Clar Goblet and Related Non-Kekulé Benzenoid LPAHs. A Theoretical Study

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Table S40. Optimized Geometry of **6**, RHF/6-31G*, $E_{\text{Tot}}=-1449.6314102$ Hartree

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Table S50. Optimized Geometry of **8**, RB3LYP/6-31G*, $E_{\text{Tot}}=-1459.0368597$ Hartree

Table S51. Optimized Geometry of **8**, RB3LYP/6-311G**, $E_{\text{Tot}}=-1459.3422149$ Hartree

Table S52. Optimized Geometry of C_{2v} -**10**, RB3LYP/6-31G*, $E_{\text{Tot}}=-731.3062756$ Hartree

Table S53. Optimized Geometry of C_{2h} -**11**, RB3LYP/6-31G*, $E_{\text{Tot}}=-1460.2299974$ Hartree

Table S54. Optimized Geometry of D_{2h} -**11**, RB3LYP/6-31G*, $E_{\text{Tot}}=-1460.2299024$ Hartree

Table S1. Semiempirical AM1 and PM3 Enthalpies of Formation ΔH_f° (kJ/mol) of the LPAHs **1**, **4–6**

^a Symm ^b			AM1 calculations				PM3 Calculation			
			C.I.=2 ^c	C.I.=4 ^c	C.I.=6 ^c	C.I.=8 ^c	C.I.=2 ^c	C.I.=4 ^c	C.I.=6 ^c	C.I.=8 ^c
1 pl	<i>D</i> _{2<i>h</i>}	T	839.71	833.80	824.94	809.41	766.46	761.03	752.46	737.82
1 pl	<i>D</i> _{2<i>h</i>}	S	839.68	827.94	818.66	812.26	766.42	755.52	753.00	740.11
4 pl	<i>C</i> _s	T	830.80	815.94	802.78	802.75	758.51	744.49	733.38	732.32
4 pl	<i>C</i> _s	S	847.29	835.00	825.70	824.94	773.34	762.02	752.62	752.03
5 tf	<i>C</i> ₁	T	830.18	821.30	805.84	799.88	764.66	756.24	741.89	735.66
5 tf	<i>C</i> ₁	S	865.02	856.44	849.55	840.27	798.52	790.63	783.84	774.95
6 pl	<i>C</i> _{2<i>v</i>}	S	743.18	732.86	720.43	723.30	669.69	659.91	648.72	651.01

^a - **pl** – planar conformation, **tf** – twisted-folded conformation; ^b - S – singlet, T – triplet; ^c - 2, 4, 6 or 8 molecular orbitals respectively were used in Configuration Interaction calculations

Table S2. *Ab Initio* Total Energies E_{Tot} (Hartree) of LPAHs **1**, **4-8**

^a	Symm	^b	UHF/ 6-31G*	UB3LYP/ STO-3G	UB3LYP/ 6-31G*	UB3LYP/ 6-311G**	UMP2/6-31G*// UHF/6-31G*
1 pl	D_{2h}	T	-1449.71124752	-1441.16891084	-1459.00565387	-1459.31024202	-1454.14236131
1 pl	D_{2h}	S	-1449.75259870	-1441.17092382	-1459.00702509	-1459.31155412	-1454.13050372
4 pl	C_s	T		-1441.17850438	-1459.01470714		
4 pl	C_s	S		-1441.17243103	-1459.00979485		
5 tf	C_1	T		-1441.17319335	-1459.00845164		
5 tf	C_1	S		-1441.16388910	-1459.00156071		
			RHF/ 6-31G*	RB3LYP/ STO-3G	RB3LYP/ 6-31G*	RB3LYP/ 6-311G**	RMP2/6-31G*// RHF/6-31G*
6 pl	C_{2v}	S	-1449.63141017	-1441.20000881	-1459.03894157	-1459.34466343	-1454.43459809
7 pl	C_{2h}	S	-1449.62572449	-1441.19671053	-1459.03576578	-1459.34144984	
8 tf	C_2	S	-1449.63304253	-1441.20308920	-1459.03685972	-1459.34221493	

all the structures were found to be minima (no imaginary frequencies) at B3LYP/STO-3G; ^a - **pl** – planar conformation, **tf** – twisted-folded conformation; ^b - S – singlet, T – triplet.

Table S3. *Ab Initio* Total E_{Tot} and Relative ΔE_{Tot} Energies of Neutral and Charged Species of **1**, **3**, **6**

^a	Symm	^b	^c		UB3LYP/ 6-31G* <i>E</i> _{Tot} (Hartree)	UB3LYP/ 6-31+G* <i>E</i> _{Tot} (Hartree)	UB3LYP/ 6-31G* ΔE _{Tot} (kJ/mol)	UB3LYP/ 6-31+G* ΔE _{Tot} (kJ/mol)
1 pl	<i>D</i> _{2h}	T	neutral		-1459.00565387	-1459.04134042	87.40 ^d	90.88 ^d
1 pl	<i>D</i> _{2h}	S	neutral		-1459.00702509	-1459.04369052	83.80 ^d	84.71 ^d
3 pl	<i>C</i> _{2v}	D	neutral	M	-730.69409016	-730.71566430	0.00	0.00
1 pl	<i>D</i> _{2h}		dianion	M	RB3LYP/ 6-31G* -1459.03130753	RB3LYP/ 6-31+G* -1459.09549335	RB3LYP/ 6-31G* 20.04 ^d	RB3LYP/ 6-31+G* -51.30 ^d
1 pl	<i>D</i> _{2h}		dikation	M	-1458.51183349	-1458.53248578	1383.92 ^d	1426.88 ^d
3 pl	<i>C</i> _{2v}	S	anion	M	-730.73698180	-730.77252462	-112.61 ^e	-149.29 ^e
3 tf	<i>C</i> _{2v}	T	kation	M	-730.48206198	-730.49554313	556.68 ^e	577.93 ^e
6 pl	<i>C</i> _{2v}	S	neutral		-1459.03894157	-1459.07595557	0.00	0.00
6 pl	<i>C</i> _{2v}	S	dianion	M	-1459.03551310		9.00 ^d	
6 tf	<i>C</i> _{2v}	S	dikation		-1459.51968120		1363.32 ^d	

^a - **pl** – planar conformation, **tf** – twisted-folded conformation; ^b - D – doublet, S – singlet, T – triplet;

^c – minimum (no imaginary frequencies, at B3LYP/6-31G*); all the structures were found to be minima at B3LYP/STO-3G; ^d - relatively to neutral **6**; ^e - relatively to neutral **3**.

Table S4. Optimized Geometry of Triplet-1, AM1 C.I.=8, $\Delta H_f^\circ=809.406$ kJ/mol

C	0.0000000000	0.0000000000	0.0000000000
C	2.8620162900	0.0000000000	0.0000000000
C	0.7004290874	0.0000000000	-1.2517276228
C	0.7004290874	0.0000000000	1.2517276228
C	2.1615872025	0.0000000000	-1.2517276228
C	2.1615872025	0.0000000000	1.2517276228
C	-1.4164758999	0.0000000000	0.0000066799
C	4.2784921899	0.0000000000	-0.0000066799
C	-0.0150180780	0.0000000000	-2.4304922079
C	-0.0150180780	0.0000000000	2.4304922079
C	2.8770343680	0.0000000000	-2.4304922079
C	2.8770343680	0.0000000000	2.4304922079
C	-1.4384891631	0.0000000000	-2.4548084920
C	-1.4384891631	0.0000000000	2.4548084920
C	4.3005054531	0.0000000000	-2.4548084920
C	4.3005054531	0.0000000000	2.4548084920
C	-2.1429387406	0.0000000000	-1.2269814537
C	-2.1429387406	0.0000000000	1.2269814537
C	5.0049550306	0.0000000000	-1.2269814537
C	5.0049550306	0.0000000000	1.2269814537
C	-3.5726266875	0.0000000000	-1.2272892615
C	-3.5726266889	0.0000000000	1.2272824370
C	6.4346429789	0.0000000000	-1.2272824370
C	6.4346429775	0.0000000000	1.2272892615
C	-4.2679244593	0.0000000000	-0.0000305449
C	7.1299348926	0.0000000000	-0.0000204014
H	0.4884970752	0.0000000000	-3.4091578530
H	0.4884970752	0.0000000000	3.4091578530
H	2.3735192147	0.0000000000	-3.4091578530
H	2.3735192147	0.0000000000	3.4091578530
C	-2.1576091623	0.0000000000	-3.6676643027
C	-2.1576091623	0.0000000000	3.6676643027
C	5.0196254523	0.0000000000	-3.6676643027
C	5.0196254523	0.0000000000	3.6676643027
C	-4.2528250673	0.0000000000	-2.4600344566
C	-4.2528309531	0.0000000000	2.4600243853
C	7.1148472431	0.0000000000	-2.4600243851
C	7.1148413573	0.0000000000	2.4600344566
H	-5.3672537008	0.0000000000	0.0002606411
H	8.2292641326	0.0000000000	0.0002760320
C	-3.5459998429	0.0000000000	-3.6609429169
C	-3.5459998429	0.0000000000	3.6609429169
C	6.4080161329	0.0000000000	-3.6609429169
C	6.4080161329	0.0000000000	3.6609429169
H	-1.6069757869	0.0000000000	-4.6199961606
H	-1.6069757869	0.0000000000	4.6199961606
H	4.4689920769	0.0000000000	-4.6199961606
H	4.4689920769	0.0000000000	4.6199961606
H	-4.0965747046	0.0000000000	-4.6142181115
H	-4.0965747046	0.0000000000	4.6142181115
H	6.9585909946	0.0000000000	-4.6142181115
H	6.9585909946	0.0000000000	4.6142181115
H	-5.3528842473	0.0000000000	-2.4679447153
H	-5.3528901333	0.0000000000	2.4679346154
H	8.2149064233	0.0000000000	-2.4679346154
H	8.2149005373	0.0000000000	2.4679447153

Table S5. Optimized Geometry of Singlet-1, AM1 C.I.=8, $\Delta H_f^\circ=812.263$ kJ/mol

C	0.0000000000	0.0000000000	0.0000000000
C	2.8629479700	0.0000000000	0.0000000000
C	0.7007675186	0.0000000000	-1.2520013002
C	0.7007675186	0.0000000000	1.2520013002
C	2.1621804513	0.0000000000	-1.2520013002
C	2.1621804513	0.0000000000	1.2520013002
C	-1.4151571898	0.0000000000	0.0000207991
C	4.2781051598	0.0000000000	-0.0000207991
C	-0.0145877457	0.0000000000	-2.4304053349
C	-0.0145877457	0.0000000000	2.4304053349
C	2.8775357157	0.0000000000	-2.4304053349
C	2.8775357157	0.0000000000	2.4304053349
C	-1.4379410992	0.0000000000	-2.4544492914
C	-1.4379410992	0.0000000000	2.4544492914
C	4.3008890692	0.0000000000	-2.4544492914
C	4.3008890692	0.0000000000	2.4544492914
C	-2.1421028817	0.0000000000	-1.2274578498
C	-2.1421028817	0.0000000000	1.2274578498
C	5.0050508517	0.0000000000	-1.2274578498
C	5.0050508517	0.0000000000	1.2274578498
C	-3.5719939416	0.0000000000	-1.2274779657
C	-3.5719939417	0.0000000000	1.2274567188
C	6.4349419117	0.0000000000	-1.2274567188
C	6.4349419116	0.0000000000	1.2274779657
C	-4.2669841015	0.0000000000	-0.0000088020
C	7.1299138325	0.0000000000	0.0000227715
H	0.4887507383	0.0000000000	-3.4091928791
H	0.4887507383	0.0000000000	3.4091928791
H	2.3741972316	0.0000000000	-3.4091928791
H	2.3741972316	0.0000000000	3.4091928791
C	-2.1574965399	0.0000000000	-3.6683099556
C	-2.1574965399	0.0000000000	3.6683099556
C	5.0204445099	0.0000000000	-3.6683099556
C	5.0204445099	0.0000000000	3.6683099556
C	-4.2521568337	0.0000000000	-2.4599605642
C	-4.2521751473	0.0000000000	2.4599292107
C	7.1151231173	0.0000000000	-2.4599292107
C	7.1151048037	0.0000000000	2.4599605642
H	-5.3663311513	0.0000000000	-0.0000301198
H	8.2292608825	0.0000000000	0.0000177890
C	-3.5450293685	0.0000000000	-3.6615061134
C	-3.5450293685	0.0000000000	3.6615061134
C	6.4079773385	0.0000000000	-3.6615061134
C	6.4079773385	0.0000000000	3.6615061134
H	-1.6061265430	0.0000000000	-4.6201772012
H	-1.6061265430	0.0000000000	4.6201772012
H	4.4690745130	0.0000000000	-4.6201772012
H	4.4690745130	0.0000000000	4.6201772012
H	-4.0962509140	0.0000000000	-4.6144311525
H	-4.0962509140	0.0000000000	4.6144311525
H	6.9591988840	0.0000000000	-4.6144311525
H	6.9591988840	0.0000000000	4.6144311525
H	-5.3521613172	0.0000000000	-2.4682011674
H	-5.3521796315	0.0000000000	2.4681697197
H	8.2151276015	0.0000000000	-2.4681697197
H	8.2151092872	0.0000000000	2.4682011674

Table S6. Optimized Geometry of Triplet-1, PM3 C.I.=8, $\Delta H_f^\circ=737.815$ kJ/mol

C	0.0000000000	0.0000000000	0.0000000000
C	2.8626797300	0.0000000000	0.0000000000
C	0.6993446675	0.0000000000	-1.2483641962
C	0.6993446675	0.0000000000	1.2483641962
C	2.1633350624	0.0000000000	-1.2483641962
C	2.1633350624	0.0000000000	1.2483641962
C	-1.4093702897	0.0000000000	-0.0000251171
C	4.2720500197	0.0000000000	0.0000251171
C	-0.0040692056	0.0000000000	-2.4292085160
C	-0.0040692056	0.0000000000	2.4292085160
C	2.8667489356	0.0000000000	-2.4292085160
C	2.8667489356	0.0000000000	2.4292085160
C	-1.4277136144	0.0000000000	-2.4510425407
C	-1.4277136144	0.0000000000	2.4510425407
C	4.2903933444	0.0000000000	-2.4510425407
C	4.2903933444	0.0000000000	2.4510425407
C	-2.1310012068	0.0000000000	-1.2275331196
C	-2.1310012068	0.0000000000	1.2275331196
C	4.9936809368	0.0000000000	-1.2275331196
C	4.9936809368	0.0000000000	1.2275331196
C	-3.5561153198	0.0000000000	-1.2263075034
C	-3.5561153415	0.0000000000	1.2263329826
C	6.4187950715	0.0000000000	-1.2263329826
C	6.4187950498	0.0000000000	1.2263075034
C	-4.2547483802	0.0000000000	0.0000220988
C	7.1174500569	0.0000000000	-0.0000158711
H	0.5385766294	0.0000000000	-3.3884689515
H	0.5385766294	0.0000000000	3.3884689515
H	2.3241031005	0.0000000000	-3.3884689515
H	2.3241031005	0.0000000000	3.3884689515
C	-2.1449750274	0.0000000000	-3.6623745282
C	-2.1449750274	0.0000000000	3.6623745282
C	5.0076547574	0.0000000000	-3.6623745282
C	5.0076547574	0.0000000000	3.6623745282
C	-4.2371802042	0.0000000000	-2.4550485126
C	-4.2371582575	0.0000000000	2.4550861682
C	7.0998379875	0.0000000000	-2.4550861682
C	7.0998599342	0.0000000000	2.4550485126
H	-5.3508607801	0.0000000000	0.0000120109
H	8.2135624565	0.0000000000	-0.0000455561
C	-3.5301941162	0.0000000000	-3.6535416542
C	-3.5301941162	0.0000000000	3.6535416542
C	6.3928738462	0.0000000000	-3.6535416542
C	6.3928738462	0.0000000000	3.6535416542
H	-1.5976317799	0.0000000000	-4.6116565502
H	-1.5976317799	0.0000000000	4.6116565502
H	4.4603115099	0.0000000000	-4.6116565502
H	4.4603115099	0.0000000000	4.6116565502
H	-4.0783970701	0.0000000000	-4.6018989153
H	-4.0783970701	0.0000000000	4.6018989153
H	6.9410768001	0.0000000000	-4.6018989153
H	6.9410768001	0.0000000000	4.6018989153
H	-5.3329684735	0.0000000000	-2.4649019514
H	-5.3329465252	0.0000000000	2.4649397874
H	8.1956262552	0.0000000000	-2.4649397874
H	8.1956482035	0.0000000000	2.4649019514

Table S7. Optimized Geometry of Singlet-1, PM3 C.I.=8, $\Delta H_f^\circ=740.109$ kJ/mol

C	0.0000000000	0.0000000000	0.0000000000
C	2.8634682300	0.0000000000	0.0000000000
C	0.6995935868	0.0000000000	-1.2486179931
C	0.6995935868	0.0000000000	1.2486179931
C	2.1638746431	0.0000000000	-1.2486179931
C	2.1638746431	0.0000000000	1.2486179931
C	-1.4081724899	0.0000000000	-0.0000021038
C	4.2716407199	0.0000000000	0.0000021038
C	-0.0036691492	0.0000000000	-2.4291393636
C	-0.0036691492	0.0000000000	2.4291393636
C	2.8671373792	0.0000000000	-2.4291393636
C	2.8671373792	0.0000000000	2.4291393636
C	-1.4272527510	0.0000000000	-2.4507478955
C	-1.4272527510	0.0000000000	2.4507478955
C	4.2907209810	0.0000000000	-2.4507478955
C	4.2907209810	0.0000000000	2.4507478955
C	-2.1302466125	0.0000000000	-1.2279898725
C	-2.1302466125	0.0000000000	1.2279898725
C	4.9937148425	0.0000000000	-1.2279898725
C	4.9937148425	0.0000000000	1.2279898725
C	-3.5556235595	0.0000000000	-1.2264489413
C	-3.5556235618	0.0000000000	1.2264510753
C	6.4190917918	0.0000000000	-1.2264510753
C	6.4190917895	0.0000000000	1.2264489413
C	-4.2539097495	0.0000000000	0.0000012693
C	7.1173798180	0.0000000000	-0.0000019101
H	0.5387764457	0.0000000000	-3.3884915060
H	0.5387764457	0.0000000000	3.3884915060
H	2.3246917842	0.0000000000	-3.3884915060
H	2.3246917842	0.0000000000	3.3884915060
C	-2.1449903381	0.0000000000	-3.6629777624
C	-2.1449903381	0.0000000000	3.6629777624
C	5.0084585681	0.0000000000	-3.6629777624
C	5.0084585681	0.0000000000	3.6629777624
C	-4.2366944590	0.0000000000	-2.4550274494
C	-4.2366926220	0.0000000000	2.4550306030
C	7.1001608520	0.0000000000	-2.4550306030
C	7.1001626890	0.0000000000	2.4550274494
H	-5.3500285395	0.0000000000	-0.0000020196
H	8.2134986080	0.0000000000	-0.0000068400
C	-3.5294501388	0.0000000000	-3.6541006908
C	-3.5294501388	0.0000000000	3.6541006908
C	6.3929183688	0.0000000000	-3.6541006908
C	6.3929183688	0.0000000000	3.6541006908
H	-1.5972532903	0.0000000000	-4.6119843878
H	-1.5972532903	0.0000000000	4.6119843878
H	4.4607215203	0.0000000000	-4.6119843878
H	4.4607215203	0.0000000000	4.6119843878
H	-4.0780723362	0.0000000000	-4.6022340833
H	-4.0780723362	0.0000000000	4.6022340833
H	6.9415405662	0.0000000000	-4.6022340833
H	6.9415405662	0.0000000000	4.6022340833
H	-5.3324293059	0.0000000000	-2.4650112844
H	-5.3324274687	0.0000000000	2.4650144537
H	8.1958956987	0.0000000000	-2.4650144537
H	8.1958975359	0.0000000000	2.4650112844

Table S8. Optimized Geometry of Triplet-4, AM1 C.I.=8, $\Delta H_f^\circ=802.745$ kJ/mol

C	0.0000000000	0.0000000000	0.0000000000
C	2.8479259300	0.0000000000	0.0000000000
C	0.6957425245	0.0000000000	-1.2401077685
C	0.6961650666	0.0000000000	1.2525188073
C	2.1404159581	0.0000000000	-1.2492261895
C	2.1507088837	0.0000000000	1.2540433239
C	-1.4196543024	0.0000000000	0.0004040762
C	4.2635031079	0.0000000000	-0.0054761154
C	-0.0475181577	0.0000000000	-2.4446542791
C	-0.0304634086	0.0000000000	2.4408538072
C	2.8609107092	0.0000000000	-2.4374815102
C	2.8722337977	0.0000000000	2.4321552437
C	-1.4185359762	0.0000000000	-2.4490545902
C	-1.4322884142	0.0000000000	2.4545170339
C	4.2760302226	0.0000000000	-2.4621661356
C	4.2938741660	0.0000000000	2.4488907678
C	-2.1545652882	0.0000000000	-1.2294725345
C	-2.1436395453	0.0000000000	1.2289543030
C	4.9863829398	0.0000000000	-1.2344255187
C	4.9926046510	0.0000000000	1.2192111970
C	-3.5479704141	0.0000000000	-1.2206810476
C	-3.5628840544	0.0000000000	1.2278743241
C	6.4129800292	0.0000000000	-1.2369369599
C	6.4246955832	0.0000000000	1.2122111738
C	-4.2773899543	0.0000000000	-0.0085231298
C	7.1110325938	0.0000000000	-0.0138798661
H	0.4759336721	0.0000000000	-3.4126456821
H	0.4823719029	0.0000000000	3.4148760141
H	2.3501329866	0.0000000000	-3.4121041956
H	2.3705148872	0.0000000000	3.4115398639
H	-1.9747474662	0.0000000000	-3.3986709337
C	-2.1748794906	0.0000000000	3.6847608377
C	4.9952932738	0.0000000000	-3.6785929869
C	5.0188665270	0.0000000000	3.6614915486
H	-4.0988147762	0.0000000000	-2.1732082226
C	-4.2786120233	0.0000000000	2.4589956808
C	7.0930592231	0.0000000000	-2.4779649504
C	7.1095434620	0.0000000000	2.4476986332
C	-5.6862010673	0.0000000000	0.0178982791
H	8.2109701614	0.0000000000	-0.0202425057
C	-6.3697698764	0.0000000000	1.2270867336
C	-3.5323493775	0.0000000000	3.6861620233
C	6.3863386465	0.0000000000	-3.6726964780
C	6.4074783852	0.0000000000	3.6483174208
H	-6.2405776904	0.0000000000	-0.9324339892
H	-1.6060116696	0.0000000000	4.6272759992
H	4.4435950534	0.0000000000	-4.6297151686
H	4.4709886868	0.0000000000	4.6148896814
H	-7.4703609653	0.0000000000	1.2311365931
H	-4.0984250363	0.0000000000	4.6304394063
H	6.9321436073	0.0000000000	-4.6288953409
H	6.9602740594	0.0000000000	4.6004266271
C	-5.6781253617	0.0000000000	2.4399504996
H	-6.2351833479	0.0000000000	3.3887215867
H	8.1930041838	0.0000000000	-2.4840910326
H	8.2093116535	0.0000000000	2.4504686681

Table S9. Optimized Geometry of Singlet-4, AM1 C.I.=8, $\Delta H_f^\circ=824.935$ kJ/mol

C	0.0000000000	0.0000000000	0.0000000000
C	2.8612713500	0.0000000000	0.0000000000
C	0.6953218682	0.0000000000	-1.2392473857
C	0.6999535154	0.0000000000	1.2574224037
C	2.1561542044	0.0000000000	-1.2516516571
C	2.1606986801	0.0000000000	1.2544125525
C	-1.4183085411	0.0000000000	0.0021362801
C	4.2718195924	0.0000000000	-0.0032209749
C	-0.0388932120	0.0000000000	-2.4301842996
C	-0.0167562653	0.0000000000	2.4352674444
C	2.8662074237	0.0000000000	-2.4304768928
C	2.8784560181	0.0000000000	2.4301114725
C	-1.4259622023	0.0000000000	-2.4355114552
C	-1.4361431408	0.0000000000	2.4554219726
C	4.2912454630	0.0000000000	-2.4575254649
C	4.3022161756	0.0000000000	2.4493757652
C	-2.1495512379	0.0000000000	-1.2253953401
C	-2.1394665717	0.0000000000	1.2333887716
C	4.9973016668	0.0000000000	-1.2350353892
C	5.0026736087	0.0000000000	1.2239072166
C	-3.5562698590	0.0000000000	-1.2126597656
C	-3.5658298513	0.0000000000	1.2343885631
C	6.4277552281	0.0000000000	-1.2366565537
C	6.4345768278	0.0000000000	1.2190521281
C	-4.2797459099	0.0000000000	-0.0014389518
C	7.1244702753	0.0000000000	-0.0084553820
H	0.4743183979	0.0000000000	-3.4039865958
H	0.4865712367	0.0000000000	3.4142504766
H	2.3612848680	0.0000000000	-3.4084987306
H	2.3772964719	0.0000000000	3.4103285913
H	-1.9732454432	0.0000000000	-3.3899825408
C	-2.1650687733	0.0000000000	3.6802406445
C	5.0084465890	0.0000000000	-3.6744334611
C	5.0254845475	0.0000000000	3.6650742730
H	-4.1042408147	0.0000000000	-2.1664207684
C	-4.2727922742	0.0000000000	2.4632153734
C	7.1050891775	0.0000000000	-2.4695069988
C	7.1162478089	0.0000000000	2.4502787445
C	-5.6898882374	0.0000000000	0.0274234293
H	8.2240257986	0.0000000000	-0.0133213234
C	-6.3721220652	0.0000000000	1.2398866632
C	-3.5317876921	0.0000000000	3.6855212196
C	6.3951297380	0.0000000000	-3.6700333290
C	6.4103817908	0.0000000000	3.6549896807
H	-6.2469312509	0.0000000000	-0.9210590304
H	-1.5996791534	0.0000000000	4.6247763529
H	4.4549705527	0.0000000000	-4.6249058615
H	4.4737575647	0.0000000000	4.6167522838
H	-7.4730513472	0.0000000000	1.2431673083
H	-4.0918284663	0.0000000000	4.6329882859
H	6.9455380295	0.0000000000	-4.6233729546
H	6.9650887938	0.0000000000	4.6060692683
C	-5.6819606403	0.0000000000	2.4470259663
H	-6.2311361102	0.0000000000	3.4000525544
H	8.2049536519	0.0000000000	-2.4810733927
H	8.2163040087	0.0000000000	2.4575498936

Table S10. Optimized Geometry of Triplet-4, PM3 C.I.=8, $\Delta H_f^\circ=732.317$ kJ/mol

C	0.0000000000	0.0000000000	0.0000000000
C	2.8498764300	0.0000000000	0.0000000000
C	0.6951141213	0.0000000000	-1.2333498600
C	0.6972950822	0.0000000000	1.2474542958
C	2.1424405755	0.0000000000	-1.2437777681
C	2.1540837136	0.0000000000	1.2495188546
C	-1.4136773037	0.0000000000	0.0013092631
C	4.2578815754	0.0000000000	-0.0056096036
C	-0.0397882653	0.0000000000	-2.4392085108
C	-0.0155762181	0.0000000000	2.4382150421
C	2.8480720035	0.0000000000	-2.4347279607
C	2.8633011502	0.0000000000	2.4307220381
C	-1.4088151967	0.0000000000	-2.4483137510
C	-1.4190556204	0.0000000000	2.4530477508
C	4.2653339454	0.0000000000	-2.4579513824
C	4.2845715308	0.0000000000	2.4458256296
C	-2.1428751182	0.0000000000	-1.2289167275
C	-2.1254813891	0.0000000000	1.2305730917
C	4.9745210785	0.0000000000	-1.2358899252
C	4.9830906383	0.0000000000	1.2194764359
C	-3.5346436407	0.0000000000	-1.2210226100
C	-3.5454112536	0.0000000000	1.2295683541
C	6.3979661049	0.0000000000	-1.2378015850
C	6.4087271402	0.0000000000	1.2105193027
C	-4.2562143554	0.0000000000	-0.0024073866
C	7.0990178320	0.0000000000	-0.0163466674
H	0.5176795854	0.0000000000	-3.3890443691
H	0.5345641805	0.0000000000	3.3934731915
H	2.2989483908	0.0000000000	-3.3904017527
H	2.3227173878	0.0000000000	3.3907111486
H	-1.9590927018	0.0000000000	-3.3963605890
C	-2.1565003276	0.0000000000	3.6845751394
C	4.9815098757	0.0000000000	-3.6734460161
C	5.0092196234	0.0000000000	3.6553236129
H	-4.0878204097	0.0000000000	-2.1681172128
C	-4.2546332731	0.0000000000	2.4568686935
C	7.0771666043	0.0000000000	-2.4742441677
C	7.0961479088	0.0000000000	2.4400239925
C	-5.6624687273	0.0000000000	0.0232815318
H	8.1952307243	0.0000000000	-0.0189778385
C	-6.3424884611	0.0000000000	1.23171113652
C	-3.5114175203	0.0000000000	3.6868485811
C	6.3684537510	0.0000000000	-3.6677140194
C	6.3945125731	0.0000000000	3.6395262797
H	-6.2176064428	0.0000000000	-0.9215285187
H	-1.5925804175	0.0000000000	4.6244452604
H	4.4324210931	0.0000000000	-4.6218102703
H	4.4666824429	0.0000000000	4.6070466541
H	-7.4377330522	0.0000000000	1.2371992611
H	-4.0721295845	0.0000000000	4.6286698392
H	6.9130636439	0.0000000000	-4.6184421406
H	6.9468418425	0.0000000000	4.5853208049
C	-5.6519698015	0.0000000000	2.4420219263
H	-6.2048431361	0.0000000000	3.3881384191
H	8.1730633895	0.0000000000	-2.4835694385
H	8.1915688866	0.0000000000	2.4436199388

Table S11. Optimized Geometry of Singlet-4, PM3 C.I.=8, $\Delta H_f^\circ=752.027$ kJ/mol

C	0.0000000000	0.0000000000	0.0000000000
C	2.8603742200	0.0000000000	0.0000000000
C	0.6933434409	0.0000000000	-1.2345382286
C	0.6979495198	0.0000000000	1.2543405299
C	2.1577918616	0.0000000000	-1.2472207850
C	2.1613243144	0.0000000000	1.2512538208
C	-1.4119402147	0.0000000000	-0.0010958919
C	4.2649167825	0.0000000000	-0.0029687201
C	-0.0275693367	0.0000000000	-2.4289058321
C	-0.0067101887	0.0000000000	2.4339571101
C	2.8554347411	0.0000000000	-2.4289757947
C	2.8665294900	0.0000000000	2.4290308012
C	-1.4125236566	0.0000000000	-2.4391545755
C	-1.4264147961	0.0000000000	2.4498445436
C	4.2808344322	0.0000000000	-2.4540713546
C	4.2913976545	0.0000000000	2.4463180779
C	-2.1344898631	0.0000000000	-1.2282810949
C	-2.1258435139	0.0000000000	1.2312989187
C	4.9854264308	0.0000000000	-1.2356116472
C	4.9905035853	0.0000000000	1.2252358718
C	-3.5411200987	0.0000000000	-1.2194606709
C	-3.5505212386	0.0000000000	1.2288907990
C	6.4116223973	0.0000000000	-1.2353532501
C	6.4181078714	0.0000000000	1.2186126180
C	-4.2595399954	0.0000000000	-0.0037379403
C	7.1114799837	0.0000000000	-0.0073870411
H	0.5272364350	0.0000000000	-3.3811157701
H	0.5365592242	0.0000000000	3.3934195821
H	2.3140156252	0.0000000000	-3.3884232501
H	2.3280034805	0.0000000000	3.3908067782
H	-1.9535269172	0.0000000000	-3.3925105023
C	-2.1544195094	0.0000000000	3.6749893746
C	4.9958198848	0.0000000000	-3.6693823777
C	5.0120851521	0.0000000000	3.6612903058
H	-4.0890435375	0.0000000000	-2.1697981582
C	-4.2536384824	0.0000000000	2.4515345504
C	7.0894981168	0.0000000000	-2.4640065590
C	7.0998596961	0.0000000000	2.4460243541
C	-5.6673072777	0.0000000000	0.0210932339
H	8.2069586835	0.0000000000	-0.0125888745
C	-6.3484305095	0.0000000000	1.2315386954
C	-3.5176031844	0.0000000000	3.6774578351
C	6.3794038663	0.0000000000	-3.6617342115
C	6.3933682703	0.0000000000	3.6489132169
H	-6.2242434614	0.0000000000	-0.9229326607
H	-1.5937628474	0.0000000000	4.6171948325
H	4.4471700382	0.0000000000	-4.6169056253
H	4.4651359535	0.0000000000	4.6103602951
H	-7.4441477485	0.0000000000	1.2340118228
H	-4.0752721623	0.0000000000	4.6212564841
H	6.9275425336	0.0000000000	-4.6095617451
H	6.9463084447	0.0000000000	4.5943956204
C	-5.6613692185	0.0000000000	2.4363999789
H	-6.2101218921	0.0000000000	3.3851677172
H	8.1844945277	0.0000000000	-2.4759871457
H	8.1953923948	0.0000000000	2.4534242247

Table S12. Optimized Geometry of Triplet-5, AM1 C.I.=8, $\Delta H_f^\circ=799.882$ kJ/mol

C	0.0000000000	0.0000000000	0.0000000000
C	2.8263299800	0.0000000000	0.0000000000
C	0.6935705488	-0.0491018871	-1.2336827058
C	0.6990371537	-0.0493978047	1.2411176217
C	2.1295231419	-0.1968455964	-1.2314759092
C	2.1128754041	0.1750285215	1.2331718539
C	-1.4262992784	0.1219312425	-0.0089997227
C	4.2443976197	0.0371453203	0.0015303195
C	-0.0355132469	0.0794842561	-2.4426057055
C	-0.0419112190	-0.3066016844	2.4501222141
C	2.8486152142	-0.4936995589	-2.3846204703
C	2.8189662381	0.5949100461	2.3624974055
C	-1.3980582575	0.2434485366	-2.4454997879
C	-1.4606038635	-0.1450140336	2.4439259724
C	4.2653083067	-0.5380689458	-2.3876303066
C	4.2315818485	0.6844405316	2.3725668899
C	-2.1260348116	0.2702397662	-1.2268018268
C	-2.1536652057	0.1026193502	1.2180029617
C	4.9687102128	-0.2422226475	-1.1887891300
C	4.9540345065	0.3676092511	1.1894778121
C	-3.5373968520	0.4494006962	-1.2058395444
C	-3.5526230428	0.2695297727	1.2140232109
C	6.3968598882	-0.2338730461	-1.1795604328
C	6.3806732717	0.4053547037	1.1899400681
C	-4.2272698986	0.4581829386	-0.0221557789
C	7.0820756620	0.0901710220	0.0090182990
H	0.5030068610	0.0699110057	-3.4023385115
C	0.5591615929	-0.7669905747	3.6282540950
H	2.3262869131	-0.7059166849	-3.3302956992
H	2.2761997920	0.8980801087	3.2714881962
H	-1.9484142308	0.3587998215	-3.3913724913
C	-2.2004191884	-0.2751824858	3.6445118272
C	4.9975152395	-0.8465662806	-3.5541961476
C	4.9447022212	1.0609104416	3.5303802215
H	-4.0630624034	0.5816534306	-2.1635638964
C	-4.2647262786	0.2147225183	2.4525515014
C	7.0859120394	-0.5472752776	-2.3698798172
C	7.0521207310	0.7689916677	2.3781696065
H	-5.3183858063	0.6009480898	-0.0078951277
H	8.1819376354	0.1024761516	0.0152608876
C	-0.1801267867	-0.9221809444	4.8057560862
C	-3.6148968121	-0.0535532151	3.6196317581
C	6.3871195284	-0.8515977250	-3.5348787116
C	6.3344107093	1.0959543419	3.5232890544
H	1.6235386440	-1.0495341556	3.6317568291
C	-1.5357865299	-0.6482192202	4.8308572235
H	4.4553198474	-1.0819965550	-4.4828341648
H	4.3860816132	1.3219009666	4.4413336913
H	0.3304976979	-1.2682653862	5.7169521439
H	-4.1632746942	-0.1144559138	4.5719263252
H	6.9444705215	-1.0968949135	-4.4528774711
H	6.8734786282	1.3857227128	4.4385461364
H	-2.1102404320	-0.7411007156	5.7639399556
H	-5.3523200115	0.3817319189	2.4342654401
H	8.1866852686	-0.5481691410	-2.3678958401
H	8.1513844235	0.7954221974	2.3873289922

Table S13. Optimized Geometry of Singlet-5, AM1 C.I.=8, $\Delta H_f^\circ=840.268$ kJ/mol

C	0.0000000000	0.0000000000	0.0000000000
C	2.8405913100	0.0000000000	0.0000000000
C	0.6951688330	-0.0462538730	-1.2342000175
C	0.6942620830	-0.0466384432	1.2444615713
C	2.1420269728	-0.2201268363	-1.2306462674
C	2.1232350668	0.2047651249	1.2351654834
C	-1.4231394487	0.1040081846	-0.0124033032
C	4.2453687471	0.0507164182	-0.0024859722
C	-0.0194099889	0.0949510787	-2.4350433222
C	-0.0318425049	-0.3196799268	2.4416692655
C	2.8514207727	-0.5433886379	-2.3677496267
C	2.8070758487	0.6661223780	2.3353346397
C	-1.3932759634	0.2584750394	-2.4423354759
C	-1.4580933977	-0.1963193555	2.4347273270
C	4.2743638479	-0.5931721312	-2.3685067788
C	4.2346816710	0.7831897016	2.3406923893
C	-2.1209042723	0.2603615917	-1.2339742251
C	-2.1532586656	0.0517838073	1.2129380884
C	4.9745188585	-0.2614632898	-1.1876382694
C	4.9558124911	0.4335811098	1.1794237413
C	-3.5404056799	0.4163665799	-1.2102410626
C	-3.5557773137	0.1916817328	1.2074338871
C	6.4088591961	-0.2405554635	-1.1801743740
C	6.3845972392	0.4887466442	1.1754130593
C	-4.2312447039	0.3907704361	-0.0312754918
C	7.0910820300	0.1325898960	-0.0023520917
H	0.5200114196	0.0912581065	-3.3950150561
C	0.5814237636	-0.7498842980	3.6335897061
H	2.3363376984	-0.7670508250	-3.3144315139
H	2.2733204464	0.9718567560	3.2497608106
H	-1.9314487635	0.3849172569	-3.3936115862
C	-2.1960352030	-0.3440125203	3.6351441439
C	5.0059512155	-0.9384171903	-3.5310655772
C	4.9371552577	1.2096397197	3.4864391438
H	-4.0638152429	0.5572132695	-2.1680255545
C	-4.2683995815	0.1019968847	2.4394851517
C	7.0925778334	-0.5878346093	-2.3542092201
C	7.0459753548	0.9030613966	2.3373184501
H	-5.3250127705	0.5130483742	-0.0157260645
H	8.1899766527	0.1558336541	0.0033091717
C	-0.1559421494	-0.9183832057	4.8059137575
C	-3.6138465222	-0.1611507709	3.6079695388
C	6.3882660973	-0.9367502620	-3.5132653322
C	6.3210885669	1.2643230732	3.4785936372
H	1.6536141051	-1.0016169109	3.6399758735
C	-1.5223050735	-0.6902254661	4.8251722412
H	4.4581915744	-1.2054137874	-4.4467155498
H	4.3743428585	1.4957070953	4.3876451584
H	0.3586056024	-1.2417107528	5.7239724520
H	-4.1650113315	-0.2456599353	4.5569586291
H	6.9489538873	-1.2093124654	-4.4208045458
H	6.8620705491	1.5946631941	4.3786023036
H	-2.0958026895	-0.7973639380	5.7574351470
H	-5.3603992194	0.2381924806	2.4217406775
H	8.1924645362	-0.5852836172	-2.3648529468
H	8.1451423497	0.9498482574	2.3523480570

Table S14. Optimized Geometry of Triplet-**5**, PM3 C.I.=8, $\Delta H_f^\circ=735.655$ kJ/mol

C	0.0000000000	0.0000000000	0.0000000000
C	2.8268399800	0.0000000000	0.0000000000
C	0.6941610073	-0.0502461643	-1.2260366865
C	0.6898307705	-0.0511137990	1.2472074961
C	2.1330294764	-0.1573933428	-1.2316470200
C	2.1142207850	0.1315667241	1.2381993660
C	-1.4254190549	0.1254409338	-0.0356672375
C	4.2425393797	0.0432778601	-0.0139679917
C	-0.0185274107	0.0239615428	-2.4486878619
C	-0.0854586701	-0.2745221768	2.4503699740
C	2.8377948455	-0.3649597490	-2.4105065586
C	2.8423562739	0.4724393031	2.3788376408
C	-1.3749447438	0.1866014525	-2.4744848133
C	-1.5007976992	-0.1081838948	2.4136852352
C	4.2514778424	-0.3985950579	-2.4269371688
C	4.2540186107	0.5629253334	2.3772619886
C	-2.1065690426	0.2536513930	-1.2592866569
C	-2.1727914131	0.1306154985	1.1758700169
C	4.9583074373	-0.1703978347	-1.2205862337
C	4.9645020537	0.3135213507	1.1782017858
C	-3.5156816555	0.4457789266	-1.2688591644
C	-3.5639077924	0.3055131680	1.1451680466
C	6.3827807120	-0.1536558426	-1.2249171790
C	6.3862685390	0.3559357469	1.1686369969
C	-4.2224122038	0.4822756468	-0.1003538230
C	7.0825462611	0.1074490095	-0.0300932089
H	0.5523611829	-0.0448675912	-3.3877455992
C	0.4776800468	-0.6989561767	3.6564319081
H	2.2846411928	-0.4895479916	-3.3553316244
H	2.3217951823	0.6754638704	3.3260162608
H	-1.9136193625	0.2644591570	-3.4256442655
C	-2.2672161872	-0.2204183941	3.5925942259
C	4.9710919280	-0.6321189796	-3.6164237599
C	4.9718424518	0.8752141604	3.5490287125
H	-4.0239614292	0.5643277030	-2.2326615757
C	-4.3047688467	0.2715122256	2.3675554487
C	7.0637983340	-0.3926388815	-2.4346709258
C	7.0671485780	0.6562868053	2.3666285044
H	-5.3077092174	0.6349837673	-0.1071280439
H	8.1788694497	0.1244164555	-0.0343721518
C	-0.2887444196	-0.8462959920	4.8139354180
C	-3.6806316023	0.0093465942	3.5445210008
C	6.3572795935	-0.6309619239	-3.6072294726
C	6.3583573207	0.9160832679	3.5315236716
H	1.5517617857	-0.9234243827	3.7139010116
C	-1.6414156333	-0.5801559480	4.8008898908
H	4.4244727569	-0.8135418121	-4.5488389014
H	4.4256945121	1.0819275541	4.4761975598
H	0.1976066735	-1.1720932622	5.7396133531
H	-4.2458203044	-0.0381279432	4.4823833351
H	6.9048229251	-0.8169101624	-4.5378055292
H	6.9020529261	1.1559633532	4.4517126808
H	-2.2380193754	-0.6651821625	5.7158922612
H	-5.3859610235	0.4461998640	2.3290423945
H	8.1597459071	-0.3876043892	-2.4446711628
H	8.1622480084	0.6880747884	2.3696600115

Table S15. Optimized Geometry of Singlet-5, PM3 C.I.=8, $\Delta H_f^\circ=774.954$ kJ/mol

C	0.0000000000	0.0000000000	0.0000000000
C	2.8441782200	0.0000000000	0.0000000000
C	0.6953374910	-0.0471197921	-1.2275629116
C	0.6843649464	-0.0480177881	1.2509574653
C	2.1478084268	-0.1767779136	-1.2327617296
C	2.1268485287	0.1652737394	1.2419455842
C	-1.4229720904	0.0922024254	-0.0387664145
C	4.2447643589	0.0520508808	-0.0154019144
C	-0.0039551308	0.0392954133	-2.4412117701
C	-0.0735430060	-0.2929067222	2.4414813730
C	2.8429587673	-0.4107375413	-2.3965343252
C	2.8313251472	0.5551383704	2.3533966938
C	-1.3727430389	0.1911046304	-2.4713046011
C	-1.4979224724	-0.1834808435	2.4043973731
C	4.2633266147	-0.4541477221	-2.4099613017
C	4.2592687910	0.6657597197	2.3509185908
C	-2.1041324036	0.2214186923	-1.2661960425
C	-2.1741890424	0.0497391449	1.1709591681
C	4.9655233324	-0.1938647670	-1.2192899807
C	4.9679585611	0.3747792103	1.1748482183
C	-3.5239439570	0.3728704051	-1.2732604840
C	-3.5709331086	0.1792653882	1.1388088151
C	6.3966876996	-0.1742731463	-1.2220913234
C	6.3923111250	0.4266382964	1.1642836078
C	-4.2320883207	0.3617708229	-0.1091718827
C	7.0947351570	0.1302705280	-0.0332820504
H	0.5683668266	-0.0169510007	-3.3806834111
C	0.5060778255	-0.6776902830	3.6619379804
H	2.2934962202	-0.5433428272	-3.3423387749
H	2.3151699602	0.7709590709	3.3005227660
H	-1.9019602433	0.2807428256	-3.4265671689
C	-2.2610555934	-0.3267397874	3.5828777067
C	4.9841302370	-0.7268192115	-3.5968732636
C	4.9674752026	1.0294188801	3.5127735781
H	-4.0314776385	0.4964760607	-2.2368306362
C	-4.3120899684	0.0969927937	2.3545371577
C	7.0735310399	-0.4499040880	-2.4144582715
C	7.0635333881	0.7779479647	2.3362491556
H	-5.3216983358	0.4801101003	-0.1141415817
H	8.1904471625	0.1477755124	-0.0345764425
C	-0.2558292376	-0.8515871985	4.8140880289
C	-3.6800810045	-0.1549224968	3.5324109418
C	6.3623587824	-0.7274898672	-3.5869225307
C	6.3472889652	1.0813078088	3.4977204352
H	1.5894396260	-0.8503411362	3.7221810334
C	-1.6220823348	-0.6535259531	4.7945287437
H	4.4324970842	-0.9364735375	-4.5199193488
H	4.4137207627	1.2677280639	4.4279772441
H	0.2400870395	-1.1469023532	5.7451519283
H	-4.2474460323	-0.2355490782	4.4667638489
H	6.9141320435	-0.9437766744	-4.5081432171
H	6.8921033088	1.3626556208	4.4054558918
H	-2.2168865547	-0.7641361444	5.7079376798
H	-5.3995524845	0.2277442066	2.3161759201
H	8.1690483845	-0.4464465717	-2.4322762455
H	8.1585554392	0.8210044047	2.3459913423

Table S16. Optimized Geometry of **6**, AM3 C.I.=8, $\Delta H_f^\circ=723.304$ kJ/mol

C	0.0000000000	0.0000000000	0.0000000000
C	2.8308616300	0.0000000000	0.0000000000
C	0.7171388595	0.0000000000	-1.2419815444
C	0.6969966179	0.0000000000	1.2380116547
C	2.1338650120	0.0000000000	1.2380116547
C	2.1137227704	0.0000000000	-1.2419815444
C	-1.4253053224	0.0000000000	-0.0028888156
C	4.2561669524	0.0000000000	-0.0028888156
C	-0.0534659097	0.0000000000	-2.4630757982
C	-0.0439930602	0.0000000000	2.4421471361
C	2.8748546902	0.0000000000	2.4421471361
C	2.8843275397	0.0000000000	-2.4630757982
C	-1.4057890571	0.0000000000	-2.4661448968
C	-1.4296382460	0.0000000000	2.4497983912
C	4.2604998760	0.0000000000	2.4497983912
C	4.2366506871	0.0000000000	-2.4661448968
C	-2.1600854763	0.0000000000	-1.2387424375
C	-2.1412837434	0.0000000000	1.2119216214
C	4.9721453734	0.0000000000	1.2119216214
C	4.9909471063	0.0000000000	-1.2387424375
C	-3.5384785575	0.0000000000	-1.2365032469
C	-3.5686392079	0.0000000000	1.2112342764
C	6.3995008379	0.0000000000	1.2112342764
C	6.3693401875	0.0000000000	-1.2365032469
C	-4.2752072407	0.0000000000	-0.0197799320
C	7.1060688707	0.0000000000	-0.0197799320
H	0.4812844253	0.0000000000	-3.4249702383
H	0.4771232009	0.0000000000	3.4114627494
H	2.3537384290	0.0000000000	3.4114627494
H	2.3495772046	0.0000000000	-3.4249702383
H	-1.9713716848	0.0000000000	-3.4112839325
C	-2.1857759768	0.0000000000	3.6778452824
C	5.0166376068	0.0000000000	3.6778452824
H	4.8022333148	0.0000000000	-3.4112839325
H	-4.0952104310	0.0000000000	-2.1866228661
C	-4.2876252631	0.0000000000	2.4409092807
C	7.1184868931	0.0000000000	2.4409092807
H	6.9260720610	0.0000000000	-2.1866228661
C	-5.6869722973	0.0000000000	-0.0012619945
C	8.5178339273	0.0000000000	-0.0012619945
C	-5.6810848923	0.0000000000	2.4194958938
C	8.5119465223	0.0000000000	2.4194958938
C	-6.3722947815	0.0000000000	1.2009050319
C	9.2031564115	0.0000000000	1.2009050319
H	-6.2349050373	0.0000000000	-0.9553436265
H	9.0657666673	0.0000000000	-0.9553436265
H	-7.4728435030	0.0000000000	1.2063679776
H	10.3037051330	0.0000000000	1.2063679776
H	-6.2436615392	0.0000000000	3.3650015331
H	9.0745231692	0.0000000000	3.3650015335
C	-3.5403380896	0.0000000000	3.6739511649
C	6.3711997196	0.0000000000	3.6739511649
H	4.4515030193	0.0000000000	4.6229103299
H	-1.6206413893	0.0000000000	4.6229103299
H	6.9432157048	0.0000000000	4.6148777760
H	-4.1123540748	0.0000000000	4.6148777760

Table S17. Optimized Geometry of **6**, PM3 C.I.=8, $\Delta H_f^\circ=651.014$ kJ/mol

C	0.0000000000	0.0000000000	0.0000000000
C	2.8203653900	0.0000000000	0.0000000000
C	0.7136179978	0.0000000000	-1.2382873386
C	0.6920274012	0.0000000000	1.2328774903
C	2.1283379887	0.0000000000	1.2328774903
C	2.1067473921	0.0000000000	-1.2382873386
C	-1.4213900607	0.0000000000	-0.0043082859
C	4.2417554507	0.0000000000	-0.0043082859
C	-0.0466806321	0.0000000000	-2.4672703906
C	-0.0381763608	0.0000000000	2.4419901772
C	2.8585417508	0.0000000000	2.4419901772
C	2.8670460221	0.0000000000	-2.4672703906
C	-1.3951663835	0.0000000000	-2.4740333144
C	-1.4201311812	0.0000000000	2.4465672206
C	4.2404965712	0.0000000000	2.4465672206
C	4.2155317735	0.0000000000	-2.4740333144
C	-2.1489002285	0.0000000000	-1.2413043405
C	-2.1286539960	0.0000000000	1.2097633864
C	4.9490193860	0.0000000000	1.2097633864
C	4.9692656185	0.0000000000	-1.2413043405
C	-3.5239358290	0.0000000000	-1.2420986310
C	-3.5542497026	0.0000000000	1.2065315114
C	6.3746150926	0.0000000000	1.2065315114
C	6.3443012190	0.0000000000	-1.2420986310
C	-4.2556044977	0.0000000000	-0.0206386658
C	7.0759698877	0.0000000000	-0.0206386658
H	0.5220477915	0.0000000000	-3.4101815066
H	0.5181576945	0.0000000000	3.3933384478
H	2.3022076954	0.0000000000	3.3933384478
H	2.2983175984	0.0000000000	-3.4101815066
H	-1.9555889964	0.0000000000	-3.4162934639
C	-2.1758585579	0.0000000000	3.6770917252
C	4.9962239479	0.0000000000	3.6770917252
H	4.7759543864	0.0000000000	-3.4162934639
H	-4.0789254461	0.0000000000	-2.1883463883
C	-4.2695414210	0.0000000000	2.4322939710
C	7.0899068110	0.0000000000	2.4322939710
H	6.8992908361	0.0000000000	-2.1883463883
C	-5.6654787866	0.0000000000	-0.0041623274
C	8.4858441766	0.0000000000	-0.0041623274
C	-5.6595100482	0.0000000000	2.4131787389
C	8.4798754382	0.0000000000	2.4131787389
C	-6.3481396837	0.0000000000	1.1955856410
C	9.1685050737	0.0000000000	1.1955856410
H	-6.2123028961	0.0000000000	-0.9538332764
H	9.0326682861	0.0000000000	-0.9538332764
H	-7.4434020738	0.0000000000	1.2003356203
H	10.2637674638	0.0000000000	1.2003356203
H	-6.2191827960	0.0000000000	3.3553353465
H	9.0395481860	0.0000000000	3.3553353465
C	-3.5264224401	0.0000000000	3.6705226821
C	6.3467878301	0.0000000000	3.6705226821
H	4.4376127251	0.0000000000	4.6201589433
H	-1.6172473351	0.0000000000	4.6201589433
H	6.9159159139	0.0000000000	4.6072470968
H	-4.0955505239	0.0000000000	4.6072470968

Table S18. Optimized Geometry of Triplet-1, UHF/6-31G*, $E_{\text{Tot}}=-1449.7112475$ Hartree

C 0. -1.454356179 0.
 C 0. 1.454356179 0.
 C -1.2468984661 -0.7556959548 0.
 C 1.2468984679 -0.7556959521 0.
 C -1.2468984679 0.7556959521 0.
 C 1.2468984661 0.7556959548 0.
 C 0. -2.8877448432 0.
 C 0. 2.8877448432 0.
 C -2.4243052859 -1.4760049974 0.
 C 2.4243052891 -1.4760049918 0.
 C -2.4243052891 1.4760049918 0.
 C 2.4243052859 1.4760049974 0.
 C -2.4564320275 -2.8971640031 0.
 C 2.456432034 -2.8971639977 0.
 C -2.456432034 2.8971639977 0.
 C 2.4564320275 2.8971640031 0.
 C -1.22770863 -3.6086594613 0.
 C 1.2277086383 -3.6086594585 0.
 C -1.2277086383 3.6086594585 0.
 C 1.22770863 3.6086594613 0.
 C -1.2310689721 -5.0423721881 0.
 C 1.2310689835 -5.0423721851 0.
 C -1.2310689835 5.0423721851 0.
 C 1.2310689721 5.0423721881 0.
 C 0. -5.7329960933 0.
 C 0. 5.7329960933 0.
 H -3.3713871177 -0.9740020105 0.
 H 3.3713871197 -0.9740020028 0.
 H -3.3713871197 0.9740020028 0.
 H 3.3713871177 0.9740020105 0.
 C -3.6771117004 -3.6166866143 0.
 C 3.6771117085 -3.6166866061 0.
 C -3.6771117085 3.6166866061 0.
 C 3.6771117004 3.6166866143 0.
 C -2.4766352714 -5.7229950195 0.
 C 2.4766352841 -5.7229950139 0.
 C -2.4766352841 5.7229950139 0.
 C 2.4766352714 5.7229950195 0.
 H 0. -6.8091602093 0.
 H 0. 6.8091602093 0.
 C -3.678787511 -5.0139166853 0.
 C 3.6787875221 -5.013916677 0.
 C -3.6787875221 5.013916677 0.
 C 3.678787511 5.0139166853 0.
 H -4.6071023827 -3.0760667437 0.
 H 4.6071023894 -3.0760667333 0.
 H -4.6071023894 3.0760667333 0.
 H 4.6071023827 3.0760667437 0.
 H -4.6128088257 -5.5466725386 0.
 H 4.6128088379 -5.5466725284 0.
 H -4.6128088379 5.5466725284 0.
 H 4.6128088257 5.5466725386 0.
 H -2.4848361893 -6.7986390405 0.
 H 2.4848362046 -6.7986390347 0.
 H -2.4848362046 6.7986390347 0.
 H 2.4848361893 6.7986390405 0.

Table S19. Optimized Geometry of Singlet-1, UHF/6-31G*, $E_{\text{Tot}}=-1449.7525987$ Hartree

C 0. 0. -1.4354022174
 C 0. 0. 1.4354022174
 C 0. -1.2475840519 -0.7266210868
 C 0. 1.2475840519 -0.7266210868
 C 0. -1.2475840519 0.7266210868
 C 0. 1.2475840519 0.7266210868
 C 0. 0. -2.8699679387
 C 0. 0. 2.8699679387
 C 0. -2.4442048598 -1.4703151352
 C 0. 2.4442048598 -1.4703151352
 C 0. -2.4442048598 1.4703151352
 C 0. 2.4442048598 1.4703151352
 C 0. -2.4648035045 -2.8827280673
 C 0. 2.4648035045 -2.8827280673
 C 0. -2.4648035045 2.8827280673
 C 0. 2.4648035045 2.8827280673
 C 0. -1.2288172805 -3.5933536084
 C 0. 1.2288172805 -3.5933536084
 C 0. -1.2288172805 3.5933536084
 C 0. 1.2288172805 3.5933536084
 C 0. -1.2310649756 -5.0261506874
 C 0. 1.2310649756 -5.0261506874
 C 0. -1.2310649756 5.0261506874
 C 0. 1.2310649756 5.0261506874
 C 0. 0. -5.7165955438
 C 0. 0. 5.7165955438
 H 0. -3.3921134013 -0.9710156149
 H 0. 3.3921134013 -0.9710156149
 H 0. -3.3921134013 0.9710156149
 H 0. 3.3921134013 0.9710156149
 C 0. -3.6842579079 -3.6103112732
 C 0. 3.6842579079 -3.6103112732
 C 0. -3.6842579079 3.6103112732
 C 0. 3.6842579079 3.6103112732
 C 0. -2.4754141175 -5.7117934333
 C 0. 2.4754141175 -5.7117934333
 C 0. -2.4754141175 5.7117934333
 C 0. 2.4754141175 5.7117934333
 H 0. 0. -6.7927636965
 H 0. 0. 6.7927636965
 C 0. -3.6810848119 -5.0071426131
 C 0. 3.6810848119 -5.0071426131
 C 0. -3.6810848119 5.0071426131
 C 0. 3.6810848119 5.0071426131
 H 0. -4.6160098195 -3.072744361
 H 0. 4.6160098195 -3.072744361
 H 0. -4.6160098195 3.072744361
 H 0. 4.6160098195 3.072744361
 H 0. -4.6130809917 -5.5434533382
 H 0. 4.6130809917 -5.5434533382
 H 0. -4.6130809917 5.5434533382
 H 0. 4.6130809917 5.5434533382
 H 0. -2.4791261989 -6.7874478726
 H 0. 2.4791261989 -6.7874478726
 H 0. -2.4791261989 6.7874478726
 H 0. 2.4791261989 6.7874478726

Table S20. Optimized Geometry of Triplet-1, UB3LYP/6-31G*, $E_{\text{Tot}}=-1459.0056539$ Hartree

C 0. -1.4445123597 0.
 C 0. 1.4445123597 0.
 C -1.2513864325 -0.7402289904 0.
 C 1.2513864325 -0.7402289904 0.
 C -1.2513864325 0.7402289904 0.
 C 1.2513864325 0.7402289904 0.
 C 0. -2.8742029511 0.
 C 0. 2.8742029511 0.
 C -2.4268326337 -1.4689337625 0.
 C 2.4268326337 -1.4689337625 0.
 C -2.4268326337 1.4689337625 0.
 C 2.4268326337 1.4689337625 0.
 C -2.458101908 -2.8873860871 0.
 C 2.458101908 -2.8873860871 0.
 C -2.458101908 2.8873860871 0.
 C 2.458101908 2.8873860871 0.
 C -1.2278611569 -3.597708531 0.
 C 1.2278611569 -3.597708531 0.
 C -1.2278611569 3.597708531 0.
 C 1.2278611569 3.597708531 0.
 C -1.2305243804 -5.0339692605 0.
 C 1.2305243804 -5.0339692605 0.
 C -1.2305243804 5.0339692605 0.
 C 1.2305243804 5.0339692605 0.
 C 0. -5.7213499219 0.
 C 0. 5.7213499219 0.
 H -3.3857744263 -0.9627451262 0.
 H 3.3857744263 -0.9627451262 0.
 H -3.3857744263 0.9627451262 0.
 H 3.3857744263 0.9627451262 0.
 C -3.676145142 -3.6104829953 0.
 C 3.676145142 -3.6104829953 0.
 C -3.676145142 3.6104829953 0.
 C 3.676145142 3.6104829953 0.
 C -2.4752893029 -5.7108229263 0.
 C 2.4752893029 -5.7108229263 0.
 C -2.4752893029 5.7108229263 0.
 C 2.4752893029 5.7108229263 0.
 H 0. -6.8088767379 0.
 H 0. 6.8088767379 0.
 C -3.6741882342 -5.0026600823 0.
 C 3.6741882342 -5.0026600823 0.
 C -3.6741882342 5.0026600823 0.
 C 3.6741882342 5.0026600823 0.
 H -4.6147821682 -3.0624604419 0.
 H 4.6147821682 -3.0624604419 0.
 H -4.6147821682 3.0624604419 0.
 H 4.6147821682 3.0624604419 0.
 H -4.6172390494 -5.5425085736 0.
 H 4.6172390494 -5.5425085736 0.
 H -4.6172390494 5.5425085736 0.
 H 4.6172390494 5.5425085736 0.
 H -2.4809354983 -6.7977241268 0.
 H 2.4809354983 -6.7977241268 0.
 H -2.4809354983 6.7977241268 0.
 H 2.4809354983 6.7977241268 0.

Table S21. Optimized Geometry of Singlet-1, UB3LYP/6-31G*, $E_{\text{Tot}}=-1459.0070251$ Hartree

C 0. 0. -1.4432285601
 C 0. 0. 1.4432285601
 C 0. -1.2511492486 -0.7389190525
 C 0. 1.2511492486 -0.7389190525
 C 0. -1.2511492486 0.7389190525
 C 0. 1.2511492486 0.7389190525
 C 0. 0. -2.873951915
 C 0. 0. 2.873951915
 C 0. -2.427773801 -1.4686878564
 C 0. 2.427773801 -1.4686878564
 C 0. -2.427773801 1.4686878564
 C 0. 2.427773801 1.4686878564
 C 0. -2.4587217058 -2.8866225604
 C 0. 2.4587217058 -2.8866225604
 C 0. -2.4587217058 2.8866225604
 C 0. 2.4587217058 2.8866225604
 C 0. -1.2275168308 -3.5972525385
 C 0. 1.2275168308 -3.5972525385
 C 0. -1.2275168308 3.5972525385
 C 0. 1.2275168308 3.5972525385
 C 0. -1.2301734699 -5.0331542337
 C 0. 1.2301734699 -5.0331542337
 C 0. -1.2301734699 5.0331542337
 C 0. 1.2301734699 5.0331542337
 C 0. 0. -5.7205223281
 C 0. 0. 5.7205223281
 H 0. -3.386435989 -0.9626876194
 H 0. 3.386435989 -0.9626876194
 H 0. -3.386435989 0.9626876194
 H 0. 3.386435989 0.9626876194
 C 0. -3.6763297758 -3.6100559637
 C 0. 3.6763297758 -3.6100559637
 C 0. -3.6763297758 3.6100559637
 C 0. 3.6763297758 3.6100559637
 C 0. -2.475709151 -5.7107332629
 C 0. 2.475709151 -5.7107332629
 C 0. -2.475709151 5.7107332629
 C 0. 2.475709151 5.7107332629
 H 0. 0. -6.8078136547
 H 0. 0. 6.8078136547
 C 0. -3.6742438024 -5.002989091
 C 0. 3.6742438024 -5.002989091
 C 0. -3.6742438024 5.002989091
 C 0. 3.6742438024 5.002989091
 H 0. -4.6151502184 -3.0627168315
 H 0. 4.6151502184 -3.0627168315
 H 0. -4.6151502184 3.0627168315
 H 0. 4.6151502184 3.0627168315
 H 0. -4.6173090699 -5.5424816578
 H 0. 4.6173090699 -5.5424816578
 H 0. -4.6173090699 5.5424816578
 H 0. 4.6173090699 5.5424816578
 H 0. -2.4810257466 -6.7973866991
 H 0. 2.4810257466 -6.7973866991
 H 0. -2.4810257466 6.7973866991
 H 0. 2.4810257466 6.7973866991

Table S22. Optimized Geometry of Triplet-1, UB3LYP/6-31+G*, $E_{\text{Tot}}=-1459.0413404$ Hartree

C 1.4459086049 0. 0.
 C -1.4459086049 0. 0.
 C 0.7410028485 0. -1.2520390373
 C 0.7410028485 0. 1.2520390373
 C -0.7410028485 0. -1.2520390373
 C -0.7410028485 0. 1.2520390373
 C 2.8769198675 0. 0.
 C -2.8769198675 0. 0.
 C 1.4705672156 0. -2.4285415864
 C 1.4705672156 0. 2.4285415864
 C -1.4705672156 0. -2.4285415864
 C -1.4705672156 0. 2.4285415864
 C 2.8901261497 0. -2.4599695458
 C 2.8901261497 0. 2.4599695458
 C -2.8901261497 0. -2.4599695458
 C -2.8901261497 0. 2.4599695458
 C 3.6009529526 0. -1.2288312914
 C 3.6009529526 0. 1.2288312914
 C -3.6009529526 0. -1.2288312914
 C -3.6009529526 0. 1.2288312914
 C 5.0381539418 0. -1.231582736
 C 5.0381539418 0. 1.231582736
 C -5.0381539418 0. -1.231582736
 C -5.0381539418 0. 1.231582736
 C 5.7262440589 0. 0.
 C -5.7262440589 0. 0.
 H 0.9649302702 0. -3.3880504214
 H 0.9649302702 0. 3.3880504214
 H -0.9649302702 0. -3.3880504214
 H -0.9649302702 0. 3.3880504214
 C 3.6135471302 0. -3.67987061
 C 3.6135471302 0. 3.67987061
 C -3.6135471302 0. -3.67987061
 C -3.6135471302 0. 3.67987061
 C 5.7162692715 0. -2.4776596877
 C 5.7162692715 0. 2.4776596877
 C -5.7162692715 0. -2.4776596877
 C -5.7162692715 0. 2.4776596877
 H 6.8142672072 0. 0.
 H -6.8142672072 0. 0.
 C 5.00758045 0. -3.6783440761
 C 5.00758045 0. 3.6783440761
 C -5.00758045 0. -3.6783440761
 C -5.00758045 0. 3.6783440761
 H 3.065766047 0. -4.6192647631
 H 3.065766047 0. 4.6192647631
 H -3.065766047 0. -4.6192647631
 H -3.065766047 0. 4.6192647631
 H 5.5475011361 0. -4.6218076816
 H 5.5475011361 0. 4.6218076816
 H -5.5475011361 0. -4.6218076816
 H -5.5475011361 0. 4.6218076816
 H 6.8035937565 0. -2.4837357629
 H 6.8035937565 0. 2.4837357629
 H -6.8035937565 0. -2.4837357629
 H -6.8035937565 0. 2.4837357629

Table S23. Optimized Geometry of Singlet-1, UB3LYP/6-31+G*, $E_{\text{Tot}}=-1459.0436905$ Hartree

C 0. 0. 1.4446255623
 C 0. 0. -1.4446255623
 C 0. 1.251727386 0.739768696
 C 0. -1.251727386 0.739768696
 C 0. 1.251727386 -0.739768696
 C 0. -1.251727386 -0.739768696
 C 0. 0. 2.8765293132
 C 0. 0. -2.8765293132
 C 0. 2.4294945353 1.4702547635
 C 0. -2.4294945353 1.4702547635
 C 0. 2.4294945353 -1.4702547635
 C 0. -2.4294945353 -1.4702547635
 C 0. 2.4604965949 2.8893213172
 C 0. -2.4604965949 2.8893213172
 C 0. 2.4604965949 -2.8893213172
 C 0. -2.4604965949 -2.8893213172
 C 0. 1.2284646017 3.6004056808
 C 0. -1.2284646017 3.6004056808
 C 0. 1.2284646017 -3.6004056808
 C 0. -1.2284646017 -3.6004056808
 C 0. 1.2311288837 5.0372679614
 C 0. -1.2311288837 5.0372679614
 C 0. 1.2311288837 -5.0372679614
 C 0. -1.2311288837 -5.0372679614
 C 0. 0. 5.7252793142
 C 0. 0. -5.7252793142
 H 0. 3.3889085687 0.9645185229
 H 0. -3.3889085687 0.9645185229
 H 0. 3.3889085687 -0.9645185229
 H 0. -3.3889085687 -0.9645185229
 C 0. 3.6797133727 3.6131138704
 C 0. -3.6797133727 3.6131138704
 C 0. 3.6797133727 -3.6131138704
 C 0. -3.6797133727 -3.6131138704
 C 0. 2.4777941757 5.7161169092
 C 0. -2.4777941757 5.7161169092
 C 0. 2.4777941757 -5.7161169092
 C 0. -2.4777941757 -5.7161169092
 H 0. 0. 6.8133204092
 H 0. 0. -6.8133204092
 C 0. 3.677979459 5.007843884
 C 0. -3.677979459 5.007843884
 C 0. 3.677979459 -5.007843884
 C 0. -3.677979459 -5.007843884
 H 0. 4.6193704816 3.0657748537
 H 0. -4.6193704816 3.0657748537
 H 0. 4.6193704816 -3.0657748537
 H 0. -4.6193704816 -3.0657748537
 H 0. 4.6215180276 5.5476354519
 H 0. -4.6215180276 5.5476354519
 H 0. 4.6215180276 -5.5476354519
 H 0. -4.6215180276 -5.5476354519
 H 0. 2.4834181341 6.803443519
 H 0. -2.4834181341 6.803443519
 H 0. 2.4834181341 -6.803443519
 H 0. -2.4834181341 -6.803443519

Table S24. Optimized Geometry of Triplet-1, UB3LYP/6-311G**, $E_{\text{Tot}}=-1459.3102420$ Hartree

C 0. -1.4431386033 0.
 C 0. 1.4431386033 0.
 C -1.2498140493 -0.7400752726 0.
 C 1.2498140493 -0.7400752726 0.
 C -1.2498140493 0.7400752726 0.
 C 1.2498140493 0.7400752726 0.
 C 0. -2.8710003255 0.
 C 0. 2.8710003255 0.
 C -2.423431507 -1.4669580853 0.
 C 2.423431507 -1.4669580853 0.
 C -2.423431507 1.4669580853 0.
 C 2.423431507 1.4669580853 0.
 C -2.4548552851 -2.8839006108 0.
 C 2.4548552851 -2.8839006108 0.
 C -2.4548552851 2.8839006108 0.
 C 2.4548552851 2.8839006108 0.
 C -1.2264041615 -3.5932533516 0.
 C 1.2264041615 -3.5932533516 0.
 C -1.2264041615 3.5932533516 0.
 C 1.2264041615 3.5932533516 0.
 C -1.2287278015 -5.0276159786 0.
 C 1.2287278015 -5.0276159786 0.
 C -1.2287278015 5.0276159786 0.
 C 1.2287278015 5.0276159786 0.
 C 0. -5.7142525329 0.
 C 0. 5.7142525329 0.
 H -3.380105965 -0.9611435785 0.
 H 3.380105965 -0.9611435785 0.
 H -3.380105965 0.9611435785 0.
 H 3.380105965 0.9611435785 0.
 C -3.6712656468 -3.6066282972 0.
 C 3.6712656468 -3.6066282972 0.
 C -3.6712656468 3.6066282972 0.
 C 3.6712656468 3.6066282972 0.
 C -2.4723499376 -5.7035354426 0.
 C 2.4723499376 -5.7035354426 0.
 C -2.4723499376 5.7035354426 0.
 C 2.4723499376 5.7035354426 0.
 H 0. -6.7996129888 0.
 H 0. 6.7996129888 0.
 C -3.6687349933 -4.9963883657 0.
 C 3.6687349933 -4.9963883657 0.
 C -3.6687349933 4.9963883657 0.
 C 3.6687349933 4.9963883657 0.
 H -4.6087245713 -3.0610514165 0.
 H 4.6087245713 -3.0610514165 0.
 H -4.6087245713 3.0610514165 0.
 H 4.6087245713 3.0610514165 0.
 H -4.6098993422 -5.5349872276 0.
 H 4.6098993422 -5.5349872276 0.
 H -4.6098993422 5.5349872276 0.
 H 4.6098993422 5.5349872276 0.
 H -2.4789849817 -6.7882184503 0.
 H 2.4789849817 -6.7882184503 0.
 H -2.4789849817 6.7882184503 0.
 H 2.4789849817 6.7882184503 0.

Table S25. Optimized Geometry of Singlet-1, UB3LYP/6-311G**, $E_{\text{Tot}}=-1459.3115541$ Hartree

C 0. 0. -1.4416859694
 C 0. 0. 1.4416859694
 C 0. -1.2495132122 -0.7385880699
 C 0. 1.2495132122 -0.7385880699
 C 0. -1.2495132122 0.7385880699
 C 0. 1.2495132122 0.7385880699
 C 0. 0. -2.8705115345
 C 0. 0. 2.8705115345
 C 0. -2.4242366548 -1.4666271999
 C 0. 2.4242366548 -1.4666271999
 C 0. -2.4242366548 1.4666271999
 C 0. 2.4242366548 1.4666271999
 C 0. -2.455338379 -2.8828898363
 C 0. 2.455338379 -2.8828898363
 C 0. -2.455338379 2.8828898363
 C 0. 2.455338379 2.8828898363
 C 0. -1.2259897887 -3.5925830749
 C 0. 1.2259897887 -3.5925830749
 C 0. -1.2259897887 3.5925830749
 C 0. 1.2259897887 3.5925830749
 C 0. -1.2282946774 -5.0265073098
 C 0. 1.2282946774 -5.0265073098
 C 0. -1.2282946774 5.0265073098
 C 0. 1.2282946774 5.0265073098
 C 0. 0. -5.7130152352
 C 0. 0. 5.7130152352
 H 0. -3.380795634 -0.9608877744
 H 0. 3.380795634 -0.9608877744
 H 0. -3.380795634 0.9608877744
 H 0. 3.380795634 0.9608877744
 C 0. -3.6711148017 -3.6059526745
 C 0. 3.6711148017 -3.6059526745
 C 0. -3.6711148017 3.6059526745
 C 0. 3.6711148017 3.6059526745
 C 0. -2.4725743241 -5.7031223358
 C 0. 2.4725743241 -5.7031223358
 C 0. -2.4725743241 5.7031223358
 C 0. 2.4725743241 5.7031223358
 H 0. 0. -6.7983101387
 H 0. 0. 6.7983101387
 C 0. -3.6684561428 -4.9964026612
 C 0. 3.6684561428 -4.9964026612
 C 0. -3.6684561428 4.9964026612
 C 0. 3.6684561428 4.9964026612
 H 0. -4.6088052066 -3.0607974583
 H 0. 4.6088052066 -3.0607974583
 H 0. -4.6088052066 3.0607974583
 H 0. 4.6088052066 3.0607974583
 H 0. -4.6097157557 -5.5348424106
 H 0. 4.6097157557 -5.5348424106
 H 0. -4.6097157557 5.5348424106
 H 0. 4.6097157557 5.5348424106
 H 0. -2.478800119 -6.7876852604
 H 0. 2.478800119 -6.7876852604
 H 0. -2.478800119 6.7876852604
 H 0. 2.478800119 6.7876852604

Table S26. Optimized Geometry of Dikation of **1**, RB3LYP/6-31G*, $E_{\text{Tot}}=-1458.5118335$ Hartree

C 0. 0. 1.4445016056
 C 0. 0. -1.4445016056
 C 0. 1.2531830104 0.7401565824
 C 0. -1.2531830104 0.7401565824
 C 0. 1.2531830104 -0.7401565824
 C 0. -1.2531830104 -0.7401565824
 C 0. 0. 2.8755537934
 C 0. 0. -2.8755537934
 C 0. 2.4283010835 1.4727740825
 C 0. -2.4283010835 1.4727740825
 C 0. 2.4283010835 -1.4727740825
 C 0. -2.4283010835 -1.4727740825
 C 0. 2.4493084644 2.8926368979
 C 0. -2.4493084644 2.8926368979
 C 0. 2.4493084644 -2.8926368979
 C 0. -2.4493084644 -2.8926368979
 C 0. 1.2209999657 3.5971539436
 C 0. -1.2209999657 3.5971539436
 C 0. 1.2209999657 -3.5971539436
 C 0. -1.2209999657 -3.5971539436
 C 0. 1.2252022227 5.0295011839
 C 0. -1.2252022227 5.0295011839
 C 0. 1.2252022227 -5.0295011839
 C 0. -1.2252022227 -5.0295011839
 C 0. 0. 5.718872379
 C 0. 0. -5.718872379
 H 0. 3.3899664485 0.9729531619
 H 0. -3.3899664485 0.9729531619
 H 0. 3.3899664485 -0.9729531619
 H 0. -3.3899664485 -0.9729531619
 C 0. 3.6585193268 3.6246412985
 C 0. -3.6585193268 3.6246412985
 C 0. 3.6585193268 -3.6246412985
 C 0. -3.6585193268 -3.6246412985
 C 0. 2.4650477175 5.7206406454
 C 0. -2.4650477175 5.7206406454
 C 0. 2.4650477175 -5.7206406454
 C 0. -2.4650477175 -5.7206406454
 H 0. 0. 6.8063352564
 H 0. 0. -6.8063352564
 C 0. 3.6659695015 5.0216275221
 C 0. -3.6659695015 5.0216275221
 C 0. 3.6659695015 -5.0216275221
 C 0. -3.6659695015 -5.0216275221
 H 0. 4.6022009041 3.0852060873
 H 0. -4.6022009041 3.0852060873
 H 0. 4.6022009041 -3.0852060873
 H 0. -4.6022009041 -3.0852060873
 H 0. 4.6087793524 5.5580991682
 H 0. -4.6087793524 5.5580991682
 H 0. 4.6087793524 -5.5580991682
 H 0. -4.6087793524 -5.5580991682
 H 0. 2.4659845829 6.8070991015
 H 0. -2.4659845829 6.8070991015
 H 0. 2.4659845829 -6.8070991015
 H 0. -2.4659845829 -6.8070991015

Table S27. Optimized Geometry of Dikation of **1**, RB3LYP/6-31+G*, $E_{\text{Tot}}=-1458.5324858$ Hartree

C 0. 0. 1.4455301188
 C 0. 0. -1.4455301188
 C 0. 1.2535289543 0.7407112905
 C 0. -1.2535289543 0.7407112905
 C 0. 1.2535289543 -0.7407112905
 C 0. -1.2535289543 -0.7407112905
 C 0. 0. 2.8776543389
 C 0. 0. -2.8776543389
 C 0. 2.4296918204 1.4734940086
 C 0. -2.4296918204 1.4734940086
 C 0. 2.4296918204 -1.4734940086
 C 0. -2.4296918204 -1.4734940086
 C 0. 2.4513512317 2.8942172991
 C 0. -2.4513512317 2.8942172991
 C 0. 2.4513512317 -2.8942172991
 C 0. -2.4513512317 -2.8942172991
 C 0. 1.222157291 3.5987286393
 C 0. -1.222157291 3.5987286393
 C 0. 1.222157291 -3.5987286393
 C 0. -1.222157291 -3.5987286393
 C 0. 1.2256868193 5.0315855498
 C 0. -1.2256868193 5.0315855498
 C 0. 1.2256868193 -5.0315855498
 C 0. -1.2256868193 -5.0315855498
 C 0. 0. 5.7218762806
 C 0. 0. -5.7218762806
 H 0. 3.3916875866 0.9736850803
 H 0. -3.3916875866 0.9736850803
 H 0. 3.3916875866 -0.9736850803
 H 0. -3.3916875866 -0.9736850803
 C 0. 3.6616268792 3.626723808
 C 0. -3.6616268792 3.626723808
 C 0. 3.6616268792 -3.626723808
 C 0. -3.6616268792 -3.626723808
 C 0. 2.4662936727 5.7239011207
 C 0. -2.4662936727 5.7239011207
 C 0. 2.4662936727 -5.7239011207
 C 0. -2.4662936727 -5.7239011207
 H 0. 0. 6.8097408741
 H 0. 0. -6.8097408741
 C 0. 3.6682962459 5.0247573421
 C 0. -3.6682962459 5.0247573421
 C 0. 3.6682962459 -5.0247573421
 C 0. -3.6682962459 -5.0247573421
 H 0. 4.606054185 3.0878778267
 H 0. -4.606054185 3.0878778267
 H 0. 4.606054185 -3.0878778267
 H 0. -4.606054185 -3.0878778267
 H 0. 4.61119737 5.5617449019
 H 0. -4.61119737 5.5617449019
 H 0. 4.61119737 -5.5617449019
 H 0. -4.61119737 -5.5617449019
 H 0. 2.4674172562 6.8107243705
 H 0. -2.4674172562 6.8107243705
 H 0. 2.4674172562 -6.8107243705
 H 0. -2.4674172562 -6.8107243705

Table S28. Optimized Geometry of Dianion of **1**, RB3LYP/6-31G*, $E_{\text{Tot}}=-1459.0313075$ Hartree

C 0. 0. 1.4461424724
 C 0. 0. -1.4461424724
 C 0. 1.2493171084 0.7421554936
 C 0. -1.2493171084 0.7421554936
 C 0. 1.2493171084 -0.7421554936
 C 0. -1.2493171084 -0.7421554936
 C 0. 0. 2.8829175565
 C 0. 0. -2.8829175565
 C 0. 2.4261307147 1.4712604251
 C 0. -2.4261307147 1.4712604251
 C 0. 2.4261307147 -1.4712604251
 C 0. -2.4261307147 -1.4712604251
 C 0. 2.469442496 2.8925705737
 C 0. -2.469442496 2.8925705737
 C 0. 2.469442496 -2.8925705737
 C 0. -2.469442496 -2.8925705737
 C 0. 1.2331512448 3.6090240666
 C 0. -1.2331512448 3.6090240666
 C 0. 1.2331512448 -3.6090240666
 C 0. -1.2331512448 -3.6090240666
 C 0. 1.230624409 5.0539192605
 C 0. -1.230624409 5.0539192605
 C 0. 1.230624409 -5.0539192605
 C 0. -1.230624409 -5.0539192605
 C 0. 0. 5.7345724023
 C 0. 0. -5.7345724023
 H 0. 3.3836068581 0.9592832577
 H 0. -3.3836068581 0.9592832577
 H 0. 3.3836068581 -0.9592832577
 H 0. -3.3836068581 -0.9592832577
 C 0. 3.6930227135 3.6074318621
 C 0. -3.6930227135 3.6074318621
 C 0. 3.6930227135 -3.6074318621
 C 0. -3.6930227135 -3.6074318621
 C 0. 2.4901012922 5.7199258612
 C 0. -2.4901012922 5.7199258612
 C 0. 2.4901012922 -5.7199258612
 C 0. -2.4901012922 -5.7199258612
 H 0. 0. 6.8248906325
 H 0. 0. -6.8248906325
 C 0. 3.6806284592 5.0019960826
 C 0. -3.6806284592 5.0019960826
 C 0. 3.6806284592 -5.0019960826
 C 0. -3.6806284592 -5.0019960826
 H 0. 4.6309676352 3.0551846772
 H 0. -4.6309676352 3.0551846772
 H 0. 4.6309676352 -3.0551846772
 H 0. -4.6309676352 -3.0551846772
 H 0. 4.6281282478 5.5442560226
 H 0. -4.6281282478 5.5442560226
 H 0. 4.6281282478 -5.5442560226
 H 0. -4.6281282478 -5.5442560226
 H 0. 2.503588561 6.8093814092
 H 0. -2.503588561 6.8093814092
 H 0. 2.503588561 -6.8093814092
 H 0. -2.503588561 -6.8093814092

Table S29. Optimized Geometry of Dianion of **1**, RB3LYP/6-31+G*, $E_{\text{Tot}}=-1459.0954933$ Hartree

C 0. 0. 1.447501985
 C 0. 0. -1.447501985
 C 0. 1.2495938541 0.7428149704
 C 0. -1.2495938541 0.7428149704
 C 0. 1.2495938541 -0.7428149704
 C 0. -1.2495938541 -0.7428149704
 C 0. 0. 2.885277852
 C 0. 0. -2.885277852
 C 0. 2.4280999832 1.4719166601
 C 0. -2.4280999832 1.4719166601
 C 0. 2.4280999832 -1.4719166601
 C 0. -2.4280999832 -1.4719166601
 C 0. 2.4721052811 2.8938831069
 C 0. -2.4721052811 2.8938831069
 C 0. 2.4721052811 -2.8938831069
 C 0. -2.4721052811 -2.8938831069
 C 0. 1.234901709 3.610444055
 C 0. -1.234901709 3.610444055
 C 0. 1.234901709 -3.610444055
 C 0. -1.234901709 -3.610444055
 C 0. 1.231746617 5.0558204885
 C 0. -1.231746617 5.0558204885
 C 0. 1.231746617 -5.0558204885
 C 0. -1.231746617 -5.0558204885
 C 0. 0. 5.7377376265
 C 0. 0. -5.7377376265
 H 0. 3.3857152242 0.9602481676
 H 0. -3.3857152242 0.9602481676
 H 0. 3.3857152242 -0.9602481676
 H 0. -3.3857152242 -0.9602481676
 C 0. 3.698598204 3.609510403
 C 0. -3.698598204 3.609510403
 C 0. 3.698598204 -3.609510403
 C 0. -3.698598204 -3.609510403
 C 0. 2.4925889529 5.7247425424
 C 0. -2.4925889529 5.7247425424
 C 0. 2.4925889529 -5.7247425424
 C 0. -2.4925889529 -5.7247425424
 H 0. 0. 6.8285051299
 H 0. 0. -6.8285051299
 C 0. 3.6860015929 5.0067070405
 C 0. -3.6860015929 5.0067070405
 C 0. 3.6860015929 -5.0067070405
 C 0. -3.6860015929 -5.0067070405
 H 0. 4.6375225651 3.0582461292
 H 0. -4.6375225651 3.0582461292
 H 0. 4.6375225651 -3.0582461292
 H 0. -4.6375225651 -3.0582461292
 H 0. 4.6331262486 5.5487326925
 H 0. -4.6331262486 5.5487326925
 H 0. 4.6331262486 -5.5487326925
 H 0. -4.6331262486 -5.5487326925
 H 0. 2.5059093859 6.8144395494
 H 0. -2.5059093859 6.8144395494
 H 0. 2.5059093859 -6.8144395494
 H 0. -2.5059093859 -6.8144395494

Table S30. Optimized Geometry of Doublet-3, UB3LYP/6-31G*, $E_{\text{Tot}}=-730.6940902$ Hartree

H 0. 0. -3.3167844395
C 0. 0. -2.2290351907
C 1.2342117434 0. -1.5449907922
C -1.2342117434 0. -1.5449907922
C 1.2354422787 0. -0.1085124652
C -1.2354422787 0. -0.1085124652
C 0. 0. 0.6029253864
C 2.4782786046 0. -2.2236041037
C -2.4782786046 0. -2.2236041037
C 2.4694133646 0. 0.603912128
C -2.4694133646 0. 0.603912128
C 0. 0. 2.0291345828
C 3.6771371731 0. -1.5168035177
C -3.6771371731 0. -1.5168035177
C 3.6823910207 0. -0.1226479876
C -3.6823910207 0. -0.1226479876
C 2.4354590293 0. 2.033066223
C -2.4354590293 0. 2.033066223
C 1.2471161011 0. 2.7159704257
C -1.2471161011 0. 2.7159704257
H 2.4834201085 0. -3.3107252811
H -2.4834201085 0. -3.3107252811
H 4.6198036737 0. -2.0578176145
H -4.6198036737 0. -2.0578176145
H 4.6236495798 0. 0.4212601335
H -4.6236495798 0. 0.4212601335
H 3.3783418205 0. 2.5747126485
H -3.3783418205 0. 2.5747126485
H 1.2417065228 0. 3.8035485357
H -1.2417065228 0. 3.8035485357

Table S31. Optimized Geometry of Doublet-3, UB3LYP/6-31+G*, $E_{\text{Tot}}=-730.7156643$ Hartree

H 0. 0. -3.3185972802
C 0. 0. -2.2304417835
C 1.2351091464 0. -1.545580405
C -1.2351091464 0. -1.545580405
C 1.2365530794 0. -0.1083321073
C -1.2365530794 0. -0.1083321073
C 0. 0. 0.6035893192
C 2.4800799216 0. -2.2256546216
C -2.4800799216 0. -2.2256546216
C 2.4714341583 0. 0.604248976
C -2.4714341583 0. 0.604248976
C 0. 0. 2.0304533447
C 3.6806679994 0. -1.5185962641
C -3.6806679994 0. -1.5185962641
C 3.6858742501 0. -0.1227671251
C -3.6858742501 0. -0.1227671251
C 2.4379246976 0. 2.0346296198
C -2.4379246976 0. 2.0346296198
C 1.2480183989 0. 2.718299215
C -1.2480183989 0. 2.718299215
H 2.4856410595 0. -3.3131330218
H -2.4856410595 0. -3.3131330218
H 4.6233717226 0. -2.0599719896
H -4.6233717226 0. -2.0599719896
H 4.6278227391 0. 0.4206147772
H -4.6278227391 0. 0.4206147772
H 3.3805810933 0. 2.5773096591
H -3.3805810933 0. 2.5773096591
H 1.2436223328 0. 3.8061928482
H -1.2436223328 0. 3.8061928482

Table S32. Optimized Geometry of Kation of **3**, RB3LYP/6-31G*, $E_{\text{Tot}}=-730.482062$ Hartree

H 0. 0. -3.3104209819
C 0. 0. -2.2225985868
C 1.2281858509 0. -1.5376018918
C -1.2281858509 0. -1.5376018918
C 1.2270482767 0. -0.1051740527
C -1.2270482767 0. -0.1051740527
C 0. 0. 0.6040466954
C 2.4691419824 0. -2.229227963
C -2.4691419824 0. -2.229227963
C 2.4587636075 0. 0.6041893482
C -2.4587636075 0. 0.6041893482
C 0. 0. 2.0336802165
C 3.6659710625 0. -1.5299813183
C -3.6659710625 0. -1.5299813183
C 3.6604909524 0. -0.1283998413
C -3.6604909524 0. -0.1283998413
C 2.4339666393 0. 2.0358828106
C -2.4339666393 0. 2.0358828106
C 1.2474799922 0. 2.7231498042
C -1.2474799922 0. 2.7231498042
H 2.469558552 0. -3.3158686744
H -2.469558552 0. -3.3158686744
H 4.6099998673 0. -2.0647783719
H -4.6099998673 0. -2.0647783719
H 4.6053542338 0. 0.4092380009
H -4.6053542338 0. 0.4092380009
H 3.3771298524 0. 2.5751029676
H -3.3771298524 0. 2.5751029676
H 1.2450798986 0. 3.8091102181
H -1.2450798986 0. 3.8091102181

Table S33. Optimized Geometry of Kation of **3**, RB3LYP/6-31+G*, $E_{\text{Tot}}=-730.4955431$ Hartree

H 0. 0. -3.3120606593
C 0. 0. -2.2239156273
C 1.2289639625 0. -1.5382050843
C -1.2289639625 0. -1.5382050843
C 1.2279965743 0. -0.1051013065
C -1.2279965743 0. -0.1051013065
C 0. 0. 0.60454563
C 2.4706495287 0. -2.2307126523
C -2.4706495287 0. -2.2307126523
C 2.4605150884 0. 0.6044201557
C -2.4605150884 0. 0.6044201557
C 0. 0. 2.0348032964
C 3.668771161 0. -1.5311539732
C -3.668771161 0. -1.5311539732
C 3.6634059003 0. -0.12854077
C -3.6634059003 0. -0.12854077
C 2.4359341913 0. 2.0371002623
C -2.4359341913 0. 2.0371002623
C 1.2482633599 0. 2.7249404733
C -1.2482633599 0. 2.7249404733
H 2.4715592051 0. -3.3176817311
H -2.4715592051 0. -3.3176817311
H 4.6128660619 0. -2.0664654085
H -4.6128660619 0. -2.0664654085
H 4.6087209883 0. 0.4088967109
H -4.6087209883 0. 0.4088967109
H 3.3789496123 0. 2.5772422695
H -3.3789496123 0. 2.5772422695
H 1.2467093968 0. 3.8112559621
H -1.2467093968 0. 3.8112559621

Table S34. Optimized Geometry of Anion of **3**, RB3LYP/6-31G*, $E_{\text{Tot}}=-730.7369818$ Hartree

H 0. 0. -3.3236830625
C 0. 0. -2.2339763662
C 1.2328932867 0. -1.5565505185
C -1.2328932867 0. -1.5565505185
C 1.2401902395 0. -0.1122224905
C -1.2401902395 0. -0.1122224905
C 0. 0. 0.6003809535
C 2.4916980074 0. -2.225114998
C -2.4916980074 0. -2.225114998
C 2.4838093858 0. 0.6036021433
C -2.4838093858 0. 0.6036021433
C 0. 0. 2.0340720601
C 3.681619219 0. -1.5121046261
C -3.681619219 0. -1.5121046261
C 3.6989053016 0. -0.1138919876
C -3.6989053016 0. -0.1138919876
C 2.4376360378 0. 2.0363662438
C -2.4376360378 0. 2.0363662438
C 1.2461533249 0. 2.7151015451
C -1.2461533249 0. 2.7151015451
H 2.5025378749 0. -3.3139903163
H -2.5025378749 0. -3.3139903163
H 4.6271380435 0. -2.0559156041
H -4.6271380435 0. -2.0559156041
H 4.6409179477 0. 0.4314971754
H -4.6409179477 0. 0.4314971754
H 3.3805624131 0. 2.5820460455
H -3.3805624131 0. 2.5820460455
H 1.2394444684 0. 3.8056624197
H -1.2394444684 0. 3.8056624197

Table S35. Optimized Geometry of Anion of **3**, RB3LYP/6-31+G*, $E_{\text{Tot}}=-730.7725246$ Hartree

H 0. 0. -3.3251754534
C 0. 0. -2.2350645509
C 1.2341583544 0. -1.5567065122
C -1.2341583544 0. -1.5567065122
C 1.2415688686 0. -0.1116913357
C -1.2415688686 0. -0.1116913357
C 0. 0. 0.6013224736
C 2.4937698674 0. -2.227843296
C -2.4937698674 0. -2.227843296
C 2.4857329478 0. 0.6042027673
C -2.4857329478 0. 0.6042027673
C 0. 0. 2.0353325276
C 3.6864321245 0. -1.5147492146
C -3.6864321245 0. -1.5147492146
C 3.7033860842 0. -0.1141905456
C -3.7033860842 0. -0.1141905456
C 2.4406140808 0. 2.0380330817
C -2.4406140808 0. 2.0380330817
C 1.2470751652 0. 2.7179447625
C -1.2470751652 0. 2.7179447625
H 2.5047946471 0. -3.3169947383
H -2.5047946471 0. -3.3169947383
H 4.6314866938 0. -2.0589342771
H -4.6314866938 0. -2.0589342771
H 4.6461335292 0. 0.4304795652
H -4.6461335292 0. 0.4304795652
H 3.3831864261 0. 2.5846749612
H -3.3831864261 0. 2.5846749612
H 1.2415077662 0. 3.8085926197
H -1.2415077662 0. 3.8085926197

Table S36. Optimized Geometry of Triplet-4, UB3LYP/6-31G*, $E_{\text{Tot}}=-1459.0147071$ Hartree

C 0. -0.3579108474 -1.2310501714
 C 0. -0.3577400701 1.6437353183
 C 0. -1.6001064197 -0.5249358615
 C 0. 0.8956218435 -0.5254542781
 C 0. -1.6072061488 0.93161497
 C 0. 0.8930665241 0.9428744766
 C 0. -0.3550740414 -2.6587892735
 C 0. -0.363100756 3.0749670013
 C 0. -2.8015923607 -1.2803775336
 C 0. 2.0781047055 -1.2618812891
 C 0. -2.7940123963 1.6655771074
 C 0. 2.0735698392 1.6802137016
 C 0. -2.8062177029 -2.6529154242
 C 0. 2.1040103555 -2.6654447263
 C 0. -2.8252793243 3.0790047332
 C 0. 2.0975345151 3.0941735914
 C 0. -1.5909989612 -3.3931347356
 C 0. 0.8696795944 -3.3811441119
 C 0. -1.5933432681 3.794291563
 C 0. 0.8616395054 3.8013934284
 C 0. -1.5722593808 -4.7922354009
 C 0. 0.8750798608 -4.8049834442
 C 0. -1.5999710894 5.2288564934
 C 0. 0.8596364909 5.2369615973
 C 0. -0.3642625091 -5.5248600821
 C 0. -0.3722813416 5.9197072078
 H 0. -3.756919269 -0.7693621488
 H 0. 3.0363452708 -0.754042109
 H 0. -3.7513074478 1.1571174855
 H 0. 3.033404439 1.1760586663
 H 0. -3.7490841317 -3.1939581671
 C 0. 3.3305668181 -3.403047219
 C 0. -4.0446100923 3.8024254435
 C 0. 3.313061123 3.8244078485
 H 0. -2.5165930627 -5.3321916083
 C 0. 2.112259564 -5.5173136191
 C 0. -2.8479664204 5.9051149826
 C 0. 2.1033265701 5.9197971697
 C 0. -0.3299545697 -6.9406368447
 H 0. -0.3759698316 7.0073125706
 C 0. 0.8804491492 -7.6216547525
 C 0. 3.3358373326 -4.7681958571
 C 0. -4.0450171179 5.1953145745
 C 0. 3.304938213 5.2168224462
 H 0. -1.2684182597 -7.4892620379
 H 0. 4.2670525138 -2.8502898059
 H 0. -4.9827732452 3.2534948208
 H 0. 4.2542025672 3.2806652923
 H 0. 0.8872635728 -8.70830859
 H 0. 4.2762208649 -5.3139153065
 H 0. -4.9893521722 5.7330281825
 H 0. 4.2459118852 5.7604133954
 C 0. 2.0917198337 -6.9239707843
 H 0. 3.0335527518 -7.4668017436
 H 0. -2.8547420091 6.991976991
 H 0. 2.1040234421 7.0066946392

Table S37. Optimized Geometry of Singlet-4, UB3LYP/6-31G*, $E_{\text{Tot}}=-1459.0097948$ Hartree

C 0. -0.3597858727 -1.2330744948
 C 0. -0.3584477509 1.6496048287
 C 0. -1.6009739503 -0.5291280961
 C 0. 0.8958227498 -0.5274672373
 C 0. -1.6097295832 0.9382162385
 C 0. 0.8932905589 0.9478663781
 C 0. -0.3565139012 -2.6606892441
 C 0. -0.3633662699 3.0775897729
 C 0. -2.797822862 -1.2804211352
 C 0. 2.073427238 -1.2604428786
 C 0. -2.7897822707 1.6660049807
 C 0. 2.0696009834 1.6814773882
 C 0. -2.8030507962 -2.6576010627
 C 0. 2.1012936961 -2.6695679471
 C 0. -2.8232241952 3.0839014027
 C 0. 2.0951977475 3.0975665445
 C 0. -1.5911093956 -3.3942425165
 C 0. 0.869508723 -3.3840359069
 C 0. -1.594796226 3.7976332744
 C 0. 0.8624546959 3.8042343718
 C 0. -1.5710394606 -4.7984942858
 C 0. 0.8757272686 -4.8085214762
 C 0. -1.6014371746 5.2334771075
 C 0. 0.8609548167 5.2410248173
 C 0. -0.3641149002 -5.5293888501
 C 0. -0.3714311341 5.9247137412
 H 0. -3.7537458431 -0.7700199682
 H 0. 3.0324087148 -0.7536444394
 H 0. -3.7475286572 1.1579420161
 H 0. 3.0296874081 1.1773744603
 H 0. -3.7467678382 -3.197118212
 C 0. 3.3265251644 -3.4032328515
 C 0. -4.043118008 3.8045929711
 C 0. 3.312690615 3.8258535108
 H 0. -2.5157637095 -5.3375603567
 C 0. 2.1123072805 -5.5188541212
 C 0. -2.8463940596 5.9069769474
 C 0. 2.1032799319 5.9211614318
 C 0. -0.3282036547 -6.9455611392
 H 0. -0.3748375333 7.0122130008
 C 0. 0.8839257016 -7.6264401694
 C 0. 3.3333860327 -4.7707360474
 C 0. -4.04437762 5.1958840013
 C 0. 3.3056849147 5.2165542491
 H 0. -1.2661087396 -7.4950607408
 H 0. 4.2627805107 -2.8500745493
 H 0. -4.9806583861 3.2546118645
 H 0. 4.252955097 3.2806563023
 H 0. 0.8906093497 -8.7132017005
 H 0. 4.2746152362 -5.3150091156
 H 0. -4.9887513167 5.7337258365
 H 0. 4.2467850444 5.7600962772
 C 0. 2.0931907176 -6.9292218025
 H 0. 3.0360447849 -7.4701900577
 H 0. -2.85480668 6.9938866875
 H 0. 2.1057840538 7.0080965247

Table S38. Optimized Geometry of Triplet-**5**, UB3LYP/6-31G*, $E_{\text{Tot}}=-1459.0084516$ Hartree

C -1.6521179476 0.0034137549 -0.6027394161
 C 1.1988248087 -0.0210961014 -0.6031534439
 C -0.9453593671 -0.0221117047 -1.8420518751
 C -0.9561989289 -0.0756844736 0.6438865952
 C 0.4989500815 -0.1899693305 -1.8389420386
 C 0.4805319571 0.128954522 0.6347531523
 C -3.0821473688 0.1339053649 -0.6177324014
 C 2.6270876132 0.0185020957 -0.6059231139
 C -1.6725952896 0.1346806101 -3.0479157332
 C -1.7194746304 -0.3375203179 1.8520955462
 C 1.2289425627 -0.4568044056 -3.0000273805
 C 1.2068714299 0.5230668718 1.7684518458
 C -3.0355922736 0.3075873261 -3.0560541383
 C -3.1439816123 -0.1696126761 1.8301041475
 C 2.6412444475 -0.5064901475 -3.0134679204
 C 2.6168233598 0.6270960298 1.7779741015
 C -3.7761175445 0.3115698424 -1.8458212269
 C -3.8192943785 0.1059871061 0.6030653881
 C 3.3502350205 -0.2359132578 -1.8054157683
 C 3.340943746 0.3263233103 0.5868858262
 C -5.1862553566 0.5011838176 -1.8312705333
 C -5.2314545324 0.2800442588 0.5869572792
 C 4.7851659792 -0.225750166 -1.8025512341
 C 4.7737854263 0.3734667805 0.5848242199
 C -5.8889967756 0.4943085653 -0.6537884104
 C 5.4658291184 0.0788909466 -0.6069392299
 H -1.1394946554 0.1567249616 -3.9917462064
 C -1.1453141749 -0.8204211846 3.0469683296
 H 0.7124618091 -0.6433676038 -3.9357524448
 H 0.6788835359 0.790954612 2.6755022517
 H -3.5625019399 0.4508597378 -3.996033369
 C -3.9065723136 -0.3203690002 3.0283844852
 C 3.3754087715 -0.789384946 -4.1942216429
 C 3.3348989123 1.0000369436 2.9431618247
 H -5.699935817 0.651019657 -2.7776989747
 C -5.9547954882 0.1995117031 1.8145133806
 C 5.4699342642 -0.5153155119 -3.0118251751
 C 5.4440750222 0.7302184768 1.7848362239
 H -6.9672547336 0.6341877466 -0.6562482935
 H 6.5532339855 0.100712933 -0.6075019611
 C -1.9023485552 -0.9984148794 4.2068162064
 C -5.3196616167 -0.0977420219 2.9862093205
 C 4.7679201086 -0.7946806382 -4.1813900664
 C 4.7274605354 1.0437490837 2.93631364
 H -0.1003047056 -1.101830403 3.0616231838
 C -3.2594215809 -0.7134819261 4.2173662416
 H 2.8342121718 -0.9981268471 -5.1133928504
 H 2.7826893945 1.2404102907 3.8479463951
 H -1.4173180577 -1.3701422922 5.105419305
 H -5.8835657425 -0.1870773513 3.9114315058
 H 5.3129857147 -1.0139829463 -5.0956067161
 H 5.2603529393 1.3241506409 3.8409769651
 H -3.8438956723 -0.829830397 5.1264587782
 H -7.031116636 0.3526674742 1.7946331498
 H 6.5568192516 -0.5139267741 -3.01200719
 H 6.5303485806 0.7661882361 1.7879744364

Table S39. Optimized Geometry of Singlet-**5**, UB3LYP/6-31G*, $E_{\text{Tot}}=-1459.0015607$ Hartree

C -1.6544624815 0.0247495076 -0.600814933
 C 1.2050093626 -0.0170772848 -0.6007137709
 C -0.9475599262 0.003962242 -1.839463923
 C -0.9604637811 -0.0651758897 0.646045394
 C 0.5030226368 -0.1869028239 -1.8366029566
 C 0.486065552 0.1462750978 0.6381562578
 C -3.0837609894 0.151534666 -0.6168099908
 C 2.6281253817 0.0182923586 -0.6042272926
 C -1.6674186512 0.1822657957 -3.0400873856
 C -1.7179391849 -0.3405848019 1.846821546
 C 1.2250944485 -0.4687319092 -2.989583846
 C 1.2039377847 0.5500373558 1.7599169593
 C -3.0343662008 0.3602967704 -3.050152701
 C -3.1460720179 -0.1874949267 1.8249292763
 C 2.6401506965 -0.5304760649 -3.0034544389
 C 2.6207659246 0.6544647244 1.7701615108
 C -3.7762695694 0.3443825745 -1.844830872
 C -3.8219147371 0.0998913037 0.601996833
 C 3.3499777151 -0.2512527819 -1.8025488996
 C 3.3429343927 0.339602722 0.5873110603
 C -5.1894140589 0.5268093293 -1.828687882
 C -5.2361483564 0.2659074262 0.5863585836
 C 4.7874121533 -0.2466303506 -1.7999376893
 C 4.7771660291 0.381931083 0.585157093
 C -5.8929819 0.4967331286 -0.653312132
 C 5.4694019728 0.0690981355 -0.6066026263
 H -1.131813119 0.2133463298 -3.9825070165
 C -1.1384483105 -0.8196929112 3.0445786984
 H 0.7068983263 -0.6538963773 -3.9249687197
 H 0.6777278407 0.8162696888 2.6687210347
 H -3.5570263915 0.518198885 -3.9900895874
 C -3.9078419931 -0.3543396294 3.0213775606
 C 3.3715857022 -0.830258447 -4.1834277574
 C 3.3360130958 1.0346139875 2.9327631918
 H -5.7024437887 0.6887523099 -2.773453184
 C -5.9592295185 0.162456117 1.8102105254
 C 5.4672554121 -0.5519222153 -3.0035378717
 C 5.4442580011 0.7487466555 1.776888632
 H -6.9720014494 0.6307482234 -0.6548748343
 H 6.5567756059 0.0864171269 -0.6067914483
 C -1.8954356196 -1.0139240195 4.2001716547
 C -5.3218808733 -0.1440201883 2.9798617705
 C 4.7613324284 -0.8417521419 -4.1713468889
 C 4.7265535893 1.0751425961 2.9268452822
 H -0.0897479637 -1.0868694858 3.0591984418
 C -3.2573377762 -0.7477149202 4.2095184283
 H 2.8279127832 -1.046425132 -5.0993879274
 H 2.7831108651 1.2840259402 3.8347053977
 H -1.4078789472 -1.3841366352 5.0980704666
 H -5.8861784796 -0.2481131165 3.9032878519
 H 5.3055429908 -1.0735394141 -5.0830094493
 H 5.2601772221 1.3625098947 3.8288570988
 H -3.8417704707 -0.8770041293 5.1168209289
 H -7.0367818238 0.3069869668 1.7919881974
 H 6.5541456747 -0.5555927438 -3.0064082072
 H 6.530653125 0.7828680438 1.7822825547

Table S40. Optimized Geometry of **6**, RHF/6-31G*, $E_{\text{Tot}}=-1449.6314102$ Hartree

C 0. -0.6967984958 -1.4125640672
 C 0. -0.6967984958 1.4125640672
 C 0. -1.9419340922 -0.6898016569
 C 0. 0.5314219167 -0.7237774716
 C 0. 0.5314219167 0.7237774716
 C 0. -1.9419340922 0.6898016569
 C 0. -0.7006683955 -2.8351008888
 C 0. -0.7006683955 2.8351008888
 C 0. -3.171448928 -1.4738598096
 C 0. 1.7271190633 -1.4722498117
 C 0. 1.7271190633 1.4722498117
 C 0. -3.171448928 1.4738598096
 C 0. -3.1724180386 -2.8056717227
 C 0. 1.7364402165 -2.8403315021
 C 0. 1.7364402165 2.8403315021
 C 0. -3.1724180386 2.8056717227
 C 0. -1.9402763447 -3.5686557047
 C 0. 0.5008996229 -3.548087934
 C 0. 0.5008996229 3.548087934
 C 0. -1.9402763447 3.5686557047
 C 0. -1.9361621934 -4.9270946263
 C 0. 0.499551203 -4.9735134689
 C 0. 0.499551203 4.9735134689
 C 0. -1.9361621934 4.9270946263
 C 0. -0.7231017828 -5.6735586785
 C 0. -0.7231017828 5.6735586785
 H 0. -4.114210973 -0.9671878418
 H 0. 2.6736547661 -0.970304844
 H 0. 2.6736547661 0.970304844
 H 0. -4.114210973 0.9671878418
 H 0. -4.1022995365 -3.3462809103
 C 0. 2.971930865 -3.6017751611
 C 0. 2.971930865 3.6017751611
 H 0. -4.1022995365 3.3462809103
 H 0. -2.8701041564 -5.4619026933
 C 0. 1.7246552972 -5.6893529238
 C 0. 1.7246552972 5.6893529238
 H 0. -2.8701041564 5.4619026933
 C 0. -0.7046269028 -7.0794226086
 C 0. -0.7046269028 7.0794226086
 C 0. 1.700118719 -7.069016288
 C 0. 1.700118719 7.069016288
 C 0. 0.4858857186 -7.7600804457
 C 0. 0.4858857186 7.7600804457
 H 0. -1.6363735591 -7.6170366333
 H 0. -1.6363735591 7.6170366333
 H 0. 0.4887351029 -8.8353707634
 H 0. 0.4887351029 8.8353707634
 H 0. 2.6256665126 -7.6173458147
 H 0. 2.6256665126 7.6173458147
 C 0. 2.9665768204 -4.9370028142
 C 0. 2.9665768204 4.9370028142
 H 0. 3.9007945258 3.0591748962
 H 0. 3.9007945258 -3.0591748962
 H 0. 3.8911517053 5.486793922
 H 0. 3.8911517053 -5.486793922

Table S41. Optimized Geometry of **6**, RB3LYP/6-31G*, $E_{\text{Tot}}=-1459.0389416$ Hartree

C 0. -0.709944826 -1.4269243958
 C 0. -0.709944826 1.4269243958
 C 0. -1.9560196605 -0.7072711899
 C 0. 0.5385594893 -0.7262390901
 C 0. 0.5385594893 0.7262390901
 C 0. -1.9560196605 0.7072711899
 C 0. -0.7130719082 -2.8531255994
 C 0. -0.7130719082 2.8531255994
 C 0. -3.1740711395 -1.4763364593
 C 0. 1.7311116828 -1.473651672
 C 0. 1.7311116828 1.473651672
 C 0. -3.1740711395 1.4763364593
 C 0. -3.1771445976 -2.8345476918
 C 0. 1.7479006193 -2.8642848683
 C 0. 1.7479006193 2.8642848683
 C 0. -3.1771445976 2.8345476918
 C 0. -1.9540948205 -3.5865808166
 C 0. 0.5060515158 -3.577938967
 C 0. 0.5060515158 3.577938967
 C 0. -1.9540948205 3.5865808166
 C 0. -1.9429904503 -4.9722830696
 C 0. 0.5054336239 -5.0006175944
 C 0. 0.5054336239 5.0006175944
 C 0. -1.9429904503 4.9722830696
 C 0. -0.7350267201 -5.7138133562
 C 0. -0.7350267201 5.7138133562
 H 0. -4.127181672 -0.9618435809
 H 0. 2.6890070631 -0.9655703938
 H 0. 2.6890070631 0.9655703938
 H 0. -4.127181672 0.9618435809
 H 0. -4.1181735954 -3.3792548184
 C 0. 2.9753900239 -3.6149735532
 C 0. 2.9753900239 3.6149735532
 H 0. -4.1181735954 3.3792548184
 H 0. -2.888376319 -5.5108559948
 C 0. 1.7405782104 -5.7211818463
 C 0. 1.7405782104 5.7211818463
 H 0. -2.888376319 5.5108559948
 C 0. -0.7092553935 -7.1279129137
 C 0. -0.7092553935 7.1279129137
 C 0. 1.7126622538 -7.1204554943
 C 0. 1.7126622538 7.1204554943
 C 0. 0.4955326624 -7.8140044134
 C 0. 0.4955326624 7.8140044134
 H 0. -1.6507506291 -7.6716602799
 H 0. -1.6507506291 7.6716602799
 H 0. 0.4980383238 -8.9007729872
 H 0. 0.4980383238 8.9007729872
 H 0. 2.6508371421 -7.6700069577
 H 0. 2.6508371421 7.6700069577
 C 0. 2.9723531455 -4.9746545112
 C 0. 2.9723531455 4.9746545112
 H 0. 3.9140554111 3.0658170107
 H 0. 3.9140554111 -3.0658170107
 H 0. 3.9088220103 5.5273346348
 H 0. 3.9088220103 -5.5273346348

Table S42. Optimized Geometry of **6**, RB3LYP/6-31+G*, $E_{\text{Tot}}=-1459.0759556$ Hartree

C 0. -0.7105837678 -1.4279470561
 C 0. -0.7105837678 1.4279470561
 C 0. -1.9571705092 -0.7076381972
 C 0. 0.5381661381 -0.7267043543
 C 0. 0.5381661381 0.7267043543
 C 0. -1.9571705092 0.7076381972
 C 0. -0.7134496775 -2.8554342941
 C 0. -0.7134496775 2.8554342941
 C 0. -3.1765350214 -1.4768327895
 C 0. 1.7318901727 -1.4744760057
 C 0. 1.7318901727 1.4744760057
 C 0. -3.1765350214 1.4768327895
 C 0. -3.1795430031 -2.8369079741
 C 0. 1.7486226584 -2.866393141
 C 0. 1.7486226584 2.866393141
 C 0. -3.1795430031 2.8369079741
 C 0. -1.9550736873 -3.5892570897
 C 0. 0.5063841407 -3.5808600687
 C 0. 0.5063841407 3.5808600687
 C 0. -1.9550736873 3.5892570897
 C 0. -1.9442255777 -4.9762962538
 C 0. 0.5060335171 -5.004772013
 C 0. 0.5060335171 5.004772013
 C 0. -1.9442255777 4.9762962538
 C 0. -0.7351559382 -5.7183644845
 C 0. -0.7351559382 5.7183644845
 H 0. -4.1304330976 -0.9635658734
 H 0. 2.6901954188 -0.9667848367
 H 0. 2.6901954188 0.9667848367
 H 0. -4.1304330976 0.9635658734
 H 0. -4.1214716056 -3.3807285047
 C 0. 2.9775368018 -3.6173332142
 C 0. 2.9775368018 3.6173332142
 H 0. -4.1214716056 3.3807285047
 H 0. -2.8900498755 -5.5149484639
 C 0. 1.7419376667 -5.7258744792
 C 0. 1.7419376667 5.7258744792
 H 0. -2.8900498755 5.5149484639
 C 0. -0.7101249238 -7.1339729703
 C 0. -0.7101249238 7.1339729703
 C 0. 1.7144268155 -7.1266845269
 C 0. 1.7144268155 7.1266845269
 C 0. 0.4959525883 -7.8213050207
 C 0. 0.4959525883 7.8213050207
 H 0. -1.6516631144 -7.678312386
 H 0. -1.6516631144 7.678312386
 H 0. 0.4983149034 -8.9083006745
 H 0. 0.4983149034 8.9083006745
 H 0. 2.6526361903 -7.6768190494
 H 0. 2.6526361903 7.6768190494
 C 0. 2.9747984915 -4.978834314
 C 0. 2.9747984915 4.978834314
 H 0. 3.9169703977 3.0689278911
 H 0. 3.9169703977 -3.0689278911
 H 0. 3.9121794736 5.5305804829
 H 0. 3.9121794736 -5.5305804829

Table S43. Optimized Geometry of **6**, RB3LYP/6-311G**, $E_{\text{Tot}}=-1459.3446634$ Hartree

C 0. -0.7082826967 -1.424792243
 C 0. -0.7082826967 1.424792243
 C 0. -1.952596356 -0.705873985
 C 0. 0.5381826776 -0.7254377777
 C 0. 0.5381826776 0.7254377777
 C 0. -1.952596356 0.705873985
 C 0. -0.7117898971 -2.84922366
 C 0. -0.7117898971 2.84922366
 C 0. -3.1698682232 -1.4739757273
 C 0. 1.7293671471 -1.4716696869
 C 0. 1.7293671471 1.4716696869
 C 0. -3.1698682232 1.4739757273
 C 0. -3.1735461949 -2.829144486
 C 0. 1.7459639116 -2.8599883266
 C 0. 1.7459639116 2.8599883266
 C 0. -3.1735461949 2.829144486
 C 0. -1.9515200403 -3.5812397022
 C 0. 0.5056690705 -3.5726433518
 C 0. 0.5056690705 3.5726433518
 C 0. -1.9515200403 3.5812397022
 C 0. -1.9408562584 -4.9645142605
 C 0. 0.5045806556 -4.9936088573
 C 0. 0.5045806556 4.9936088573
 C 0. -1.9408562584 4.9645142605
 C 0. -0.7342465829 -5.7052791861
 C 0. -0.7342465829 5.7052791861
 H 0. -4.1206250751 -0.9599026896
 H 0. 2.6850433654 -0.9642240357
 H 0. 2.6850433654 0.9642240357
 H 0. -4.1206250751 0.9599026896
 H 0. -4.1132134024 -3.371625081
 C 0. 2.9720276297 -3.6109746599
 C 0. 2.9720276297 3.6109746599
 H 0. -4.1132134024 3.371625081
 H 0. -2.8844337107 -5.5016483722
 C 0. 1.7377841601 -5.7134702565
 C 0. 1.7377841601 5.7134702565
 H 0. -2.8844337107 5.5016483722
 C 0. -0.7084956537 -7.1176653047
 C 0. -0.7084956537 7.1176653047
 C 0. 1.7095249547 -7.1104834715
 C 0. 1.7095249547 7.1104834715
 C 0. 0.4939583007 -7.8023899106
 C 0. 0.4939583007 7.8023899106
 H 0. -1.6474847853 -7.6609732911
 H 0. -1.6474847853 7.6609732911
 H 0. 0.4961383559 -8.8867363664
 H 0. 0.4961383559 8.8867363664
 H 0. 2.6452371155 -7.6594993683
 H 0. 2.6452371155 7.6594993683
 C 0. 2.96857274 -4.967662244
 C 0. 2.96857274 4.967662244
 H 0. 3.909497204 3.0643396318
 H 0. 3.909497204 -3.0643396318
 H 0. 3.9032648669 5.5188031272
 H 0. 3.9032648669 -5.5188031272

Table S44. Optimized Geometry of Dikation of **6**, RB3LYP/6-31G*, $E_{\text{Tot}}=-1458.5196812$ Hartree

C 0. -0.6992583909 -1.4357773041
 C 0. -0.6992583909 1.4357773041
 C 0. -1.9357135587 -0.7335087259
 C 0. 0.5626068605 -0.7355232594
 C 0. 0.5626068605 0.7355232594
 C 0. -1.9357135587 0.7335087259
 C 0. -0.7067156243 -2.8608221747
 C 0. -0.7067156243 2.8608221747
 C 0. -3.1467657795 -1.4691131854
 C 0. 1.7354169632 -1.4741855152
 C 0. 1.7354169632 1.4741855152
 C 0. -3.1467657795 1.4691131854
 C 0. -3.1568087711 -2.8473423244
 C 0. 1.7505293409 -2.8909489713
 C 0. 1.7505293409 2.8909489713
 C 0. -3.1568087711 2.8473423244
 C 0. -1.9446250866 -3.5781877409
 C 0. 0.5093271876 -3.590935083
 C 0. 0.5093271876 3.590935083
 C 0. -1.9446250866 3.5781877409
 C 0. -1.9384759527 -4.9887858543
 C 0. 0.5002450719 -5.0079717083
 C 0. 0.5002450719 5.0079717083
 C 0. -1.9384759527 4.9887858543
 C 0. -0.7421955932 -5.7193709158
 C 0. -0.7421955932 5.7193709158
 H 0. -4.099839759 -0.9579112791
 H 0. 2.6986569841 -0.9776028828
 H 0. 2.6986569841 0.9776028828
 H 0. -4.099839759 0.9579112791
 H 0. -4.102676333 -3.3812550385
 C 0. 2.96838494 -3.62974748
 C 0. 2.96838494 3.62974748
 H 0. -4.102676333 3.3812550385
 H 0. -2.8879570928 -5.5189570791
 C 0. 1.725290826 -5.7272877517
 C 0. 1.725290826 5.7272877517
 H 0. -2.8879570928 5.5189570791
 C 0. -0.7301102006 -7.1427400019
 C 0. -0.7301102006 7.1427400019
 C 0. 1.6834081651 -7.1389106349
 C 0. 1.6834081651 7.1389106349
 C 0. 0.4698397951 -7.8380785238
 C 0. 0.4698397951 7.8380785238
 H 0. -1.6741734579 -7.6805653027
 H 0. -1.6741734579 7.6805653027
 H 0. 0.4722403379 -8.9228442719
 H 0. 0.4722403379 8.9228442719
 H 0. 2.6186374421 -7.6928339053
 H 0. 2.6186374421 7.6928339053
 C 0. 2.9574312585 -5.0030606797
 C 0. 2.9574312585 5.0030606797
 H 0. 3.9119610363 3.092394883
 H 0. 3.9119610363 -3.092394883
 H 0. 3.8922821353 5.5560009334
 H 0. 3.8922821353 -5.5560009334

Table S45. Optimized Geometry of Dianion of **6**, RB3LYP/6-31G*, $E_{\text{Tot}}=-1459.0355131$ Hartree

C 0. 1.4468424648 0.7321058169
 C 0. -1.4468424648 0.7321058169
 C 0. 0.7327987478 1.9645916426
 C 0. 0.7391206275 -0.5314069498
 C 0. -0.7391206275 -0.5314069498
 C 0. -0.7327987478 1.9645916426
 C 0. 2.8854780265 0.7288435558
 C 0. -2.8854780265 0.7288435558
 C 0. 1.4925296188 3.1560118426
 C 0. 1.4787761606 -1.7033017448
 C 0. -1.4787761606 -1.7033017448
 C 0. -1.4925296188 3.1560118426
 C 0. 2.8733249265 3.1678114902
 C 0. 2.8927423432 -1.7355437162
 C 0. -2.8927423432 -1.7355437162
 C 0. -2.8733249265 3.1678114902
 C 0. 3.6246521187 1.964610586
 C 0. 3.6150730541 -0.5017472624
 C 0. -3.6150730541 -0.5017472624
 C 0. -3.6246521187 1.964610586
 C 0. 5.0353927549 1.9385313615
 C 0. 5.0465163137 -0.5102868746
 C 0. -5.0465163137 -0.5102868746
 C 0. -5.0353927549 1.9385313615
 C 0. 5.767983504 0.7422974354
 C 0. -5.767983504 0.7422974354
 H 0. 0.9781609922 4.1136459208
 H 0. 0.9712526985 -2.6646060877
 H 0. -0.9712526985 -2.6646060877
 H 0. -0.9781609922 4.1136459208
 H 0. 3.4088608727 4.1173525304
 C 0. 3.6266142239 -2.9514430255
 C 0. -3.6266142239 -2.9514430255
 H 0. -3.4088608727 4.1173525304
 H 0. 5.5739945312 2.8868237619
 C 0. 5.7618758173 -1.754344971
 C 0. -5.7618758173 -1.754344971
 H 0. -5.5739945312 2.8868237619
 C 0. 7.1958272526 0.6887181513
 C 0. -7.1958272526 0.6887181513
 C 0. 7.178651766 -1.7447701529
 C 0. -7.178651766 -1.7447701529
 C 0. 7.8651128093 -0.5276769081
 C 0. -7.8651128093 -0.5276769081
 H 0. 7.75245558 1.6253260219
 H 0. -7.75245558 1.6253260219
 H 0. 8.9571601607 -0.5330547306
 H 0. -8.9571601607 -0.5330547306
 H 0. 7.7186002457 -2.6906041405
 H 0. -7.7186002457 -2.6906041405
 C 0. 5.0008438094 -2.9650525528
 C 0. -5.0008438094 -2.9650525528
 H 0. -3.0705420661 -3.8896861236
 H 0. 3.0705420661 -3.8896861236
 H 0. -5.5397577408 -3.9128834981
 H 0. 5.5397577408 -3.9128834981

Table S46. Optimized Geometry of **7**, RHF/6-31G*, $E_{\text{Tot}}=-1449.6257245$ Hartree

C 0. -0.0033252775 -1.4065910664
 C 0. 0.0033252775 1.4065910664
 C 0. -1.2297101177 -0.7104373166
 C 0. 1.2340891376 -0.7010887436
 C 0. -1.2340891376 0.7010887436
 C 0. 1.2297101177 0.7104373166
 C 0. 0.0063056563 -2.8405976123
 C 0. -0.0063056563 2.8405976123
 C 0. -2.4553743154 -1.4864358816
 C 0. 2.4423266578 -1.4626397722
 C 0. -2.4423266578 1.4626397722
 C 0. 2.4553743154 1.4864358816
 C 0. -2.4554392973 -2.8221149343
 C 0. 2.4526217359 -2.818756092
 C 0. -2.4526217359 2.818756092
 C 0. 2.4554392973 2.8221149343
 C 0. -1.2238083546 -3.5742115759
 C 0. 1.2103276911 -3.5432562829
 C 0. -1.2103276911 3.5432562829
 C 0. 1.2238083546 3.5742115759
 C 0. -1.2106572844 -4.9421673583
 C 0. 1.2183449493 -4.9608417373
 C 0. -1.2183449493 4.9608417373
 C 0. 1.2106572844 4.9421673583
 C 0. -0.0007697293 -5.6703820616
 C 0. 0.0007697293 5.6703820616
 H 0. -3.3981894509 -0.9794220258
 H 0. 3.3871064989 -0.9581107325
 H 0. -3.3871064989 0.9581107325
 H 0. 3.3981894509 0.9794220258
 H 0. -3.384316599 -3.3643886384
 C 0. 3.6925196458 -3.5802249239
 C 0. -3.6925196458 3.5802249239
 H 0. 3.384316599 3.3643886384
 H 0. -2.1421367272 -5.4812506714
 C 0. 2.4524122924 -5.6753457506
 C 0. -2.4524122924 5.6753457506
 H 0. 2.1421367272 5.4812506714
 C 0. 0.0304633385 -7.0861400271
 C 0. -0.0304633385 7.0861400271
 C 0. 2.436386268 -7.0467047582
 C 0. -2.436386268 7.0467047582
 C 0. 1.2192511294 -7.7523841586
 C 0. -1.2192511294 7.7523841586
 H 0. -0.8985313229 -7.6283408791
 H 0. 0.8985313229 7.6283408791
 H 0. 1.2342075405 -8.8275483522
 H 0. -1.2342075405 8.8275483522
 H 0. 3.3643179682 -7.5908983448
 H 0. -3.3643179682 7.5908983448
 C 0. 3.6927449722 -4.9130881596
 C 0. -3.6927449722 4.9130881596
 H 0. -4.6188801119 3.0333723551
 H 0. 4.6188801119 -3.0333723551
 H 0. -4.6194626104 5.4592464118
 H 0. 4.6194626104 -5.4592464118

Table S47. Optimized Geometry of **7**, RB3LYP/6-31G*, $E_{\text{Tot}}=-1459.0357658$ Hartree

C 0. -0.0036422457 -1.4245482463
 C 0. 0.0036422457 1.4245482463
 C 0. -1.2429174936 -0.7209896197
 C 0. 1.2483259969 -0.7117820867
 C 0. -1.2483259969 0.7117820867
 C 0. 1.2429174936 0.7209896197
 C 0. 0.0032083772 -2.8549145866
 C 0. -0.0032083772 2.8549145866
 C 0. -2.4567567243 -1.487547811
 C 0. 2.4477097826 -1.4627472461
 C 0. -2.4477097826 1.4627472461
 C 0. 2.4567567243 1.487547811
 C 0. -2.456970067 -2.8487078318
 C 0. 2.4675559718 -2.8478010638
 C 0. -2.4675559718 2.8478010638
 C 0. 2.456970067 2.8487078318
 C 0. -1.2329982574 -3.5922288511
 C 0. 1.225281965 -3.5717051808
 C 0. -1.225281965 3.5717051808
 C 0. 1.2329982574 3.5922288511
 C 0. -1.2142711524 -4.9828434364
 C 0. 1.2321151258 -4.9917130622
 C 0. -1.2321151258 4.9917130622
 C 0. 1.2142711524 4.9828434364
 C 0. -0.005654719 -5.712848178
 C 0. 0.005654719 5.712848178
 H 0. -3.4108497983 -0.974914328
 H 0. 3.4039166094 -0.952412324
 H 0. -3.4039166094 0.952412324
 H 0. 3.4108497983 0.974914328
 H 0. -3.3965255616 -3.3955528318
 C 0. 3.6992114461 -3.5957074626
 C 0. -3.6992114461 3.5957074626
 H 0. 3.3965255616 3.3955528318
 H 0. -2.1571710204 -5.5254171456
 C 0. 2.4721494389 -5.7080441188
 C 0. -2.4721494389 5.7080441188
 H 0. 2.1571710204 5.5254171456
 C 0. 0.0294850483 -7.131066547
 C 0. -0.0294850483 7.131066547
 C 0. 2.4517425014 -7.1039662331
 C 0. -2.4517425014 7.1039662331
 C 0. 1.2355186042 -7.8073633529
 C 0. -1.2355186042 7.8073633529
 H 0. -0.9091239711 -7.6794224348
 H 0. 0.9091239711 7.6794224348
 H 0. 1.246415991 -8.8938940876
 H 0. -1.246415991 8.8938940876
 H 0. 3.3923634183 -7.649042955
 H 0. -3.3923634183 7.649042955
 C 0. 3.7019336358 -4.9540356616
 C 0. -3.7019336358 4.9540356616
 H 0. -4.6354210634 3.0426669608
 H 0. 4.6354210634 -3.0426669608
 H 0. -4.6406172646 5.5026312172
 H 0. 4.6406172646 -5.5026312172

Table S48. Optimized Geometry of **7**, RB3LYP/6-311G**, $E_{\text{Tot}}=-1459.3414498$ Hartree

C 0. -0.0037454369 -1.4226378625
 C 0. 0.0037454369 1.4226378625
 C 0. -1.2410830132 -0.7202415705
 C 0. 1.2467493744 -0.7107893991
 C 0. -1.2467493744 0.7107893991
 C 0. 1.2410830132 0.7202415705
 C 0. 0.003089269 -2.8512532441
 C 0. -0.003089269 2.8512532441
 C 0. -2.4537611396 -1.4859918079
 C 0. 2.4449695474 -1.4606360957
 C 0. -2.4449695474 1.4606360957
 C 0. 2.4537611396 1.4859918079
 C 0. -2.454300875 -2.8440276742
 C 0. 2.464502854 -2.8432895958
 C 0. -2.464502854 2.8432895958
 C 0. 2.454300875 2.8440276742
 C 0. -1.2315408285 -3.5872062305
 C 0. 1.2237159496 -3.5663510579
 C 0. -1.2237159496 3.5663510579
 C 0. 1.2315408285 3.5872062305
 C 0. -1.213035874 -4.9756383134
 C 0. 1.2303077736 -4.9843161913
 C 0. -1.2303077736 4.9843161913
 C 0. 1.213035874 4.9756383134
 C 0. -0.0057843816 -5.7042668707
 C 0. 0.0057843816 5.7042668707
 H 0. -3.4055271259 -0.9736197456
 H 0. 3.3986275311 -0.950373494
 H 0. -3.3986275311 0.950373494
 H 0. 3.4055271259 0.9736197456
 H 0. -3.3921744959 -3.3891144155
 C 0. 3.694580771 -3.5912904426
 C 0. -3.694580771 3.5912904426
 H 0. 3.3921744959 3.3891144155
 H 0. -2.1538262373 -5.5170576006
 C 0. 2.468512574 -5.6997820298
 C 0. -2.468512574 5.6997820298
 H 0. 2.1538262373 5.5170576006
 C 0. 0.0297783909 -7.1210142991
 C 0. -0.0297783909 7.1210142991
 C 0. 2.44806864 -7.0932919283
 C 0. -2.44806864 7.0932919283
 C 0. 1.2334374857 -7.7954014295
 C 0. -1.2334374857 7.7954014295
 H 0. -0.9061262462 -7.6692090923
 H 0. 0.9061262462 7.6692090923
 H 0. 1.2443295732 -8.8795981661
 H 0. -1.2443295732 8.8795981661
 H 0. 3.3863289855 -7.6376109944
 H 0. -3.3863289855 7.6376109944
 C 0. 3.6970558317 -4.9463835531
 C 0. -3.6970558317 4.9463835531
 H 0. -4.6293440793 3.0403633986
 H 0. 4.6293440793 -3.0403633986
 H 0. -4.6338540892 5.4936268136
 H 0. 4.6338540892 -5.4936268136

Table S49. Optimized Geometry of **8**, RHF/6-31G*, $E_{\text{Tot}}=-1449.6330425$ Hartree

C -0.0980272641 0.0047316115 -1.3928763331
 C -0.0981393259 0.0006366832 1.3928763331
 C 0.0342656962 -1.2223605959 -0.7168941342
 C -0.1128525455 1.2298440493 -0.676637323
 C -0.1799450916 -1.2218313495 0.676637323
 C 0.1010665835 1.2186570929 0.7168941342
 C -0.2774558429 0.017981335 -2.8257630844
 C -0.2780239996 -0.0027800743 2.8257630844
 C 0.3401874529 -2.4323554539 -1.5020334699
 C -0.4419617919 2.4316512588 -1.4069328113
 C -0.5742898544 -2.4038405174 1.4069328113
 C 0.4727063516 2.410109803 1.5020334699
 C 0.144421728 -2.4115234457 -2.9053135454
 C -0.665184861 2.4205517303 -2.7286980964
 C -0.7965717864 -2.3805492995 2.7286980965
 C 0.2760943002 2.4000156046 2.9053135454
 C -0.2086731423 -1.1906271899 -3.5674077689
 C -0.5630747516 1.2106672772 -3.4913525987
 C -0.6284446639 -1.1780601582 3.4913525987
 C -0.1432441875 1.2002577591 3.5674077689
 C -0.4108245357 -1.1773554159 -4.9516768121
 C -0.7882750705 1.1992768402 -4.8843473114
 C -0.8526849762 -1.1543703294 4.8843473114
 C -0.345818873 1.1980617185 4.9516768121
 C -0.715145174 0.0409865916 -5.5940863749
 C -0.7163164334 -0.0018132149 5.5940863749
 C 0.9030573793 -3.5724597655 -0.9462605127
 H -0.585004045 3.3420411879 -0.8630714201
 H -0.7669081915 -3.3050447592 0.8630714201
 C 1.0970873349 3.5177238075 0.9462605127
 C 0.3571135043 -3.5746645594 -3.6713113752
 H -0.9551450747 3.3248138717 -3.234116041
 H -1.1355530605 -3.2675998289 3.234116041
 C 0.5520811429 3.5497835397 3.6713113752
 C -0.2719062005 -2.4000559032 -5.6932258655
 H -1.0187824268 2.1253652336 -5.3808367955
 H -1.1334960751 -2.0664659825 5.3808367955
 C -0.1402376925 2.4113346325 5.6932258655
 H -0.8793455245 0.0447392429 -6.6572323577
 H -0.8804762657 0.0034200382 6.6572323577
 C 1.1418666972 -4.711918083 -1.7102319496
 C 1.397857393 4.6424159964 1.7102319496
 C 0.8392499922 -4.7304467316 -3.0483226795
 C 1.096706958 4.6774673359 3.0483226795
 H 1.1879022791 -3.5829640023 0.0861131645
 H 1.3820804021 3.5126338591 -0.0861131645
 H 1.5696815357 -5.5794260254 -1.2405773406
 H 1.8724768431 5.4852279231 1.2405773406
 H 1.0058347013 -5.6172171642 -3.6339729858
 H 1.3115407408 5.5537998705 3.6339729858
 C 0.1038656351 -3.536541624 -5.0868627684
 C 0.2971273205 3.5255680512 5.0868627684
 H 0.2340126246 -4.4418671702 -5.6529827772
 H 0.4765927177 4.4224207452 5.6529827772
 H -0.4510857736 -2.3795635559 -6.7537421534
 H -0.3202698398 2.4006724727 6.7537421534

Table S50. Optimized Geometry of **8**, RB3LYP/6-31G*, $E_{\text{Tot}}=-1459.0368597$ Hartree

C -0.1264860459 0.0054818058 -1.4084368056
 C -0.1265965431 0.0014440521 1.4084368056
 C 0.0096304259 -1.2342130597 -0.7248893176
 C -0.1528838008 1.2435362484 -0.6827732573
 C -0.2206652739 -1.2333137049 0.6827732573
 C 0.0771164078 1.2318391459 0.7248893176
 C -0.2849191215 0.0196696011 -2.8376565334
 C -0.2855684411 -0.0040576391 2.8376565334
 C 0.3250491265 -2.434812421 -1.499754715
 C -0.4906566026 2.4363436893 -1.4051093102
 C -0.6231684187 -2.405862755 1.4051093102
 C 0.4577250565 2.4133910236 1.499754715
 C 0.1598166802 -2.4090135679 -2.9199011177
 C -0.7048397877 2.429416917 -2.7522199514
 C -0.8366522088 -2.3872324487 2.7522199514
 C 0.2913289433 2.3966675173 2.9199011177
 C -0.1864815941 -1.1922361526 -3.5841944913
 C -0.5765352858 1.2310319986 -3.5161237449
 C -0.6429988198 -1.1976582296 3.5161237449
 C -0.120997857 1.2006506349 3.5841944913
 C -0.3669548533 -1.1761543891 -4.994519409
 C -0.7774700858 1.2155806215 -4.9194939644
 C -0.8427878338 -1.1712406451 4.9194939644
 C -0.3020805347 1.1944632108 4.994519409
 C -0.6757703195 0.0480202674 -5.6377426966
 C -0.6773851893 -0.0109898153 5.6377426966
 C 0.862708322 -3.5998652141 -0.9276270136
 H -0.6468313766 3.3534388796 -0.8511877812
 H -0.8292663393 -3.3130439912 0.8511877812
 C 1.0582974995 3.547294971 0.9276270136
 C 0.3838302072 -3.5901042802 -3.6921503885
 H -1.0020162322 3.3430880201 -3.2612432817
 H -1.1833534993 -3.2832831945 3.2612432817
 C 0.579602274 3.5637389881 3.6921503885
 C -0.2047515151 -2.3922472418 -5.7305866148
 H -1.0137491045 2.1501831779 -5.4223443506
 H -1.1298276052 -2.0915220601 5.4223443506
 C -0.0736105797 2.3998648986 5.7305866148
 H -0.8213138846 0.0518431619 -6.7152405904
 H -0.8229200011 -0.0068470593 6.7152405904
 C 1.1083271556 -4.744760901 -1.6916644029
 C 1.3661642571 4.6770439718 1.6916644029
 C 0.8387396594 -4.7576533201 -3.0512196294
 C 1.0976853456 4.7046611156 3.0512196294
 H 1.1280240213 -3.6089690201 0.1222282571
 H 1.3237140041 3.5418747601 -0.1222282571
 H 1.5202323432 -5.6272583065 -1.2097051489
 H 1.8257176572 5.5356930425 1.2097051489
 H 1.011014171 -5.6543479442 -3.641288697
 H 1.3187431795 5.5905918072 3.641288697
 C 0.165253557 -3.5472478182 -5.1079410222
 C 0.3590088975 3.5329008525 5.1079410222
 H 0.313581721 -4.4596657057 -5.6802680163
 H 0.5570161454 4.4358409255 5.6802680163
 H -0.3595605291 -2.3711213788 -6.8066468817
 H -0.2293432903 2.3872373201 6.8066468817

Table S51. Optimized Geometry of **8**, RB3LYP/6-311G**, $E_{\text{Tot}}=-1459.3422149$ Hartree

C -0.1218226235 0.0052570649 -1.4060759211
 C -0.1219278089 0.0014134092 1.4060759211
 C 0.0155629513 -1.2323208463 -0.723635107
 C -0.1457135308 1.2415393726 -0.681921932
 C -0.2133965242 -1.2317119673 0.681921932
 C 0.082936567 1.2296253086 0.723635107
 C -0.285608162 0.0188993249 -2.8330674227
 C -0.2862143232 -0.0032508314 2.8330674227
 C 0.3311179227 -2.4310265707 -1.4987714752
 C -0.4839058303 2.4331437947 -1.4030813251
 C -0.6162527445 -2.4030368564 1.4030813251
 C 0.4635777176 2.4092789307 1.4987714752
 C 0.159569764 -2.4064242089 -2.9158516572
 C -0.7039097085 2.4257390708 -2.7460194525
 C -0.8355223764 -2.3836109741 2.7460194525
 C 0.2909407819 2.3940955378 2.9158516572
 C -0.1914082342 -1.1919315594 -3.5782547403
 C -0.5801428679 1.2277980117 -3.5092517883
 C -0.6464241324 -1.1942317805 3.5092517883
 C -0.125933782 1.2006159407 3.5782547403
 C -0.3792072974 -1.1769876839 -4.9850480049
 C -0.7889390686 1.2109705154 -4.9096573964
 C -0.8539875199 -1.1660101883 4.9096573964
 C -0.3142690672 1.1959653573 4.9850480049
 C -0.6913015315 0.0452973877 -5.6263074526
 C -0.692744239 -0.0074215927 5.6263074526
 C 0.8770457378 -3.5910255615 -0.9298481479
 H -0.633525079 3.349419064 -0.8507865166
 H -0.815760109 -3.3097579272 0.8507865166
 C 1.0721300071 3.5376844202 0.9298481479
 C 0.3836708181 -3.5851617005 -3.6875534218
 H -1.0029632432 3.337339821 -3.2524775745
 H -1.183984718 -3.2774918056 3.2524775745
 C 0.5791728086 3.5588125229 3.6875534218
 C -0.2187421631 -2.3922926757 -5.7204185542
 H -1.0277151657 2.1428013225 -5.4112575212
 H -1.1433690424 -2.0833874346 5.4112575212
 C -0.0875778034 2.4006754276 5.7204185542
 H -0.8429401875 0.0488079239 -6.7005079479
 H -0.8443479361 -0.002633599 6.7005079479
 C 1.1252117345 -4.7322929335 -1.693781344
 C 1.3823416791 4.6636712296 1.693781344
 C 0.8482661957 -4.7478375837 -3.0492623038
 C 1.1066607908 4.694339054 3.0492623038
 H 1.1443323554 -3.5996334714 0.1169307424
 H 1.339487359 3.5316612639 -0.1169307424
 H 1.5451090725 -5.609954677 -1.2153322453
 H 1.8496108006 5.5170547768 1.2153322453
 H 1.0217660712 -5.6423500725 -3.637692248
 H 1.3288228116 5.5780238598 3.637692248
 C 0.156872161 -3.5433478316 -5.1008191843
 C 0.3504267514 3.5294650901 5.1008191843
 H 0.3041013253 -4.4533310954 -5.6727216964
 H 0.5472034923 4.4300342887 5.6727216964
 H -0.3797463746 -2.3729350846 -6.7931597444
 H -0.2493997307 2.3901522962 6.7931597444

Table S52. Optimized Geometry of C_{2v} -**10**, RB3LYP/6-31G*, $E_{Tot}=-731.3062756$ Hartree

H 0. -2.9967975653 0.8722541122
 C 0. -2.3268426008 0.
 C 1.2840615937 -1.522233373 0.
 C -1.2840615937 -1.522233373 0.
 C 1.2510822656 -0.1039898444 0.
 C -1.2510822656 -0.1039898444 0.
 C 0. 0.6100054824 0.
 C 2.5072539463 -2.1744763163 0.
 C -2.5072539463 -2.1744763163 0.
 C 2.4781093752 0.6269398393 0.
 C -2.4781093752 0.6269398393 0.
 C 0. 2.020193203 0.
 C 3.7178421646 -1.4571433907 0.
 C -3.7178421646 -1.4571433907 0.
 C 3.7039881711 -0.0768555327 0.
 C -3.7039881711 -0.0768555327 0.
 C 2.4350177202 2.0570231936 0.
 C -2.4350177202 2.0570231936 0.
 C 1.245199254 2.7244841946 0.
 C -1.245199254 2.7244841946 0.
 H 2.5309370332 -3.2624873569 0.
 H -2.5309370332 -3.2624873569 0.
 H 4.661957563 -1.9954430381 0.
 H -4.661957563 -1.9954430381 0.
 H 4.6341938244 0.4863307265 0.
 H -4.6341938244 0.4863307265 0.
 H 3.3748293895 2.6040177553 0.
 H -3.3748293895 2.6040177553 0.
 H 1.2243275542 3.8118186014 0.
 H -1.2243275542 3.8118186014 0.
 H 0. -2.9967975653 -0.8722541122

Table S53. Optimized Geometry of C_{2h} -**11**, RB3LYP/6-31G*, $E_{\text{Tot}}=-1460.2299974$ Hartree

C 0. 1.4002826396 0.4083763708
 C 0. -1.4002826396 -0.4083763708
 C 1.2521191008 0.7053797069 0.2232784342
 C -1.2521191008 0.7053797069 0.2232784342
 C -1.2521191008 -0.7053797069 -0.2232784342
 C 1.2521191008 -0.7053797069 -0.2232784342
 C 0. 2.7584713317 0.80527438
 C 0. -2.7584713317 -0.80527438
 C 1.2416237076 3.4507089724 1.0348058757
 C -1.2416237076 3.4507089724 1.0348058757
 C -1.2416237076 -3.4507089724 -1.0348058757
 C 1.2416237076 -3.4507089724 -1.0348058757
 C 1.2759507498 4.8162663745 1.4193228045
 C -1.2759507498 4.8162663745 1.4193228045
 C -1.2759507498 -4.8162663745 -1.4193228045
 C 1.2759507498 -4.8162663745 -1.4193228045
 C 0. 5.6244901008 1.484746562
 C 0. -5.6244901008 -1.484746562
 C 2.4253436459 1.3751767131 0.4933105509
 C -2.4253436459 1.3751767131 0.4933105509
 C -2.4253436459 -1.3751767131 -0.4933105509
 C 2.4253436459 -1.3751767131 -0.4933105509
 C 2.4639529286 2.7340585316 0.9000157175
 C -2.4639529286 2.7340585316 0.9000157175
 C -2.4639529286 -2.7340585316 -0.9000157175
 C 2.4639529286 -2.7340585316 -0.9000157175
 C 2.494826563 5.4191797561 1.6860581726
 C -2.494826563 5.4191797561 1.6860581726
 C -2.494826563 -5.4191797561 -1.6860581726
 C 2.494826563 -5.4191797561 -1.6860581726
 H 0. 6.248454135 2.3881400799
 H 0. 6.337692597 0.6448007487
 H 0. -6.337692597 -0.6448007487
 H 0. -6.248454135 -2.3881400799
 C 3.6912491488 3.3872693609 1.1713315949
 C -3.6912491488 3.3872693609 1.1713315949
 C -3.6912491488 -3.3872693609 -1.1713315949
 C 3.6912491488 -3.3872693609 -1.1713315949
 C 3.7047154391 4.7083623839 1.5645587173
 C -3.7047154391 4.7083623839 1.5645587173
 C -3.7047154391 -4.7083623839 -1.5645587173
 C 3.7047154391 -4.7083623839 -1.5645587173
 H 3.3804541446 0.8688767109 0.4090056415
 H -3.3804541446 0.8688767109 0.4090056415
 H -3.3804541446 -0.8688767109 -0.4090056415
 H 3.3804541446 -0.8688767109 -0.4090056415
 H 4.6186553827 2.8296272309 1.0657565486
 H -4.6186553827 2.8296272309 1.0657565486
 H -4.6186553827 -2.8296272309 -1.0657565486
 H 4.6186553827 -2.8296272309 -1.0657565486
 H 4.6459114247 5.2073980523 1.7788435159
 H -4.6459114247 5.2073980523 1.7788435159
 H -4.6459114247 -5.2073980523 -1.7788435159
 H 4.6459114247 -5.2073980523 -1.7788435159
 H 2.516724538 6.4640892154 1.9885097592
 H -2.516724538 6.4640892154 1.9885097592
 H -2.516724538 -6.4640892154 -1.9885097592
 H 2.516724538 -6.4640892154 -1.9885097592

Table S54. Optimized Geometry of D_{2h} -**11**, RB3LYP/6-31G*, $E_{\text{Tot}}=-1460.2299024$ Hartree

C 0. -1.459573572 0.
 C 0. 1.459573572 0.
 C -1.2521029063 -0.7401642235 0.
 C 1.2521029063 -0.7401642235 0.
 C -1.2521029063 0.7401642235 0.
 C 1.2521029063 0.7401642235 0.
 C 0. -2.8750698142 0.
 C 0. 2.8750698142 0.
 C -2.4265644459 -1.4597293806 0.
 C 2.4265644459 -1.4597293806 0.
 C -2.4265644459 1.4597293806 0.
 C 2.4265644459 1.4597293806 0.
 C -2.4658785419 -2.877765471 0.
 C 2.4658785419 -2.877765471 0.
 C -2.4658785419 2.877765471 0.
 C 2.4658785419 2.877765471 0.
 C -1.241733734 -3.6044834743 0.
 C 1.241733734 -3.6044834743 0.
 C -1.241733734 3.6044834743 0.
 C 1.241733734 3.6044834743 0.
 C -1.2782365377 -5.0226918833 0.
 C 1.2782365377 -5.0226918833 0.
 C -1.2782365377 5.0226918833 0.
 C 1.2782365377 5.0226918833 0.
 C 0. -5.831343392 0.
 C 0. 5.831343392 0.
 H -3.3845943285 -0.9521566702 0.
 H 3.3845943285 -0.9521566702 0.
 H -3.3845943285 0.9521566702 0.
 H 3.3845943285 0.9521566702 0.
 C -3.6968772073 -3.5779702776 0.
 C 3.6968772073 -3.5779702776 0.
 C -3.6968772073 3.5779702776 0.
 C 3.6968772073 3.5779702776 0.
 C -2.5020434192 -5.6735815789 0.
 C 2.5020434192 -5.6735815789 0.
 C -2.5020434192 5.6735815789 0.
 C 2.5020434192 5.6735815789 0.
 H 0. -6.5007659325 0.8726046489
 H 0. 6.5007659325 0.8726046489
 C -3.7134725414 -4.9562873137 0.
 C 3.7134725414 -4.9562873137 0.
 C -3.7134725414 4.9562873137 0.
 C 3.7134725414 4.9562873137 0.
 H -4.6246349592 -3.0108631284 0.
 H 4.6246349592 -3.0108631284 0.
 H -4.6246349592 3.0108631284 0.
 H 4.6246349592 3.0108631284 0.
 H -4.6578019451 -5.494129564 0.
 H 4.6578019451 -5.494129564 0.
 H -4.6578019451 5.494129564 0.
 H 4.6578019451 5.494129564 0.
 H -2.5252681388 -6.7615114989 0.
 H 2.5252681388 -6.7615114989 0.
 H -2.5252681388 6.7615114989 0.
 H 2.5252681388 6.7615114989 0.
 H 0. 6.5007659325 -0.8726046489
 H 0. -6.5007659325 -0.8726046489