-3.757497	-0.553199
C	1.052319	-3.499233	-1.910120
C	1.873052	-2.640561	-2.687237
C	-1.892430	-3.648038	0.904915
C	-1.075335	-3.975406	-0.208846
C	-1.388978	-3.481241	-1.498777
C	-0.288286	-3.298700	-2.348722
C	-3.056923	-2.942029	0.729923
C	-0.282728	-1.803161	3.613750
C	-1.386644	-2.365383	2.945899
C	-1.073625	-3.405218	2.045568
C	0.278266	0.360288	-4.023078
C	1.378020	-0.475328	-3.751340
C	1.057502	-1.831279	-3.529910
C	-0.287237	-2.270738	-3.349593
C	-1.382851	-1.409611	-3.510246
C	-1.068071	-0.110316	-3.964930
C	-3.052588	0.805175	-2.908667
C	-1.882165	0.996642	-3.601232
C	-3.448306	-2.515955	-0.593342
C	-2.585487	-2.670800	-1.693257
C	-2.585750	-1.620758	-2.706391
C	-3.449448	-0.526733	-2.532293
C	-4.257049	-1.012809	0.976278
C	-4.271250	-1.371397	-0.421825
C	-4.272315	-0.380343	-1.377664
C	-4.258612	0.311575	1.344733
C	-2.574172	-0.165560	3.110969
C	-2.586908	-1.561003	2.729965
C	-3.451211	-1.952420	1.682525
C	-3.431488	0.736179	2.421476
C	-1.851061	2.577829	2.607463
C	-1.034519	1.748449	3.401515
C	-1.372198	0.389433	3.682771
C	-0.282329	-0.425259	3.980385
C	-3.046511	2.071625	2.119688
C	-0.280024	4.149065	-0.271767
C	-1.449085	3.866855	0.541136
C	-1.068493	3.579019	1.945142
C	-4.290010	1.005296	-0.996641
C	-3.455821	1.726878	-1.892764
C	-2.591899	2.761359	-1.462016
C	-4.264492	1.348279	0.338341

Supporting Information

C	-3.476464	2.428885	0.800305
C	-2.577142	3.153282	-0.045178
Th	0.008032	1.893895	0.535683

Th@C₈₄-T_d(20)

C	1.946542	0.437832	-3.970511
C	2.283142	-0.950712	-3.703230
C	0.643914	0.791903	-4.323021
C	1.294654	-1.939430	-3.795285
C	1.236278	-2.970843	-2.791202
C	-0.558521	4.130422	0.582697
C	0.420269	3.874921	-0.476689
C	0.052876	1.975633	-3.758426
C	2.679835	1.273000	-3.041198
C	2.082293	2.387797	-2.363813
C	0.708732	2.756157	-2.730083
C	-0.112965	3.496495	-1.780159
C	3.580811	0.388410	-2.341641
C	2.620509	2.770023	-1.047874
C	1.783667	3.519428	-0.102164
C	4.083705	0.745679	-1.112179
C	3.712802	2.006771	-0.515942
C	3.216799	-0.989991	-2.606748
C	3.111922	-1.934718	-1.529142
C	2.076499	-2.970282	-1.625574
C	-1.353237	1.686823	-3.645884
C	-1.571045	3.411617	-1.892095
C	-2.126235	2.373169	-2.719479
C	-2.005511	4.030560	0.470835
C	-2.539024	3.651980	-0.833139
C	-3.610601	-1.274767	1.852975
C	-3.891857	0.057009	1.580867
C	-3.576728	2.614464	-0.929902
C	-2.505316	3.374707	1.688274
C	-3.534806	2.345264	1.592378
C	-4.072757	1.963607	0.278267
C	-3.313805	1.125319	2.353120
C	1.074648	3.411357	2.289444
C	-0.227326	3.721450	1.922196
C	-1.359900	3.079096	2.535130
C	-1.126279	1.846254	3.290434
C	-2.155166	0.817293	3.194676
C	2.123479	3.446186	1.303447
C	3.941537	1.855127	0.906528
C	3.150253	2.572293	1.804226
C	-3.234645	1.747833	-2.047223
C	-4.176003	0.512986	0.245616
C	-3.818280	-0.364247	-0.871406
C	-3.322707	0.286031	-2.078885
C	-2.493265	-0.446817	-3.027995

Supporting Information

C	-1.623848	0.298307	-3.914460
C	-0.390348	-0.242638	-4.419217
C	-2.154311	-1.849853	-2.758194
C	-0.978911	-2.386520	-3.381882
C	-0.064630	-1.573737	-4.157756
C	-3.548708	-2.227335	0.774986
C	-2.654677	-2.506329	-1.539172
C	-3.492622	-1.757941	-0.593600
C	-0.159000	-3.352266	-2.690036
C	-0.626552	-3.965557	-1.550983
C	-1.939280	-3.646538	-1.042480
C	-2.184449	-2.918884	2.567582
C	-2.720329	-3.299679	1.257255
C	-1.919254	-4.007097	0.360469
C	-0.877058	-3.266615	2.908547
C	1.315609	2.386441	3.271530
C	0.240866	1.495656	3.656263
C	0.579235	0.092242	3.925061
C	-0.459532	-0.946594	3.828321
C	-1.833586	-0.579042	3.463120
C	-2.679974	-1.609950	2.899438
C	-0.043356	-2.299434	3.592848
C	2.972589	0.583969	3.267150
C	2.652017	1.918702	3.018182
C	2.281782	-1.617899	3.277193
C	1.950023	-0.305649	3.778532
C	1.311253	-2.588462	3.186709
C	4.277135	0.465894	1.171510
C	3.297534	-1.505989	2.248505
C	3.800773	-0.158805	2.331644
C	-0.558988	-4.371429	0.720879
C	0.273850	-4.233247	-0.446392
C	1.575785	-3.626752	-0.406077
C	-0.046800	-4.007547	1.973209
C	1.299912	-3.503968	2.062312
C	2.112184	-3.245419	0.905557
C	3.151192	-2.206350	1.002371
C	3.650252	-1.552137	-0.212858
C	4.252045	-0.254438	-0.075875
Th	-1.614013	1.586802	0.202588

Th@C₈₄-D₂(21)

C	0.527393	-2.479465	3.176695
C	-0.867227	-2.423097	3.089537
C	-1.476045	-3.323823	2.175309
C	-2.714721	-2.996420	1.540503
C	-3.378252	-1.868924	1.899717
C	-0.741399	0.000635	3.735410
C	-1.532516	-1.178109	3.419427
C	-2.826714	-0.986883	2.895849

Supporting Information

C	-1.331780	1.261686	3.539476
C	-2.614468	1.411109	2.936468
C	-3.330961	0.298009	2.594758
C	0.705303	-0.063109	3.732154
C	1.483800	1.104180	3.392316
C	1.306400	-1.326443	3.546733
C	2.792021	0.927138	2.873149
C	-4.071343	-0.344851	-1.361279
C	-4.003396	-1.435786	-0.459917
C	-4.075379	-1.089471	0.907409
C	-4.074925	0.998374	-0.923978
C	-3.991732	1.343392	0.445682
C	-4.052241	0.256490	1.343183
C	-3.269079	-2.629150	-0.845977
C	-2.676640	-3.420929	0.163217
C	-3.341473	-0.379057	-2.603033
C	-2.605214	-1.474537	-2.933376
C	-2.601217	-2.640864	-2.095207
C	-2.838850	0.925518	-2.897246
C	-1.320721	-1.330355	-3.548352
C	-0.731298	-0.060863	-3.714376
C	-1.529433	1.116492	-3.401801
C	-2.724979	2.935377	-1.548217
C	-3.387064	1.791083	-1.919977
C	-1.493562	3.252521	-2.165359
C	-0.885155	2.351278	-3.048639
C	0.536517	2.417388	-3.079423
C	-2.612488	2.563665	2.090613
C	-3.259441	2.544873	0.838936
C	-2.683221	3.352226	-0.177059
C	-1.357016	-3.275112	-2.278471
C	-0.740178	-4.005252	-1.242104
C	-1.444349	-4.078527	-0.020078
C	0.672625	-4.060031	-1.214521
C	-0.556864	-2.456501	-3.172230
C	0.838190	-2.409193	-3.062980
C	1.450299	-3.314044	-2.144960
C	3.349790	-1.834986	-1.869457
C	2.681672	-2.997214	-1.517949
C	1.284137	1.275904	-3.399982
C	0.699240	-0.004755	-3.663428
C	1.493220	-1.160506	-3.370157
C	2.811352	-0.964329	-2.849376
C	1.387777	-4.087524	0.018641
C	0.697484	-4.005489	1.250885
C	-0.710866	-4.039229	1.232203
C	1.306072	-3.280613	2.299791
C	2.565107	-2.624908	2.107574
C	3.205972	-2.612879	0.856104
C	2.635492	-3.416524	-0.164902

Supporting Information

C	4.057868	-1.071561	-0.891710
C	3.953717	-1.407095	0.467819
C	4.039681	-0.323706	1.376130
C	3.314359	-0.355067	2.597297
C	2.573037	-1.470918	2.947685
C	4.055908	0.301367	-1.332707
C	3.986867	1.416047	-0.453969
C	4.032997	1.037588	0.925522
C	2.657995	2.692871	-2.125376
C	2.575725	1.456166	-2.851980
C	3.307770	0.323535	-2.537514
C	2.733586	3.504620	0.170214
C	3.374719	2.696792	-0.860877
C	-0.694044	3.990096	-1.214889
C	1.428509	4.164136	-0.031423
C	0.705472	4.087877	-1.274687
C	1.352411	3.326559	-2.306491
C	-1.358734	3.209056	2.274777
C	0.660329	3.972410	1.169130
C	-0.764449	3.938304	1.235124
C	-1.455128	4.015436	0.015544
C	3.342561	1.805775	1.888987
C	2.676124	2.962971	1.497514
C	1.419288	3.217134	2.090943
C	0.812973	2.331895	3.044987
C	-0.567458	2.407241	3.170131
Th	1.200257	1.722889	-0.398104

Th@C₈₄-D₂(22)

C	-2.599801	1.782906	2.813684
C	-3.234375	2.147051	1.604482
C	-2.589469	3.218766	0.871082
C	-1.270959	2.310551	3.147394
C	-0.605380	3.317350	2.386913
C	-1.360358	3.881423	1.267634
C	-4.021457	1.142551	0.870827
C	-4.111196	1.251631	-0.556409
C	-2.676962	0.438201	3.319715
C	-3.424100	-0.530865	2.627683
C	-4.121327	-0.177289	1.414892
C	-1.412375	0.088567	3.899441
C	-0.865428	-1.234564	3.750374
C	0.548491	-1.331932	3.843248
C	0.856787	1.157375	3.745816
C	-0.558529	1.258970	3.822455
C	1.399988	-0.157747	3.909005
C	1.594491	2.176179	2.979166
C	1.477265	3.876629	1.118629
C	0.869619	3.263315	2.305428
C	2.913227	1.802434	2.522293

Supporting Information

C	-3.438132	-2.401918	1.259564
C	-4.126146	-1.348707	0.547121
C	-4.024338	-1.235909	-0.873362
C	-4.117713	0.092700	-1.416692
C	-2.717407	-3.373167	0.565368
C	-1.609861	-2.247181	2.982202
C	-2.911658	-1.878226	2.501804
C	-1.484931	-3.873292	1.101696
C	-0.872261	-3.293783	2.264502
C	-2.631804	-3.317953	-0.889482
C	-3.240287	-2.248788	-1.611118
C	-2.575155	-1.863413	-2.823133
C	-2.654803	-0.505783	-3.315613
C	-3.404986	0.454365	-2.626936
C	0.694604	-4.272835	0.019399
C	-0.686845	-4.272823	-0.041732
C	-1.348607	-3.857571	-1.266864
C	-0.588044	-3.329483	-2.360675
C	-1.269197	-2.366524	-3.170796
C	1.274989	-2.377787	3.156755
C	0.594044	-3.337190	2.342673
C	1.355735	-3.859623	1.246092
C	-2.680627	3.276565	-0.560069
C	-3.416604	2.306670	-1.260567
C	-2.912338	1.808192	-2.510159
C	-1.398881	-0.142497	-3.909481
C	0.558306	1.275044	-3.812904
C	-0.856390	1.172076	-3.735908
C	-1.595243	2.187597	-2.963347
C	-0.875409	3.281734	-2.290363
C	-1.489614	3.895453	-1.100914
C	1.491842	-3.867809	-1.121921
C	0.878606	-3.284224	-2.282128
C	1.614576	-2.232999	-2.995037
C	0.868365	-1.218093	-3.758489
C	-0.544509	-1.317718	-3.851534
C	1.413895	0.107213	-3.900664
C	1.268467	2.325635	-3.132305
C	0.599315	3.330079	-2.369097
C	1.353069	3.881629	-1.244832
C	0.720649	4.405477	-0.020084
C	-0.731407	4.414486	0.044184
C	3.425144	-0.514053	-2.629928
C	2.675667	0.456010	-3.316260
C	2.595828	1.799355	-2.801184
C	3.234143	2.159549	-1.592767
C	2.584341	3.222704	-0.853401
C	2.724031	-3.367618	-0.583320
C	3.442089	-2.392643	-1.273136
C	2.915335	-1.863944	-2.512050

Supporting Information

C	2.579782	-1.872847	2.812181
C	3.245866	-2.252155	1.599178
C	2.638269	-3.318421	0.872294
C	4.119563	0.091553	1.416230
C	3.406894	0.447052	2.630330
C	2.657419	-0.516435	3.310876
C	4.127335	-1.338967	-0.554336
C	4.028165	-1.234781	0.866897
C	2.674405	3.272317	0.577602
C	4.122716	-0.165223	-1.415382
C	4.022259	1.153083	-0.864098
C	4.111855	1.253433	0.563063
C	3.412981	2.304451	1.275345
Th	-0.035507	2.106459	-0.007038

Th@C₈₄-D_{2d}(23)

C	-3.413430	-1.437973	-2.045971
C	-3.858982	-0.056792	-1.840923
C	-1.493359	-3.586318	-1.888657
C	-1.491249	-2.735269	-2.992382
C	-2.447180	-1.649750	-3.074175
C	-0.246327	-4.045522	-1.333168
C	-0.241762	-2.317184	-3.574466
C	1.012680	-2.631817	-2.958652
C	1.010242	-3.532613	-1.790586
C	3.167215	-2.535786	-1.037210
C	2.106847	-3.457543	-0.810433
C	1.860386	-3.808287	0.562896
C	-1.802701	-0.567867	-3.809456
C	-2.022198	0.792712	-3.420779
C	-3.078381	1.005152	-2.467650
C	-3.075776	2.140094	-1.592704
C	-2.016555	3.112526	-1.631754
C	-1.791994	3.833571	-0.414863
C	-0.486710	-1.014478	-4.169751
C	-0.942246	1.777252	-3.507460
C	-0.939427	2.942947	-2.608412
C	0.551490	-0.089169	-4.276734
C	0.310164	1.328355	-4.037693
C	1.869350	-0.427363	-3.821323
C	3.169606	-1.654118	-2.180558
C	2.111685	-1.666889	-3.132344
C	-3.854751	1.806277	-0.404374
C	-2.434562	3.399323	0.819597
C	-3.404001	2.353874	0.878360
C	-1.475584	3.593508	1.888289
C	-1.477848	2.742481	2.991990
C	0.561826	4.156924	-1.001810
C	-0.473721	4.291717	-0.077402
C	-0.226004	4.046542	1.333487

Supporting Information

C	0.315656	3.566494	-2.311841
C	-4.405223	0.459537	-0.582553
C	-2.439037	1.661492	3.073082
C	-3.406138	1.454683	2.044448
C	-3.858509	0.075830	1.839378
C	-4.407253	-0.437721	0.580967
C	-0.482359	1.016609	4.169253
C	-1.800379	0.576607	3.808095
C	-2.026468	-0.782893	3.419442
C	-3.083106	-0.989801	2.465891
C	0.550994	0.086288	4.276451
C	-0.230632	2.318400	3.574510
C	1.025672	2.627267	2.959771
C	1.028125	3.528053	1.791605
C	-2.451531	-3.387398	-0.820566
C	-3.415545	-2.337201	-0.879682
C	-3.863223	-1.786977	0.402677
C	-3.086150	-2.124551	1.590998
C	-2.032174	-3.102484	1.630547
C	-1.811205	-3.824831	0.414277
C	0.540698	-4.160077	1.002208
C	-0.495334	-4.289678	0.077428
C	0.302670	-1.330193	4.037758
C	-0.951714	-1.772619	3.506734
C	-0.954517	-2.938334	2.607754
C	0.297273	-3.568067	2.311750
C	2.505410	-0.824934	3.408533
C	1.548629	-1.893278	3.599650
C	1.546228	-3.005042	2.742390
C	3.842690	0.405653	1.802628
C	3.428859	-0.863150	2.322774
C	1.879828	3.799191	-0.561908
C	2.124482	3.447423	0.811627
C	3.180053	2.520369	1.038703
C	3.177652	1.638547	2.182085
C	2.119707	1.656683	3.133695
C	1.870844	0.418197	3.822286
C	1.559152	1.885392	-3.599269
C	1.561637	2.996917	-2.741676
C	3.436730	2.020104	-1.416038
C	2.515781	3.081720	-1.657455
C	3.846640	1.838770	-0.055621
C	4.256283	-0.568356	-0.429410
C	3.840980	-0.424461	-1.801062
C	3.433841	0.846245	-2.321429
C	2.510545	0.812673	-3.407878
C	4.259495	0.547727	0.431308
C	2.500090	-3.094587	1.658809
C	3.426067	-2.037093	1.417497
C	3.836971	-1.857467	0.057331

Supporting Information

Th -2.105927 0.005806 -0.000885

Th@C₈₄-D_{6h}(24)

C	-4.125983	0.788481	-1.213229
C	-4.349554	0.043452	-0.004323
C	-4.128362	0.794728	1.200558
C	-3.610388	2.129776	-1.214728
C	-3.251133	2.853470	-0.010930
C	-3.613603	2.136756	1.196152
C	-4.100552	-1.402072	-0.000217
C	-3.660976	-2.038916	1.212999
C	-3.566780	0.122300	-2.379916
C	-3.347063	-1.245143	-2.388900
C	-3.658191	-2.045121	-1.209023
C	-1.647537	3.136236	-2.329794
C	-2.735591	2.252997	-2.369399
C	-2.615703	0.993806	-3.036772
C	-1.390118	4.084986	1.220567
C	-2.192825	3.887410	-0.012921
C	-1.387543	4.077828	-1.245490
C	-1.900147	-3.027518	-2.389289
C	-2.748120	-3.150797	-1.202974
C	-2.211881	-3.700914	0.007788
C	-2.750399	-3.144638	1.214356
C	-0.607133	-3.521656	-2.380768
C	1.670077	-3.163574	-2.379424
C	0.444778	-2.789070	-3.048636
C	2.748911	-2.296297	-2.386486
C	-0.421866	2.718261	-2.953368
C	-0.213702	1.396941	-3.513474
C	-1.357400	0.495332	-3.549547
C	-1.136307	-0.944377	-3.566858
C	-2.188448	-1.788595	-3.060398
C	1.151601	0.890096	-3.547980
C	1.383430	-0.547925	-3.565175
C	0.237161	-1.468031	-3.561315
C	2.643343	-1.028437	-3.057286
C	-0.065752	-4.175692	-1.198840
C	-0.834326	-4.225315	0.010532
C	-0.068296	-4.169617	1.221131
C	-0.612011	-3.509680	2.398615
C	-1.905094	-3.015449	2.401785
C	2.099816	-3.764360	0.012367
C	1.352001	-3.946511	1.222116
C	1.354400	-3.952607	-1.198047
C	-3.571540	0.134661	2.372002
C	-3.352296	-1.232976	2.388925
C	-2.194731	-1.772762	3.065404
C	0.438543	-2.773710	3.064792
C	1.376035	-0.529535	3.570872

Supporting Information

C	0.229829	-1.449745	3.569683
C	-1.143613	-0.925968	3.569405
C	2.189014	1.766565	3.028679
C	1.144028	0.908525	3.545288
C	-0.220912	1.414956	3.505539
C	-1.364489	0.513835	3.543709
C	-2.621884	1.009534	3.025735
C	2.744066	-2.284208	2.404785
C	1.665203	-3.151602	2.400120
C	2.636991	-1.012614	3.068322
C	3.592473	-2.153577	-1.199084
C	3.249832	-2.842246	0.011198
C	3.589793	-2.147477	1.218386
C	-2.740431	2.265239	2.351079
C	-1.652202	3.148332	2.309183
C	-0.427946	2.733533	2.937214
C	2.789118	3.144467	1.200111
C	1.917150	2.998283	2.354018
C	0.610491	3.505027	2.310983
C	2.791142	3.137304	-1.210687
C	2.225593	3.716066	-0.007511
C	3.573520	-0.143271	2.393007
C	3.693389	2.018856	-1.208248
C	4.133670	1.378068	0.000977
C	3.690789	2.025055	1.205340
C	3.362054	1.225643	2.376168
C	3.367116	1.213309	-2.375429
C	3.578101	-0.155516	-2.384340
C	4.118793	-0.821664	-1.204193
C	4.340681	-0.074009	0.005054
C	4.116579	-0.815360	1.217885
C	0.615398	3.492946	-2.328732
C	1.922053	2.986039	-2.366513
C	2.195334	1.750867	-3.033703
C	0.074734	4.316395	1.221798
C	0.901197	4.376239	-0.010989
C	0.077483	4.309240	-1.244882
Th	-0.342884	2.226340	-0.004813

PBE0/def2-TZVPP/Th-ECP optimized structures of 6 selected Th@C₈₄ non-IPR isomersTh@C₈₄-C_i(51499)

C	-0.9695384	-1.8389356	3.5550806
C	-0.5647385	-0.5621353	4.0472932
C	-1.5410312	0.4081570	3.6773724
C	-2.3078293	-1.6788913	3.0927664
C	-2.6594528	-0.2887772	3.1209789
C	-2.7742743	-2.5008160	2.1081786
C	-1.9117423	-3.4619069	1.5108265
C	-0.0580373	-2.7075551	2.9274016
C	-0.5475869	-3.5398866	1.8392397
C	1.3515618	-2.3444191	2.9840333
C	0.7596658	-0.2255256	4.0803696
C	1.7405036	-1.1426883	3.6038616
C	1.1616195	1.1084066	3.7982079
C	-1.1728464	1.6945544	3.2527047
C	0.2352222	2.0589236	3.3203602
C	-2.0790192	2.3565238	2.3412990
C	-3.4788686	0.2773710	2.1484960
C	-3.2558601	1.6750392	1.8249616
C	-3.6635585	-1.9698865	1.1237791
C	-4.0759013	-0.6279542	1.1594067
C	-2.3619559	-3.5913916	0.1560680
C	-3.4003746	-2.6501669	-0.1017629
C	-1.4813993	-3.9162918	-0.8379945
C	0.3652916	-3.9669679	0.7920901
C	-0.1176914	-4.1724378	-0.5168162
C	2.2191949	-2.8465326	1.9897570
C	1.7307507	-3.6247173	0.9073643
C	3.3192105	-2.0716147	1.5126579
C	2.8307375	-0.3519819	3.1050968
C	2.4922389	1.0177235	3.2827890
C	3.5840549	-0.7660514	1.9887999
C	2.9563753	1.9611812	2.3892927
C	0.7462112	3.0867975	2.4392898
C	2.0965391	3.0193526	1.9890001
C	-1.5597288	3.4507946	1.6153683
C	-0.1641065	3.7476859	1.6085848
C	-2.0538584	3.7539152	0.3200581
C	-3.8382952	2.1506942	0.6212611
C	-3.1538384	3.1171996	-0.1837261
C	-4.4916696	-0.0997405	-0.0782046
C	-4.5257404	1.2920609	-0.2689264
C	-3.4532230	-1.9541275	-1.3309213
C	-4.0919043	-0.7131310	-1.3080364
C	-1.5537686	-3.2599616	-2.1153977
C	-2.4395318	-2.1863258	-2.3333686
C	0.6586874	-3.8053574	-1.6660752
C	-0.2390327	-3.2777954	-2.6410065
C	2.5211038	-3.3297302	-0.2423851

Supporting Information

C	3.5144564	-2.4021799	0.1501444
C	1.9615899	-3.2988333	-1.5438567
C	3.9169579	-1.4132666	-0.7413984
C	4.0642021	0.2394319	1.0554484
C	3.7708570	1.5873163	1.2956955
C	4.2620070	-0.1072066	-0.3201674
C	2.4494128	3.3716099	0.6672943
C	3.4734370	2.4776209	0.1879711
C	0.2081676	4.1566878	0.2863806
C	-0.9615837	4.0456002	-0.5374386
C	1.4818719	3.8910181	-0.2090140
C	-0.8955249	3.4424995	-1.8011213
C	-3.1646256	2.6498690	-1.5407590
C	-4.0647042	1.5634034	-1.5789525
C	-3.7042048	0.3528251	-2.1912735
C	-1.9836087	2.6243519	-2.2920127
C	-1.9783966	-1.0665893	-3.1431970
C	-2.5321112	0.2578661	-2.9620384
C	-1.6856827	1.4372846	-3.0853210
C	0.1718934	-2.2632127	-3.4803693
C	-0.7035355	-1.1656687	-3.7218390
C	2.3980800	-2.2681248	-2.4718375
C	3.4102368	-1.3438214	-2.0598826
C	1.5030058	-1.7941897	-3.4374747
C	4.1206451	0.8034900	-1.4492835
C	3.6726185	2.1531288	-1.1801085
C	3.5596186	0.0112396	-2.5457524
C	1.5935810	3.4656332	-1.5640009
C	0.4116945	3.1923337	-2.2871420
C	2.6685824	2.6731757	-2.0895365
C	-0.3550993	1.2556423	-3.5640138
C	0.1022505	-0.0170514	-3.9146007
C	1.4881511	-0.3846402	-3.7581037
C	2.5137069	0.5166775	-3.4068288
C	0.6871977	2.1679983	-3.2059229
C	2.0883315	1.8626447	-3.1568401
Th	1.7539571	0.6227604	-1.0123205

Th@C₈₄-C₇(51383)

C	1.7177275	-1.1065928	3.5548091
C	2.4635052	0.0886763	3.3494366
C	1.5887941	1.2147085	3.4484057
C	0.4280794	-0.6951903	4.0059176
C	0.3135110	0.7204550	3.8618312
C	-0.6565000	-1.5122908	3.8031005
C	-0.5113202	-2.7390743	3.0980718
C	1.8898304	-2.2360051	2.7303106
C	0.7310120	-3.0867060	2.5144538
C	2.9643229	-2.2013276	1.7429021
C	3.4950648	0.1044146	2.4613970

Supporting Information

C	3.7975202	-1.0674967	1.7024438
C	3.7423755	1.2731740	1.6775226
C	1.7145176	2.3193615	2.6119893
C	2.8551326	2.3601800	1.6962178
C	0.5133522	3.0844798	2.3415868
C	-0.8775666	1.3141956	3.4238189
C	-0.7910589	2.5540026	2.6868990
C	-1.9123101	-0.9364657	3.4958697
C	-2.0248692	0.4432192	3.2823128
C	-1.7476072	-2.9815843	2.4266896
C	-2.6270714	-1.8820229	2.6827743
C	-1.7824394	-3.6468505	1.1856861
C	0.6712251	-3.8609417	1.3377822
C	-0.5626502	-4.1345864	0.6787523
C	2.8334515	-2.9759185	0.5186269
C	1.6927895	-3.7874978	0.3528436
C	3.4541943	-2.5122311	-0.6647285
C	4.4119046	-0.6095989	0.4907850
C	4.3796246	0.8287905	0.4725727
C	4.2253854	-1.3158397	-0.6742999
C	4.1474186	1.4964603	-0.7130375
C	2.7322454	3.1248588	0.4755957
C	3.3198788	2.6492067	-0.7101867
C	0.5901905	4.0501587	1.3145553
C	1.6220759	3.9651041	0.3206637
C	-0.5694880	4.5229228	0.6734075
C	-1.9392482	2.9709908	1.9086409
C	-1.7995300	3.9182616	0.8861226
C	-3.0576155	0.8366897	2.3943137
C	-3.0282358	2.0706254	1.7294343
C	-3.5547442	-1.4617310	1.7262391
C	-3.8457839	-0.0710747	1.6390369
C	-2.7765515	-3.2504261	0.2446801
C	-3.6573553	-2.1822218	0.5148262
C	-2.5061442	-3.2606132	-1.1549988
C	-0.3065512	-4.1847110	-0.7283146
C	1.0888244	-3.9832658	-0.9194285
C	-1.2412477	-3.6840946	-1.6570980
C	2.7794540	-2.5950463	-1.9228767
C	1.5794257	-3.3018612	-2.0576835
C	3.9535046	-0.6164455	-1.9023075
C	3.8916550	0.7579926	-1.9161558
C	3.0161369	-1.3729010	-2.6448401
C	2.5489375	2.6245697	-1.9222377
C	2.8345679	1.4180326	-2.6128004
C	1.0050821	4.1506099	-0.9549822
C	-0.3174397	4.5657429	-0.7345560
C	1.3100419	3.2578673	-2.0159398
C	-2.4027721	3.6555737	-0.4125546
C	-1.3667314	3.9457065	-1.3924783

Supporting Information

C	-3.8364542	1.9667851	0.5447287
C	-4.3444026	0.6040237	0.4608486
C	-3.4005609	2.7034632	-0.6083479
C	-3.9544968	-1.4901670	-0.7154447
C	-3.2124647	-2.1860741	-1.7375047
C	-4.3736575	-0.1218162	-0.8025365
C	-2.6490775	-1.4585630	-2.8097799
C	-0.7476530	-3.0208286	-2.8116705
C	0.6419941	-2.8150795	-2.9972867
C	-1.4278010	-1.8831556	-3.3348972
C	1.9703850	-0.7396529	-3.3516241
C	1.8172931	0.7046521	-3.2710867
C	0.8319879	-1.5341587	-3.5995497
C	-0.4301836	-0.9446511	-3.7752441
C	0.2417770	2.5963686	-2.7337912
C	-1.1141158	2.9893494	-2.4070418
C	0.4987248	1.3069655	-3.3352076
C	-0.6136723	0.4386993	-3.6163441
C	-3.3734781	1.9688612	-1.8400269
C	-3.8673770	0.6025799	-1.9542850
C	-2.9472216	-0.0703936	-2.8458107
C	-2.1725528	2.0770908	-2.6278259
C	-1.9208811	0.8357280	-3.2328283
Th	-2.0560369	0.4355518	-0.3492659

Th@C₈₄-C_s(51365)

C	2.2585055	2.4903267	2.2918400
C	2.3399527	1.2507191	2.9456695
C	3.4299434	0.5242183	2.3559508
C	3.2291557	2.4784450	1.2017353
C	3.8950489	1.2405831	1.2043989
C	2.9165653	3.1271517	0.0000486
C	1.7975513	3.9979343	0.0002722
C	1.0724822	3.2288997	2.2479899
C	0.9866252	4.1878627	1.1713337
C	-0.1506206	2.6290607	2.7743943
C	1.2048076	0.6106315	3.4742070
C	-0.0729932	1.3010763	3.3666911
C	1.2703287	-0.8289770	3.5905428
C	3.4156513	-0.8346995	2.3619067
C	2.3770981	-1.5309388	3.0347857
C	3.8346534	-1.5779126	1.1958191
C	4.2130597	0.5540958	-0.0003801
C	4.1732893	-0.8980102	-0.0005418
C	3.2289378	2.4787524	-1.2018533
C	3.8948281	1.2408931	-1.2049442
C	2.2580774	2.4909167	-2.2917770
C	0.9864019	4.1881926	-1.1705954
C	1.0720663	3.2295037	-2.2475250
C	-0.2743635	4.6527855	0.7179878

Supporting Information

C	-0.2745147	4.6529913	-0.7168742
C	-1.4455443	3.1131006	2.2520693
C	-1.4946316	4.0981821	1.1903278
C	-2.5292052	2.2223019	2.2762040
C	-1.2729704	0.5031433	3.4955536
C	-2.4776280	0.9782780	2.9280394
C	0.0743215	-1.5525875	3.6666824
C	-1.1846961	-0.8891371	3.6448859
C	-0.0850112	-2.8262500	3.0669402
C	2.2062244	-2.7593597	2.3562223
C	3.0956049	-2.7724223	1.1998661
C	0.9651019	-3.4087068	2.3179074
C	2.6839547	-3.3960646	-0.0006734
C	3.8344171	-1.5776278	-1.1969855
C	3.0953746	-2.7721439	-1.2011463
C	3.4295084	0.5247952	-2.3565792
C	2.3394158	1.2514543	-2.9459150
C	3.4151984	-0.8341182	-2.3628207
C	1.2041449	0.6114797	-3.4743487
C	-0.1511608	2.6297978	-2.7738269
C	-0.0736353	1.3019129	-3.3664040
C	-1.4948967	4.0985256	-1.1890983
C	-2.2934038	3.8323272	0.0006791
C	-1.4459936	3.1136974	-2.2511008
C	-3.5016245	2.1137669	1.2058342
C	-3.2715059	2.8004171	0.0006709
C	-3.4310618	0.1121057	2.3279376
C	-4.0080196	0.7999599	1.2143203
C	-2.1356537	-1.7746361	3.0517475
C	-1.4471616	-2.9521791	2.6579463
C	-3.2297155	-1.2783532	2.3074245
C	-1.7728014	-3.6019120	1.4446841
C	0.6232020	-4.1372156	1.1466251
C	1.4645433	-4.1147544	-0.0006035
C	-0.7281316	-4.2173330	0.7131562
C	0.6229806	-4.1369227	-1.1476624
C	-0.7282730	-4.2171622	-0.7139266
C	2.2057645	-2.7587991	-2.3572963
C	2.3765090	-1.5302070	-3.0356371
C	1.2696420	-0.8281087	-3.5909960
C	0.9646500	-3.4081342	-2.3188395
C	0.0736086	-1.5516981	-3.6670287
C	-0.0856038	-2.8254963	-3.0675118
C	-1.2736326	0.5039764	-3.4951630
C	-1.1853891	-0.8882672	-3.6448204
C	-2.5296296	2.2228445	-2.2751520
C	-3.5018307	2.1140493	-1.2046022
C	-2.4781734	0.9789707	-2.9272695
C	-4.2797071	0.1033358	0.0004615
C	-4.0082281	0.8002453	-1.2132967

Supporting Information

C	-3.4314838	0.1126601	-2.3271771
C	-3.6352752	-1.9915206	1.1530759
C	-2.8947713	-3.1167384	0.7118461
C	-4.1159931	-1.2949464	0.0002796
C	-1.7730680	-3.6015595	-1.4450866
C	-1.4476570	-2.9515216	-2.6582699
C	-2.1362305	-1.7739118	-3.0516661
C	-3.2301297	-1.2778056	-2.3070197
C	-2.8949020	-3.1165667	-0.7119294
C	-3.6354793	-1.9912498	-1.1527620
Th	-0.2867951	2.2995878	0.0001455

Th@C₈₄-C_s(51550)

C	1.2888338	-3.8716397	1.3948681
C	2.4931312	-3.5939528	0.6839786
C	3.2180003	-2.5735847	1.4090145
C	1.3690143	-3.1445329	2.6282571
C	2.4911622	-2.2533499	2.5821776
C	0.2235084	-2.7685658	3.2718371
C	-1.0479133	-3.0850931	2.7225325
C	0.0583459	-4.0560482	0.7289150
C	-1.1509983	-3.6804940	1.4466495
C	0.0583440	-4.0560408	-0.7289364
C	2.4931233	-3.5939461	-0.6840009
C	1.2888277	-3.8716336	-1.3948910
C	3.2179922	-2.5735801	-1.4090318
C	3.8921058	-1.5929005	0.7175246
C	3.8921007	-1.5929034	-0.7175500
C	3.8044460	-0.2458615	1.1591188
C	2.3875168	-0.9233639	3.0511789
C	3.0719038	0.1155184	2.3001984
C	0.1569276	-1.5120586	3.9383483
C	1.2106529	-0.5840766	3.8208820
C	-1.9475868	-2.0602544	3.1498165
C	-1.2089673	-1.1001380	3.9032156
C	-3.0396845	-1.6654654	2.3499458
C	-2.3113870	-3.3664915	0.7109200
C	-3.2448213	-2.3856124	1.1530788
C	-1.1509998	-3.6804862	-1.4466704
C	-2.3113903	-3.3664918	-0.7109410
C	-1.0479198	-3.0850860	-2.7225490
C	1.3689997	-3.1445239	-2.6282666
C	2.4911401	-2.2533481	-2.5821866
C	0.2234998	-2.7685568	-3.2718387
C	2.3874922	-0.9233713	-3.0511770
C	3.8044387	-0.2458692	-1.1591313
C	3.8496237	0.5959924	-0.0000078
C	3.0718824	0.1155026	-2.3002070
C	3.3746647	1.9003802	0.0000014
C	2.6394653	1.4929642	2.3717563

Supporting Information

C	2.8923270	2.4243985	1.2800613
C	0.8612847	0.7763683	3.9401824
C	1.6103995	1.7880515	3.2940676
C	-1.5558902	0.2676230	3.8685532
C	-0.5048034	1.1989843	3.9767909
C	-3.4294211	-0.2983856	2.3817934
C	-2.6961827	0.6516052	3.1267786
C	-3.9215466	0.3395293	1.2037010
C	-3.8082224	-1.7630638	-0.0000081
C	-3.2448248	-2.3856127	-1.1531004
C	-4.0969122	-0.3849595	-0.0000143
C	-1.9475940	-2.0602597	-3.1498311
C	-3.0396820	-1.6654641	-2.3499622
C	0.1569102	-1.5120554	-3.9383471
C	1.2106403	-0.5840808	-3.8208784
C	-1.2089683	-1.1001424	-3.9032151
C	0.8612930	0.7763489	-3.9401909
C	2.6394583	1.4929421	-2.3717476
C	2.8923118	2.4243783	-1.2800631
C	1.6104034	1.7880214	-3.2940620
C	2.1497869	3.6543467	-1.2513040
C	2.1497876	3.6543676	1.2513283
C	1.8503171	4.2791990	0.0000015
C	0.7149738	2.8764469	3.0560568
C	-0.5947036	2.4769194	3.3512001
C	0.9655858	3.7908577	2.0509124
C	-2.7064239	1.8802785	2.3878543
C	-3.4514103	1.6775541	1.1960842
C	-1.6594060	2.7995170	2.4382985
C	-3.1093564	2.3505502	-0.0000182
C	-3.9215553	0.3395278	-1.2037318
C	-3.4294218	-0.2983876	-2.3818178
C	-3.4514287	1.6775553	-1.1961113
C	-1.5558803	0.2676048	-3.8685372
C	-0.5047889	1.1989469	-3.9767569
C	-2.6961872	0.6516049	-3.1267937
C	-2.7064428	1.8802705	-2.3878728
C	0.7149836	2.8764040	-3.0559937
C	0.9655815	3.7908078	-2.0508977
C	-0.5946861	2.4768365	-3.3510829
C	-1.6593875	2.7994637	-2.4382571
C	0.4688821	4.6735209	-0.0000050
C	-0.1226662	4.3018524	1.2481507
C	-1.3908358	3.6402389	1.2804445
C	-2.0700683	3.3489783	0.0000134
C	-0.1226627	4.3018227	-1.2481391
C	-1.3908265	3.6402044	-1.2804150
Th	0.5117845	2.2174466	0.0000519

Th@C₈₄-C₁(51483)

Supporting Information

C	-3.9102814	-0.5802340	-1.9480742
C	-4.2241757	-1.2621694	-0.7109988
C	-3.4774920	-2.4696939	-0.6744240
C	-2.9803293	-1.3593285	-2.6748218
C	-2.8350470	-2.5916390	-1.9617349
C	-1.8753778	-0.7751585	-3.3459121
C	-1.7267073	0.6681077	-3.2910045
C	-3.8230123	0.7890670	-1.9705930
C	-2.7375642	1.4084406	-2.6585373
C	-4.0822379	1.5466458	-0.7795168
C	-4.4143251	-0.5401608	0.4431522
C	-4.3442852	0.9023858	0.4163603
C	-3.8377742	-1.0055953	1.6588556
C	-2.8487202	-2.9341040	0.4969545
C	-3.0268803	-2.1540663	1.7171106
C	-1.6636392	-3.7635958	0.3374719
C	-1.6967163	-3.3241311	-2.0834737
C	-1.1376784	-3.9915903	-0.9563730
C	-0.7111309	-1.6060819	-3.5369004
C	-0.6502263	-2.8877605	-2.9507860
C	0.5240726	-0.9748696	-3.7744165
C	-0.4069121	1.2843577	-3.3917980
C	0.6574307	0.4347885	-3.7173219
C	-0.1026694	2.5787333	-2.8041038
C	-2.4420403	2.6325738	-1.9995032
C	-3.2281217	2.6725029	-0.7811121
C	-1.1946573	3.2453026	-2.0985828
C	-2.6592800	3.1337567	0.4133221
C	-3.7322477	1.3400428	1.6279013
C	-3.5109035	0.1727320	2.4197694
C	-2.8127950	2.4102904	1.6413287
C	-2.4874421	0.1420676	3.3162872
C	-2.0048077	-2.2036149	2.7546612
C	-1.7767537	-1.0581141	3.5576817
C	-0.7442680	-3.8443160	1.3984313
C	-0.9121753	-3.0683595	2.5869899
C	0.6484855	-4.0184968	1.1776546
C	0.2591983	-4.0930027	-1.1950031
C	0.5612520	-3.4170727	-2.4300913
C	1.1822725	-4.0889888	-0.1325010
C	1.7593607	-1.5536145	-3.3642589
C	1.7891652	-2.7561620	-2.6136491
C	1.9962108	0.7312861	-3.3269754
C	2.6725903	-0.5023216	-3.0902988
C	1.2941832	2.9366035	-2.4890534
C	2.3151950	1.9165299	-2.6621839
C	1.5590450	3.9500290	-1.4777324
C	-0.8776847	4.1237169	-1.0205250
C	-1.5008719	3.9274342	0.2548581
C	0.4518073	4.5399119	-0.7872859

Supporting Information

C	-0.5026847	4.0579281	1.2656901
C	0.6841364	4.5143744	0.6254430
C	-1.6790648	2.3625425	2.5693542
C	-1.5821908	1.2526954	3.4140298
C	-0.4559051	3.1001238	2.3206578
C	-0.4648176	-0.6832567	3.9612351
C	-0.3394158	0.7425622	3.8429358
C	0.3807637	-2.7601934	3.0936639
C	1.3507723	-3.3397753	2.2186364
C	0.6320163	-1.5265295	3.7282581
C	2.5852598	-2.7090239	1.9725893
C	2.4601153	-3.5253698	-0.3619902
C	2.7685210	-2.8776755	-1.5945856
C	3.1595484	-2.8530115	0.6778519
C	3.6277367	-0.6179277	-2.0551513
C	3.6759309	-1.8219713	-1.3214683
C	3.9250204	-1.8100613	0.0911264
C	3.4156937	1.8245261	-1.7481305
C	3.9947915	0.5822348	-1.3955896
C	2.5349548	3.6908441	-0.4307151
C	1.9584156	3.9324877	0.8822631
C	3.4166051	2.6264870	-0.5765294
C	0.8515601	2.5697418	2.6979888
C	0.8781931	1.3473210	3.4626735
C	2.0638218	2.9336494	1.9216236
C	1.8901727	-0.9124403	3.5248646
C	2.8699669	-1.5066398	2.6820535
C	2.0050693	0.4987549	3.4152003
C	4.1382062	-0.5961863	0.7749267
C	4.2510557	0.5927641	0.0127613
C	3.8203778	1.8409480	0.5281826
C	3.1138491	1.9435687	1.7754532
C	3.6258300	-0.4688390	2.0863743
C	3.0867321	0.7767647	2.5421344
Th	0.5859253	2.1555124	-0.1230526

Th@C₈₄-C₁(51482)

C	-3.5900660	2.3018326	-0.6314703
C	-3.3077846	1.8895785	-1.9724134
C	-2.2155081	2.6744149	-2.4226771
C	-2.6357663	3.2757811	-0.2274046
C	-1.8182997	3.5668792	-1.3674807
C	-2.1112996	3.2654419	1.0761969
C	-2.5871667	2.3159098	2.0497712
C	-4.0758872	1.4166243	0.2966897
C	-3.6398163	1.4608702	1.6448112
C	-4.3176604	0.0448403	-0.0875896
C	-3.4545997	0.5369988	-2.3575163
C	-3.9962013	-0.4103911	-1.3872127
C	-2.5523568	0.0565734	-3.3315337

Supporting Information

C	-1.2455606	2.1388730	-3.2954912
C	-1.4333530	0.8212879	-3.7504235
C	0.0918663	2.5875964	-3.1645433
C	-0.4884506	3.9619851	-1.2269984
C	0.4655740	3.5313255	-2.1802474
C	-0.7813453	3.7530379	1.1982890
C	0.0139962	4.1372337	0.0922908
C	0.0800717	3.3481257	2.2336081
C	-1.6970609	1.8602462	3.1004156
C	-0.3515015	2.3685614	3.1755061
C	-1.9174699	0.5729004	3.6533887
C	-3.7380116	0.1197462	2.1329651
C	-4.1212250	-0.7605176	1.0547857
C	-2.9014151	-0.3154955	3.1133157
C	-3.6013358	-2.0700666	0.9713820
C	-3.6292299	-1.7682572	-1.4768401
C	-3.4439635	-2.5813366	-0.3323088
C	-2.1434958	-1.3119092	-3.3431170
C	-2.6830034	-2.2151890	-2.4717089
C	-0.3172157	-0.0679080	-3.9487077
C	-0.7532625	-1.3857894	-3.6658336
C	1.1861434	1.7072408	-3.3808323
C	0.9996112	0.3293422	-3.6788537
C	1.8254606	3.2941012	-1.8008958
C	2.2512315	2.1459478	-2.5766860
C	1.4022980	4.0424706	0.4503751
C	1.4353952	3.5543801	1.8200812
C	2.3817059	3.6367908	-0.5327985
C	2.4568057	2.6653872	2.2770975
C	0.6843793	1.5716262	3.6871660
C	2.0143907	1.6485477	3.1474622
C	-0.8403455	-0.2481518	4.0566203
C	0.4466981	0.2282551	4.0634275
C	-2.3758878	-1.6554685	3.0801565
C	-2.6959223	-2.5281261	2.0187610
C	-1.0769134	-1.6019586	3.6346461
C	-1.7095634	-3.4684675	1.6920933
C	-2.4021259	-3.5334893	-0.6408616
C	-1.8795251	-3.2520585	-1.9397712
C	-1.5731713	-3.9731220	0.3558281
C	0.0979972	-2.3397856	-3.0917610
C	-0.4921881	-3.3325683	-2.2111857
C	1.9507553	-0.6324819	-3.2052143
C	1.5054758	-1.9986547	-2.9940862
C	3.2136478	1.2521169	-2.1061124
C	3.1253970	-0.1403356	-2.4933694
C	3.4521053	2.7929944	-0.0639837
C	3.4842337	2.3197621	1.3320771
C	3.8487336	1.6491357	-0.8805210
C	3.9139883	0.9365778	1.3025387

Supporting Information

C	4.2783584	0.6092080	-0.0184001
C	2.5113092	0.2870035	3.1208164
C	1.5394832	-0.5841871	3.6342257
C	3.4097540	-0.1215373	2.1386209
C	-0.0143227	-2.4057898	3.1484387
C	-0.3963105	-3.3953501	2.2324954
C	1.3433068	-1.8821644	3.0903914
C	-0.2020170	-4.2111902	0.0777692
C	0.3323700	-3.9300217	-1.1950872
C	0.5295819	-3.8759629	1.2601968
C	2.3080560	-2.8462985	-2.2097996
C	1.7141067	-3.7062641	-1.2355371
C	3.8905419	-1.0576577	-1.7418831
C	4.3619674	-0.6973881	-0.4324628
C	3.5455403	-2.4084386	-1.6936443
C	3.3651789	-1.4868598	1.6851752
C	2.2758649	-2.3574631	2.1178397
C	1.8513748	-3.4241982	1.2171360
C	2.4894144	-3.5810041	-0.0386985
C	4.0234608	-1.7686298	0.4570298
C	3.6509363	-2.8569673	-0.3435051
Th	1.4590380	1.5113483	0.2555878

PBE0/def2-TZVPP/Th-ECP optimized structures of 9 ThC₂@C₈₂ structuresThC₂@C₈₂-C₂(1)

C	3.215351	-1.169479	2.247628
C	4.174845	-0.901217	1.214222
C	4.514515	0.457587	0.833630
C	2.666956	-0.035435	3.009930
C	3.085100	1.287514	2.657335
C	3.958718	1.529402	1.527623
C	0.656626	-1.422859	3.618241
C	1.355470	-0.163843	3.667398
C	0.529331	0.979090	3.855779
C	0.917812	2.250431	3.326668
C	2.164504	2.400765	2.718977
C	-0.931849	0.893031	3.736206
C	-1.624260	-0.342365	3.614611
C	-0.794939	-1.549831	3.698809
C	4.112167	1.609844	-1.315916
C	3.477614	2.701078	-0.592087
C	4.654889	0.516948	-0.616692
C	3.452008	2.689350	0.807130
C	2.297128	3.189801	1.508775
C	2.301025	3.117557	-1.318977
C	1.135377	3.593636	-0.658463
C	1.137767	3.653768	0.810696
C	-1.343104	3.694280	0.775148
C	-0.141938	3.596354	1.521732
C	-0.238133	2.901172	2.770073
C	3.782121	-1.040807	-2.331566
C	3.179311	0.083110	-3.024211
C	4.483486	-0.832507	-1.126042
C	3.334411	1.386467	-2.521458
C	2.213966	2.294944	-2.519736
C	1.893193	-0.325357	-3.537214
C	0.794481	0.568245	-3.596061
C	0.956784	1.931407	-3.067912
C	-1.331306	3.743079	-0.672659
C	-0.127194	3.501279	-1.394025
C	-0.208372	2.676263	-2.610358
C	-1.480695	2.195150	-3.031583
C	3.394057	-2.821915	-0.130315
C	2.697949	-3.055559	-1.384104
C	4.238235	-1.706041	0.012273
C	2.858690	-2.157632	-2.450563
C	1.698563	-1.726632	-3.188140
C	1.396838	-3.592784	-1.089090
C	0.245774	-3.235389	-1.848312
C	0.404697	-2.251316	-2.928778
C	-1.640003	0.853586	-3.573337
C	-0.534042	-0.026564	-3.681408
C	-0.728606	-1.445292	-3.354151

Supporting Information

C	-2.019446	-1.888195	-2.961985
C	1.170484	-2.511480	2.836260
C	2.417938	-2.394644	2.116571
C	2.515776	-3.190001	0.939183
C	1.303443	-3.772634	0.345057
C	0.062230	-3.836194	1.022310
C	0.051723	-3.331860	2.400562
C	-2.367322	-2.806426	2.257204
C	-1.152555	-2.781618	3.008806
C	-2.186045	-2.863531	-1.900615
C	-1.059643	-3.429206	-1.221708
C	-1.166864	-3.743991	0.216668
C	-2.387550	-3.373901	0.909848
C	-4.004179	-1.372994	-1.809509
C	-3.406698	-2.549787	-1.202316
C	-3.473052	-2.740665	0.190383
C	-4.596245	-0.383364	-0.999000
C	-3.612046	1.393189	-2.411097
C	-2.955368	0.373897	-3.210726
C	-3.146604	-0.984582	-2.916239
C	-4.398971	1.022485	-1.304292
C	-3.377097	2.833954	0.029927
C	-2.606651	3.253021	-1.130585
C	-2.690890	2.517616	-2.318903
C	-4.232513	1.729875	-0.037970
C	-1.393376	2.094448	3.088657
C	-2.561916	2.098272	2.274801
C	-2.567986	3.048879	1.201400
C	-4.029085	-1.698395	1.026628
C	-3.253963	-1.646398	2.250409
C	-2.866852	-0.367729	2.814124
C	-4.544479	-0.526448	0.449318
C	-4.246406	0.755186	1.039155
C	-3.356436	0.865971	2.166817
Th	-0.622785	-1.127528	1.101869
C	0.847654	0.263480	-0.144252
C	-0.341544	0.578983	-0.486484

ThC₂@C₈₂-C_S(2)

C	-3.313318	0.728919	-2.661941
C	-3.776219	1.483947	-1.532426
C	-4.427314	0.731895	-0.505922
C	-4.399563	1.172422	0.882619
C	-3.662464	2.315269	1.225674
C	-2.149826	1.161450	-3.421533
C	-1.511083	2.347778	-3.108365
C	-1.971334	3.159109	-1.988438
C	-3.061313	2.720770	-1.171087
C	-2.991810	3.094827	0.207659
C	-1.365925	0.013121	-3.816026

Supporting Information

C	0.067215	0.010657	-3.762058
C	0.738853	-1.258244	-3.471984
C	-3.547803	-0.002299	2.889075
C	-2.737245	1.157839	3.198112
C	-4.371756	0.002468	1.738934
C	-2.813614	2.304959	2.404751
C	-1.621837	3.071916	2.110806
C	-1.435204	0.713698	3.667250
C	-0.252249	1.455424	3.398646
C	-0.344610	2.692096	2.597808
C	1.818001	3.761283	-0.329118
C	0.691951	3.830443	0.574472
C	0.827792	3.182334	1.873986
C	2.088926	2.583525	2.217090
C	-1.771339	3.621935	0.780144
C	-0.817638	3.799816	-1.432230
C	-0.640463	3.949601	-0.016534
C	-3.670674	-2.309834	1.212910
C	-2.821850	-2.309326	2.392114
C	-4.403746	-1.162515	0.876137
C	-2.741508	-1.166984	3.191855
C	-1.437743	-0.730188	3.663444
C	-1.632783	-3.079022	2.094162
C	-0.354142	-2.706824	2.583639
C	-0.257377	-1.474833	3.391207
C	2.196242	1.392263	3.028040
C	0.993247	0.712684	3.466550
C	0.990912	-0.736892	3.463077
C	2.192054	-1.418403	3.021503
C	-1.982396	-3.141252	-2.005818
C	-3.070923	-2.703845	-1.186060
C	-3.002726	-3.085945	0.190567
C	-1.784043	-3.620404	0.760240
C	-0.654278	-3.947345	-0.038173
C	-0.830953	-3.788892	-1.453109
C	1.578167	-3.434930	-1.752169
C	0.306735	-3.423427	-2.277259
C	2.080394	-2.604363	2.203644
C	0.816641	-3.196841	1.857021
C	0.678413	-3.836434	0.553737
C	1.804911	-3.765647	-0.349676
C	-3.781426	-1.462588	-1.540618
C	-4.429909	-0.714060	-0.509927
C	-1.519262	-2.325056	-3.121111
C	-2.153799	-1.134864	-3.427786
C	-3.315861	-0.702731	-2.665941
C	-0.082782	-2.407090	-3.223741
C	4.067966	-1.467278	1.579270
C	3.223932	-2.618212	1.315103
C	3.031982	-3.145640	0.012528

Supporting Information

C	4.615765	-0.728529	0.448264
C	4.071279	1.442949	1.586117
C	3.426722	0.702884	2.680482
C	3.425347	-0.731266	2.677459
C	4.616806	0.709200	0.452108
C	3.509867	2.334390	-1.104988
C	3.042958	3.134972	0.029642
C	3.232276	2.598824	1.328779
C	4.224703	1.151777	-0.895525
C	0.318811	3.435419	-2.258493
C	2.530575	2.425178	-2.159867
C	1.590357	3.439849	-1.733708
C	3.501676	-2.339935	-1.117655
C	2.521663	-2.420914	-2.172554
C	2.096296	-1.265082	-2.917612
C	4.221237	-1.161349	-0.901683
C	3.892773	-0.001819	-1.713260
C	2.790916	0.002947	-2.653223
C	2.101158	1.274997	-2.911031
C	0.743435	1.275666	-3.465415
C	-0.074337	2.425621	-3.210629
Th	1.994736	-0.012782	0.587806
C	-0.156547	0.644921	-0.226197
C	-0.179704	-0.630155	-0.200542

ThC₂@C₈₂-C₂(3)

C	3.817565	0.471461	-2.378328
C	3.134231	1.743744	-2.413198
C	4.451349	0.051655	-1.148846
C	3.189398	2.669531	-1.337900
C	2.066750	3.503638	-1.041611
C	1.872033	1.585589	-3.108323
C	0.724244	2.378927	-2.807752
C	0.828849	3.401347	-1.758297
C	-1.645514	3.401565	-1.586409
C	-0.391965	3.830431	-1.074607
C	-0.359979	4.130858	0.324868
C	3.566625	-2.276099	-1.448209
C	2.885365	-1.844545	-2.673715
C	4.315749	-1.302053	-0.664993
C	2.979813	-0.484813	-3.116788
C	1.773966	0.198660	-3.528804
C	1.573312	-2.477201	-2.708242
C	0.373617	-1.834290	-3.216801
C	0.479051	-0.441397	-3.620640
C	-1.733230	2.477026	-2.699190
C	-0.575034	1.833368	-3.204588
C	-0.687852	0.422160	-3.622921
C	-1.951742	-0.224181	-3.529945
C	1.314261	-3.767639	1.196912

Supporting Information

C	2.517302	-3.211963	0.689910
C	2.656683	-3.166009	-0.755093
C	1.477908	-3.363423	-1.581992
C	0.221387	-3.811201	-1.059825
C	0.202287	-4.134487	0.325676
C	-2.198667	-3.661546	0.420474
C	-1.010328	-3.956061	1.079295
C	-2.062546	-1.611999	-3.133263
C	-0.914659	-2.396320	-2.829097
C	-1.002915	-3.398108	-1.749723
C	-2.222190	-3.488343	-1.019346
C	3.209545	-2.166127	1.470997
C	4.054690	-1.229689	0.776856
C	0.735935	-3.286954	2.435757
C	1.364959	-2.272724	3.156149
C	2.603489	-1.705661	2.681973
C	-1.470264	0.053435	3.726868
C	0.570565	-1.237879	3.767092
C	-0.861515	-1.224852	3.629462
C	-1.534667	-2.280064	2.860062
C	-2.810292	-1.992074	2.179159
C	-0.711650	-3.326140	2.339724
C	-3.153234	-2.766723	1.025948
C	2.598892	-0.304886	3.060453
C	3.256015	0.673581	2.265457
C	4.079129	0.165550	1.191969
C	4.344574	0.947960	0.010437
C	3.781159	2.231280	-0.085796
C	1.407070	2.313724	2.867071
C	2.673637	2.022428	2.168223
C	3.010470	2.793004	1.010971
C	0.582335	3.348843	2.340797
C	0.872293	3.966580	1.069154
C	2.053333	3.691354	0.408160
C	1.350164	-0.025227	3.730823
C	-0.687276	1.268462	3.776336
C	0.735633	1.256138	3.638797
C	-2.733778	1.725846	2.691211
C	-1.486347	2.298698	3.159239
C	-0.866769	3.315742	2.445928
C	-4.191601	1.241128	0.820966
C	-3.353141	2.185489	1.486102
C	-3.951364	-2.216579	-0.056207
C	-4.511006	-0.943917	0.049339
C	-4.236194	-0.147150	1.229935
C	-3.400207	-0.650446	2.281755
C	-2.726510	0.339231	3.060569
C	-3.953607	-0.467891	-2.310567
C	-3.309831	-1.762545	-2.399245
C	-3.355321	-2.644838	-1.316714

Supporting Information

C	-4.564711	-0.063907	-1.106555
C	-3.657087	2.219624	-1.382144
C	-3.007045	1.795886	-2.607394
C	-3.122253	0.472277	-3.042321
C	-4.383034	1.290897	-0.619951
C	-1.447755	3.779783	1.196423
C	-2.661947	3.217011	0.693415
C	-2.788510	3.179999	-0.732035
Th	1.786347	-0.471591	-0.733281
C	-0.068821	0.691294	0.258701
C	-0.399623	-0.540661	0.209243

ThC₂@C₈₂-C₅(4)

C	-4.323033	0.002296	-1.553936
C	-3.700149	1.166321	-2.149310
C	-4.647230	0.004552	-0.180095
C	-3.513408	2.326446	-1.392016
C	-2.338576	3.138232	-1.595432
C	-2.642106	0.721295	-3.040601
C	-1.439502	1.465482	-3.204029
C	-1.294370	2.743386	-2.481817
C	1.167863	2.585769	-2.781589
C	0.047728	3.262447	-2.203776
C	0.313184	4.007298	-1.019857
C	-3.828942	-2.315620	0.042469
C	-3.510952	-2.322883	-1.377435
C	-4.343576	-1.157940	0.631232
C	-3.695216	-1.164951	-2.141326
C	-2.641391	-0.726504	-3.036005
C	-2.336289	-3.136618	-1.579135
C	-1.293226	-2.745451	-2.467111
C	-1.437798	-1.472936	-3.198429
C	1.024873	1.392856	-3.559075
C	-0.261775	0.719654	-3.637449
C	-0.262349	-0.732107	-3.635319
C	1.027584	-1.402857	-3.555846
C	-0.727865	-4.149234	-0.003651
C	-2.821809	-3.110739	0.728685
C	-2.017871	-3.735778	-0.297441
C	0.315870	-4.001850	-0.994046
C	1.169068	-2.592387	-2.762656
C	0.049636	-3.261836	-2.185374
C	-0.179983	-3.931591	1.305675
C	-0.863131	-3.134552	2.273175
C	-2.240745	-2.701464	1.966295
C	-2.763776	-1.460669	2.558882
C	-3.791788	-0.712684	1.897813
C	-1.910393	-0.700932	3.405326
C	1.262553	-3.856370	1.122527
C	2.051923	-3.133051	2.002804

Supporting Information

C	1.413141	-2.381270	3.062756
C	-0.027651	-2.345901	3.189734
C	-0.563906	-1.150984	3.738373
C	2.493727	-2.592478	-2.153290
C	2.661637	-3.125245	-0.815038
C	1.579284	-3.884848	-0.296288
C	-1.910481	0.726960	3.406926
C	-2.763980	1.484033	2.552766
C	-3.790940	0.734600	1.896126
C	-4.340990	1.173077	0.625243
C	-3.828232	2.325970	0.030654
C	-0.858220	3.142619	2.251698
C	-2.239019	2.717631	1.952323
C	-2.820193	3.125375	0.712109
C	-0.173862	3.933538	1.281294
C	-0.724118	4.153791	-0.028979
C	-2.018502	3.742499	-0.316208
C	-0.566944	1.170982	3.734891
C	1.419277	2.383119	3.045066
C	-0.023723	2.353004	3.172894
C	2.227977	-1.229692	3.315488
C	1.647198	0.002788	3.751132
C	0.246439	0.005817	4.014886
C	2.235566	1.230102	3.308133
C	3.201891	2.387497	1.503352
C	2.055858	3.124391	1.983081
C	1.267399	3.850272	1.097430
C	4.179397	1.161204	-0.391110
C	3.513697	2.342331	0.104848
C	3.318581	-1.229774	2.348104
C	4.292193	-0.009247	0.461190
C	3.838868	-0.003776	1.826619
C	3.327320	1.222723	2.351084
C	3.224977	-1.463693	-2.668455
C	4.097896	-0.730708	-1.775591
C	4.173990	-1.178922	-0.379346
C	3.513729	-2.362920	0.115675
C	3.200739	-2.400104	1.516952
C	3.232151	1.447125	-2.687640
C	2.314110	0.705467	-3.553174
C	2.306122	-0.720448	-3.549828
C	4.109842	0.715077	-1.782278
C	1.579372	3.874695	-0.315744
C	2.656720	3.104566	-0.832222
C	2.494010	2.577035	-2.169979
Th	1.645464	0.034287	-1.091555
C	-0.236086	0.628676	0.261229
C	-0.184757	-0.646270	0.292539

ThC₂@C₈₂-C₂(5)

Supporting Information

C	-3.838097	-0.211742	-2.213881
C	-3.040793	0.666067	-3.053655
C	-4.369376	0.261878	-1.009566
C	-2.835715	1.999169	-2.682454
C	-1.552827	2.606951	-2.906137
C	-1.944477	-0.098821	-3.593353
C	-0.645286	0.452953	-3.770364
C	-0.445261	1.873317	-3.427071
C	1.992857	1.461873	-3.199595
C	0.896967	2.350260	-3.068626
C	1.059781	3.398405	-2.103779
C	-2.265158	-3.408002	-1.113526
C	-3.291065	-2.412788	-1.142881
C	-3.271928	-1.541594	-2.281483
C	-2.135383	-1.481130	-3.168286
C	-1.038160	-2.368881	-3.043979
C	-1.190547	-3.411077	-2.071087
C	1.235531	-3.588123	-1.827395
C	-0.025433	-3.965600	-1.415112
C	1.797544	0.076941	-3.614299
C	0.496463	-0.475916	-3.773698
C	0.300187	-1.894255	-3.419763
C	1.413259	-2.624729	-2.906269
C	-3.836072	-1.908548	0.132053
C	-4.351713	-0.574104	0.173827
C	-1.722153	-3.896877	0.144486
C	-2.220319	-3.399727	1.350805
C	-3.288988	-2.424187	1.359518
C	0.920850	-2.400374	3.064639
C	-1.303800	-3.115838	2.423578
C	0.105187	-3.272325	2.253935
C	0.645261	-3.781390	0.988587
C	2.000748	-3.391289	0.550066
C	-0.310538	-4.153145	-0.010262
C	2.292892	-3.407313	-0.850479
C	-3.072509	-1.576739	2.498379
C	-3.428745	-0.195627	2.461836
C	-4.104971	0.289509	1.306451
C	-2.571845	0.720318	3.173550
C	-1.850348	-1.994675	3.184029
C	0.391554	-1.364019	3.949638
C	-1.039916	-1.100568	3.959085
C	-1.444026	0.303883	3.992013
C	-2.299443	2.020075	2.622503
C	-2.892883	2.491558	1.395934
C	-3.891380	1.649887	0.820744
C	-4.115012	1.636434	-0.600441
C	-3.374725	2.493812	-1.421192
C	-0.743125	3.787667	0.973191
C	-2.103331	3.395115	0.551537

Supporting Information

C	-2.410582	3.402508	-0.846044
C	0.202040	4.153217	-0.038229
C	-0.098197	3.957051	-1.438794
C	-1.363521	3.576923	-1.835210
C	-0.996468	2.420240	3.061687
C	1.221290	3.130360	2.391357
C	-0.189538	3.286303	2.235964
C	1.379371	-0.279132	3.980422
C	0.974876	1.125540	3.945325
C	-0.457117	1.388981	3.947675
C	1.776033	2.013844	3.153394
C	3.194669	2.432066	1.310096
C	2.126025	3.407545	1.306969
C	1.615121	3.897734	0.102988
C	4.244791	0.575021	0.124108
C	3.728607	1.909029	0.079841
C	2.498025	-0.700840	3.151377
C	4.010492	-0.281727	1.264661
C	3.346879	0.210420	2.424318
C	2.990655	1.591671	2.456392
C	3.250849	-2.502272	-1.441568
C	4.000140	-1.640096	-0.634097
C	3.791845	-1.644895	0.789425
C	2.799437	-2.482660	1.380329
C	2.219363	-2.003355	2.610057
C	3.705689	0.198174	-2.255676
C	2.899565	-0.684680	-3.081641
C	2.698450	-2.015559	-2.699963
C	4.250008	-0.268143	-1.054241
C	2.144546	3.401140	-1.157785
C	3.170011	2.405639	-1.192113
C	3.138793	1.527633	-2.325239
Th	-0.037944	0.011598	1.739248
C	0.575585	0.014433	-0.555876
C	-0.700525	-0.031380	-0.541913

ThC₂@C₈₂-C₅(6)

C	3.199616	-0.957772	2.549706
C	3.898041	-0.339694	1.465044
C	3.814180	1.095500	1.339224
C	4.052269	-1.105934	0.268455
C	3.462385	-2.401853	0.135650
C	2.648729	-2.974407	1.170696
C	2.613334	-2.261428	2.411893
C	4.049107	-0.455312	-1.050683
C	3.891990	0.960187	-1.170643
C	3.811181	1.733824	0.044880
C	3.188509	1.443401	-2.318649
C	1.999096	-3.300900	-1.629726
C	3.114959	-2.564537	-1.268944

Supporting Information

C	3.457317	-1.350421	-1.996050
C	2.638894	-0.879095	-3.077337
C	2.600443	0.539559	-3.267269
C	0.345234	-3.824279	1.660820
C	1.470759	-3.769271	0.782538
C	1.166799	-3.918478	-0.609832
C	2.337235	2.625913	-2.224444
C	2.208945	3.334016	-0.996518
C	2.994677	2.910756	0.130809
C	0.933684	3.935661	-0.695380
C	0.307911	0.440589	-4.181702
C	1.410824	1.189565	-3.794609
C	1.206970	2.443851	-3.111257
C	-0.107822	2.876288	-2.750364
C	-0.192942	3.666609	-1.551479
C	1.161971	-2.869118	-2.737782
C	1.460912	-1.672959	-3.467880
C	0.332307	-1.011673	-4.042657
C	0.455738	4.165420	0.672458
C	1.229787	3.693529	1.821115
C	2.484111	3.039245	1.496023
C	0.460468	3.064832	2.894405
C	-1.001185	4.004635	0.611604
C	-2.961410	2.723683	1.352110
C	-1.756892	3.405586	1.685650
C	-0.996297	2.917240	2.810400
C	-2.557394	2.956239	-1.111454
C	-1.383066	3.705649	-0.751101
C	-3.414235	2.591321	-0.027712
C	-2.513390	2.140006	-2.333655
C	-1.032678	0.924929	-3.930752
C	-1.281086	2.095432	-3.146642
C	-3.402959	1.021332	-2.389941
C	0.942648	1.841777	3.544524
C	2.218177	1.239805	3.247624
C	2.999090	1.878395	2.223052
C	2.350086	-0.164941	3.433841
C	-0.181238	0.998080	3.858800
C	-0.092837	-0.433649	3.961418
C	1.222678	-0.980944	3.833297
C	0.323908	-3.050697	2.897743
C	1.426608	-2.286059	3.252768
C	-3.409357	1.547730	2.088587
C	-2.548224	0.911175	3.034968
C	-1.374036	1.654663	3.405950
C	-2.501252	-0.555260	3.131268
C	-1.266129	-1.225180	3.586617
C	-1.016824	-2.559006	3.133841
C	-4.238320	0.772770	1.203808
C	-4.223433	-0.623504	1.297589

Supporting Information

C	-3.392400	-1.282233	2.280966
C	-4.230634	-0.813284	-1.170319
C	-4.229224	0.640661	-1.265914
C	-4.241361	1.416211	-0.100931
C	-4.227694	-1.432704	0.085889
C	-1.856721	-0.250154	-3.797629
C	-3.408913	-1.346230	-2.225656
C	-3.015503	-0.210317	-3.049517
C	-0.181350	-3.246230	-2.414435
C	-3.403094	-2.592948	0.302544
C	-2.514524	-3.093352	-0.697170
C	-2.517521	-2.442360	-2.017124
C	-1.309372	-2.504167	-2.860423
C	-1.012860	-1.432906	-3.766909
C	-3.004732	-2.554403	1.703852
C	-1.843202	-3.169889	2.123396
C	-1.001556	-3.864074	1.163494
C	-1.303449	-3.797888	-0.237097
C	-0.178295	-3.893838	-1.101137
Th	0.263133	1.548679	0.755269
C	-0.819311	-0.358499	-0.167244
C	0.432010	-0.598892	-0.255613

ThC₂@C₈₂-C_{C₂v}(7)

C	-0.803996	-4.184014	1.252249
C	-1.210750	-3.414179	2.428975
C	-1.635745	-4.173603	0.083640
C	-2.424657	-2.688233	2.431909
C	-2.433998	-1.359192	3.017310
C	2.303131	-2.666727	2.294781
C	0.633653	-4.031142	1.115221
C	1.098025	-3.338745	2.298018
C	3.556208	-0.739743	2.404810
C	2.442133	-1.423459	3.016676
C	3.565567	0.652077	2.394447
C	-2.398115	1.470352	3.028781
C	-1.239359	0.781387	3.525197
C	-1.255499	-0.688249	3.515209
C	0.001691	-1.439916	3.512185
C	-0.033404	-2.794448	3.011293
C	0.042944	1.490177	3.522563
C	1.305838	0.735085	3.519390
C	1.288596	-0.730049	3.519040
C	2.476845	1.379566	3.005344
C	3.131582	-2.650700	1.107492
C	2.606312	-3.100286	-0.149501
C	1.308243	-3.810562	-0.146597
C	0.464952	-3.801283	-1.343359
C	-0.987458	-3.945322	-1.191395
C	0.921028	-3.089880	-2.487916

Supporting Information

C	3.971474	-1.485842	1.220269
C	4.344770	-0.786886	0.065635
C	3.891937	-1.231957	-1.220935
C	3.035003	-2.377517	-1.353195
C	2.179633	-2.395059	-2.498936
C	0.006165	-2.371679	-3.368826
C	-1.388903	-2.309608	-3.068573
C	-1.876935	-3.130898	-1.998391
C	-2.105246	-1.109541	-3.363437
C	0.694254	-1.229573	-3.886917
C	0.724273	1.228765	-3.897124
C	0.001242	0.020293	-4.110696
C	-1.426859	0.038450	-3.881356
C	3.691933	-0.043788	-2.040024
C	2.739184	-0.030751	-3.097540
C	2.042200	-1.252353	-3.368217
C	2.074779	1.206446	-3.375683
C	-3.167742	-0.645728	-2.477533
C	-3.573863	-1.386921	-1.333116
C	-3.012139	-2.734639	-1.186115
C	-2.901320	-3.416700	0.086860
C	-3.299661	-2.691568	1.258508
C	-3.965296	0.828436	-0.132717
C	-3.976387	-0.651223	-0.133131
C	-3.846232	-1.352693	1.126525
C	-3.812957	1.501052	1.125207
C	-3.430256	0.760971	2.309186
C	-3.451782	-0.618630	2.309485
C	-3.151491	0.791869	-2.485261
C	-2.932541	2.847989	-1.203378
C	-3.536449	1.551091	-1.336354
C	0.067308	2.406568	-3.370495
C	-1.335991	2.405515	-3.087054
C	-2.083105	1.213791	-3.357563
C	-1.794445	3.236227	-2.025897
C	-1.471944	4.161216	0.076923
C	-2.749809	3.454583	0.083945
C	-3.184184	2.792140	1.238680
C	-0.672507	4.172533	1.218119
C	0.994675	3.083235	-2.503634
C	0.556031	3.810347	-1.354046
C	-0.862748	3.995117	-1.217962
C	3.922666	1.134264	-1.230356
C	2.678667	3.040043	-0.159612
C	3.087760	2.296812	-1.360654
C	2.235199	2.341630	-2.506843
C	0.764536	4.030032	1.098474
C	1.409085	3.799126	-0.156323
C	1.199279	3.340061	2.290584
C	2.383035	2.632225	2.287467

Supporting Information

C	3.191959	2.578635	1.092139
C	3.998214	1.380022	1.205988
C	4.362317	0.673210	0.061811
C	-2.325808	2.776830	2.419930
C	-1.104288	3.444014	2.406576
C	0.054230	2.827986	3.011645
C	-0.354257	0.649130	0.060120
C	0.744233	-0.001658	0.087625
Th	-0.974661	-1.634356	0.320432

ThC₂@C₈₂-C_{3v}(8)

C	-0.401876	4.148594	-0.324965
C	-1.543186	3.764947	-1.099327
C	-2.755114	3.353402	-0.392739
C	-1.247968	3.141850	-2.363064
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C	-3.209844	1.603647	-2.216115
C	-3.520213	2.242075	-0.937853
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C	-1.272497	1.257722	-3.761860
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C	-4.067542	-0.567817	-1.281487
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Supporting Information

C	-1.547999	-0.905053	3.773128
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C	-1.239734	2.623901	2.940152
C	-1.551204	3.504667	1.839229
C	-2.770784	3.229995	1.072239
C	-0.403236	4.007799	1.138428
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Th	-1.195659	1.356241	0.248202
C	-0.186172	-0.745808	-0.150863
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ThC₂@C₈₂-C_{3v}(9)

C	3.841080	1.158387	-1.215341
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Supporting Information

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C	3.353596	-0.767237	2.416573
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C	3.043269	1.514658	-2.388707
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C	1.423369	0.113613	-3.705949
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Supporting Information

C	2.791005	-2.037671	-2.395891
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C	-0.485726	-3.465783	-2.400142
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C	-0.485907	-4.159366	0.005736
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C	-2.571284	-2.427021	2.401922
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C	-4.054187	-0.861726	1.205897
C	-3.945944	-1.615858	-0.009262
C	-4.047202	-0.866793	-1.228311
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C	-0.499059	-3.455840	2.408454
C	-1.294115	-2.469042	3.097776
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C	1.652367	-3.675947	1.218490
Th	-0.058953	1.814579	0.011845
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