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Supporting Information

Revival of Hückel Aromatic (Poly)benzenoid Subunits in Triplet State Polycyclic Aromatic Hydrocarbons by Silicon Substitution

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Revival of Hückel

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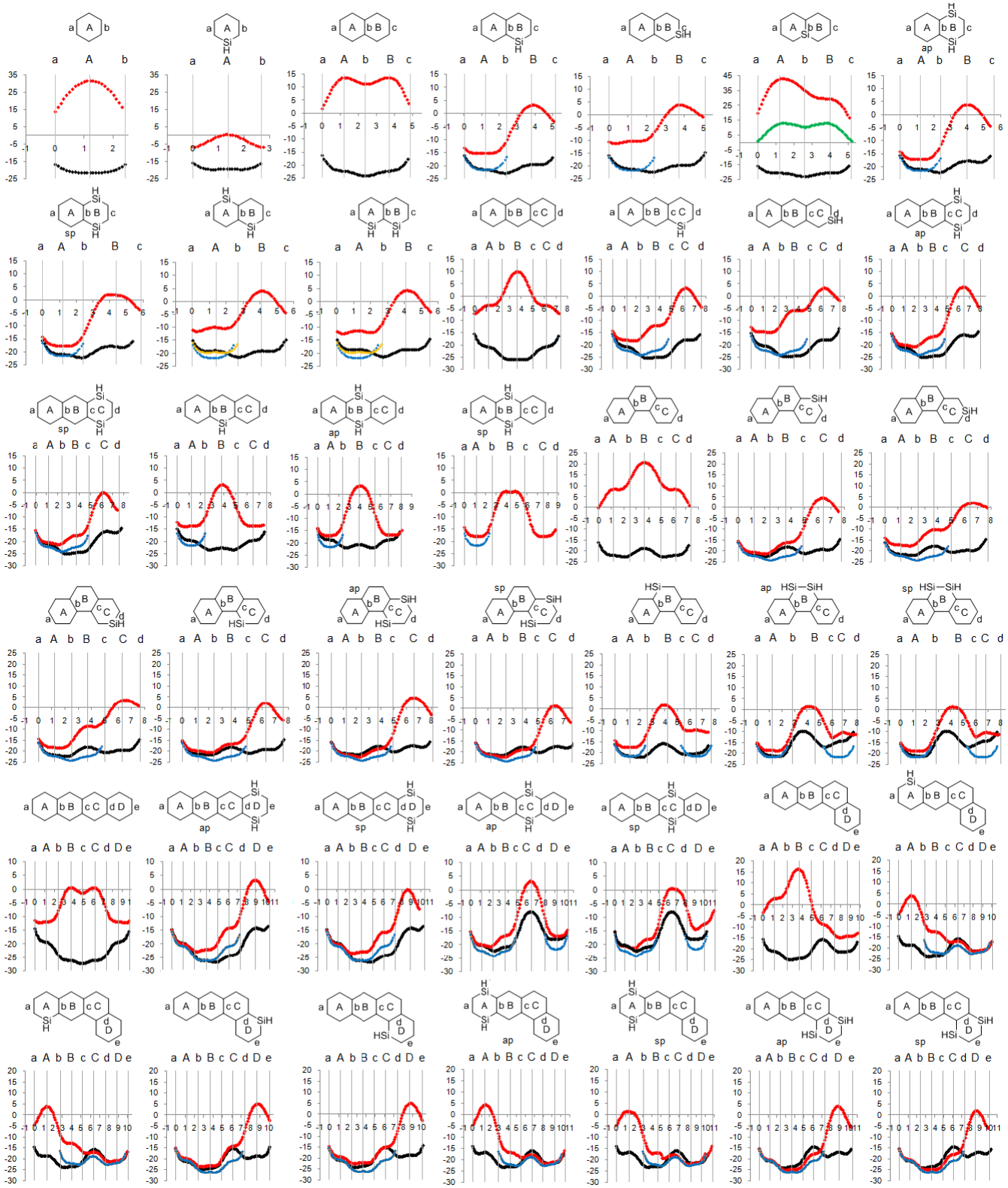


Figure S1. NICS$_{zz}$-xy scans for the studied molecules. Black curves refer to singlet state, red curves to triplet state, green curve is for nonplanar geometry of T_1 9-silanaphthalene, blue curves are scans for carbocyclic structures in their singlet state and the yellow ones are for silabenzene in its singlet state; the latter two are shown for comparison; the ap/sp corresponds to the Si–H bonds spatial orientation in disilicon-substituted molecules: antiperiplanar/synperiplanar; x-axis: distance in Å, y-axis: NICS values in ppm.

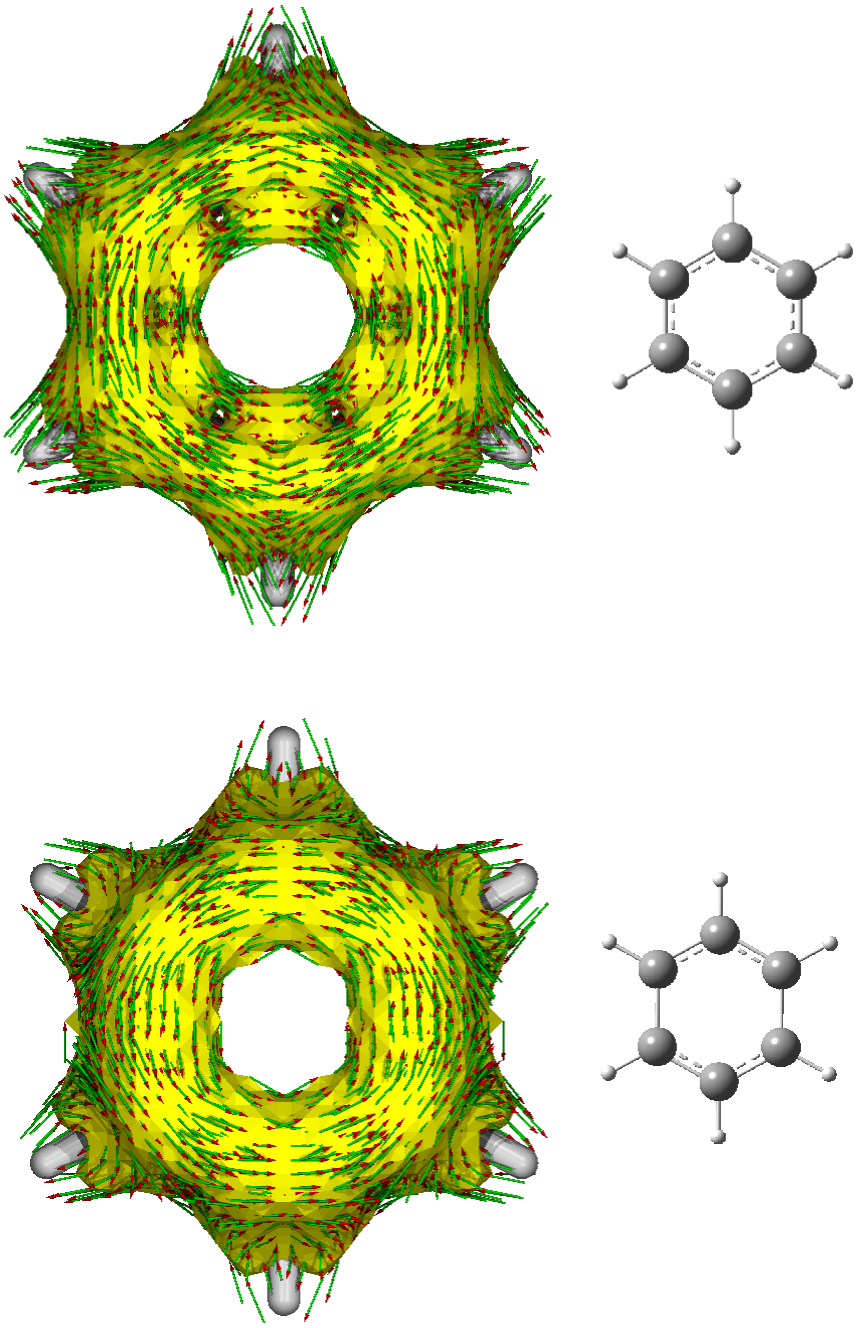


Figure S2. AICD plots of S_0 (top) and T_1 (bottom) benzene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

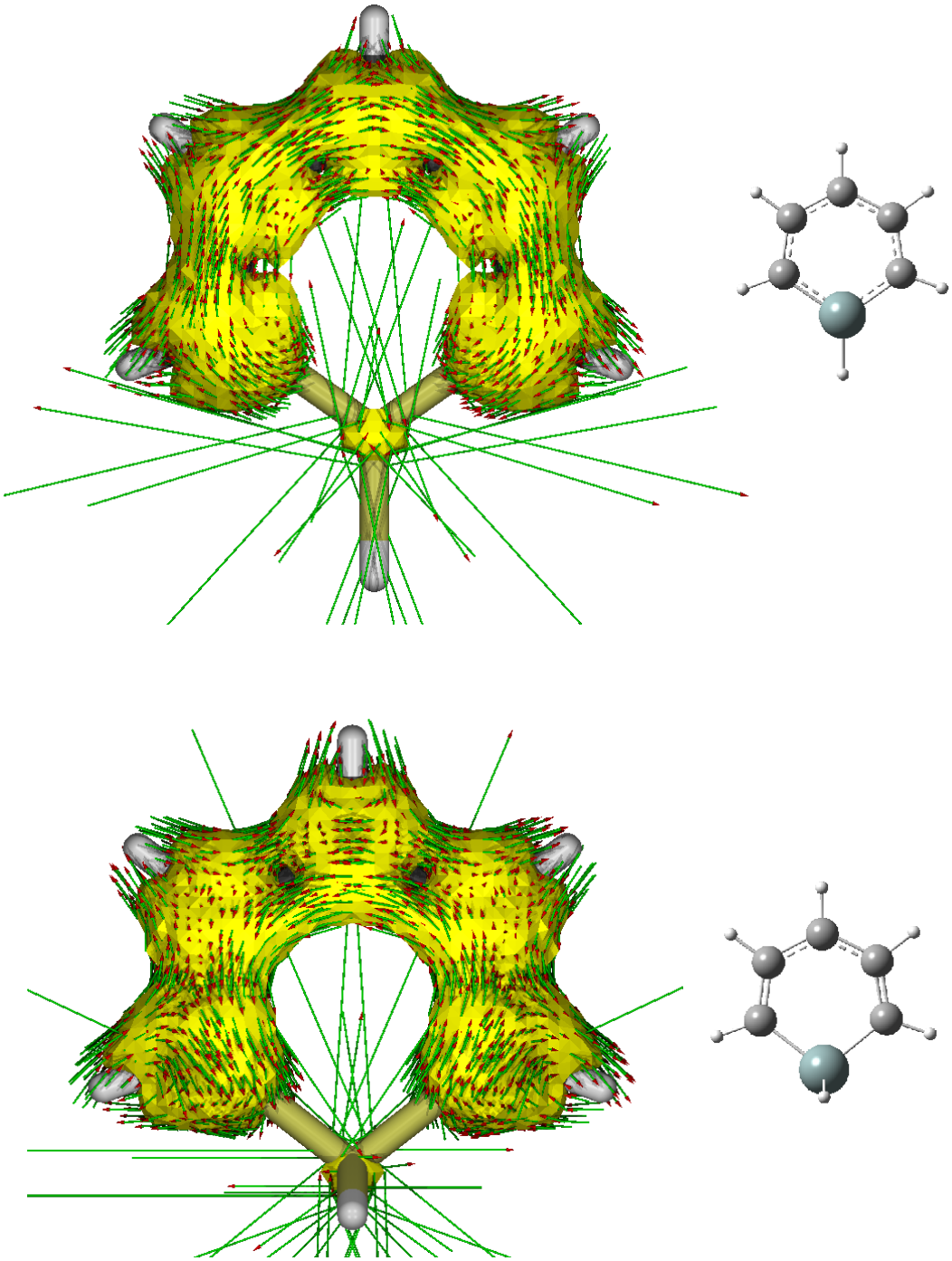


Figure S3. AICD plots of S_0 (top) and T_1 (bottom) silabenzene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

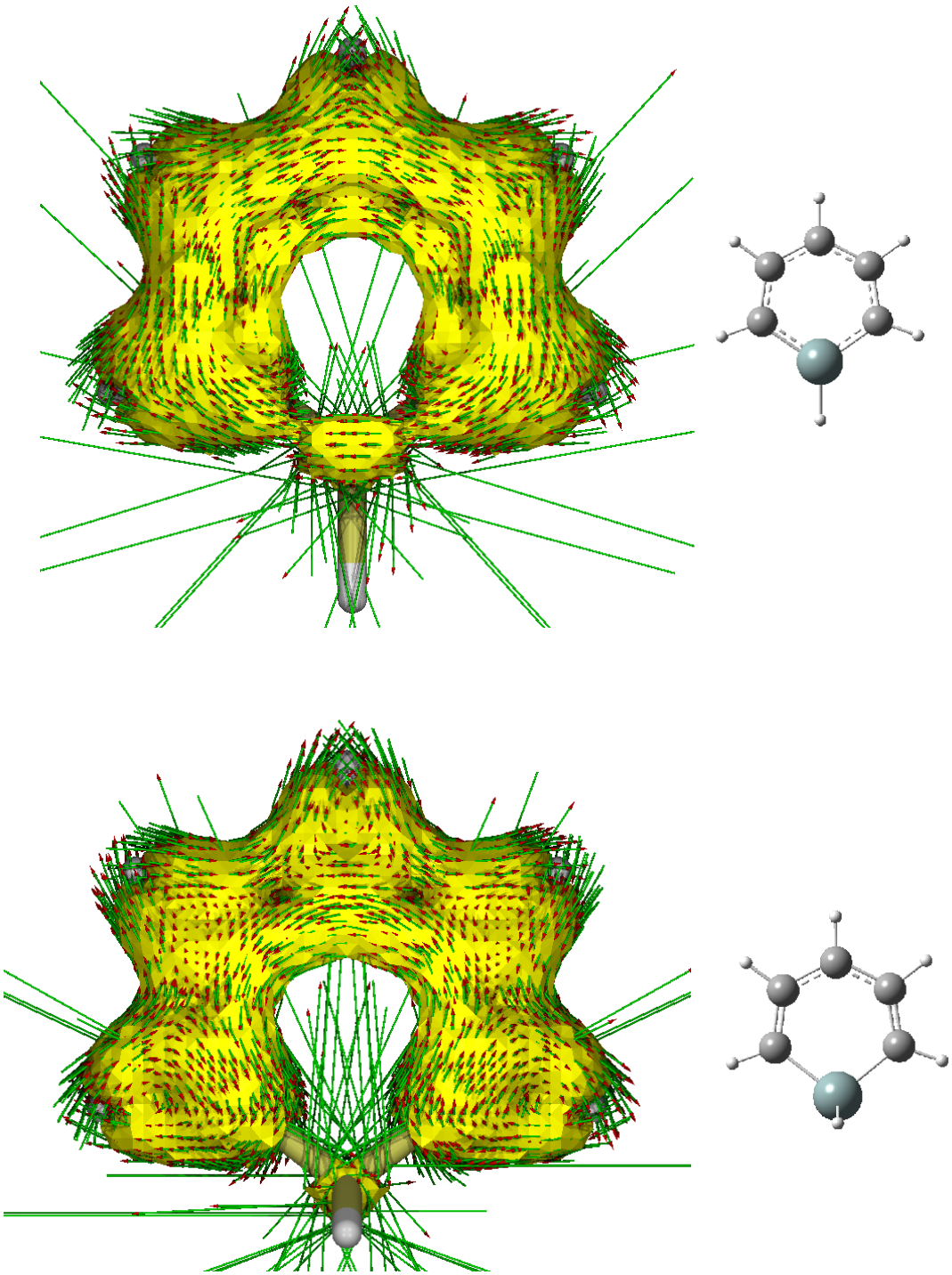


Figure S4. AICD plots of S_0 (top) and T_1 (bottom) silabenzene at an isovalue of 0.03 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

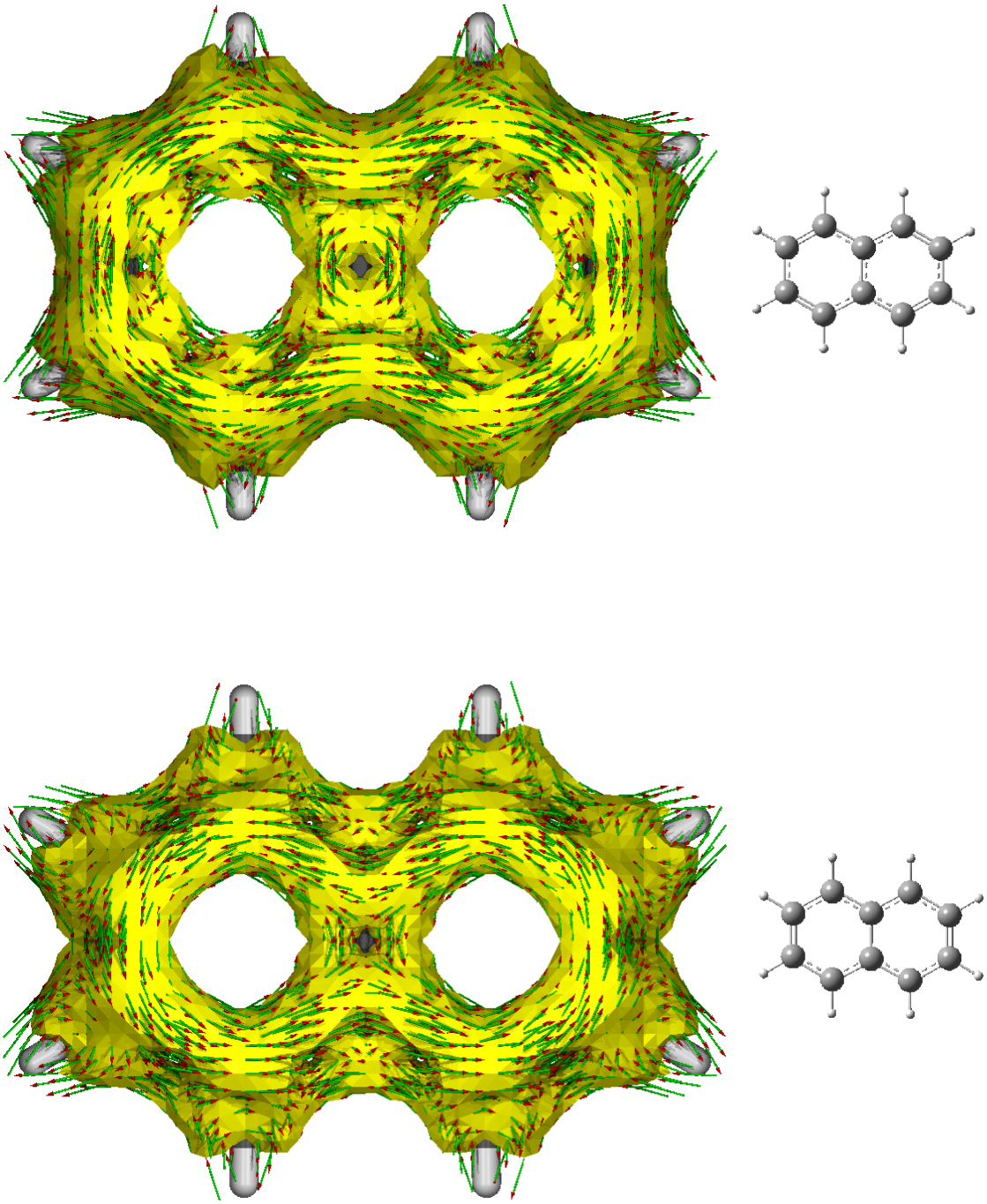


Figure S5. AICD plots of S_0 (top) and T_1 (bottom) naphthalene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

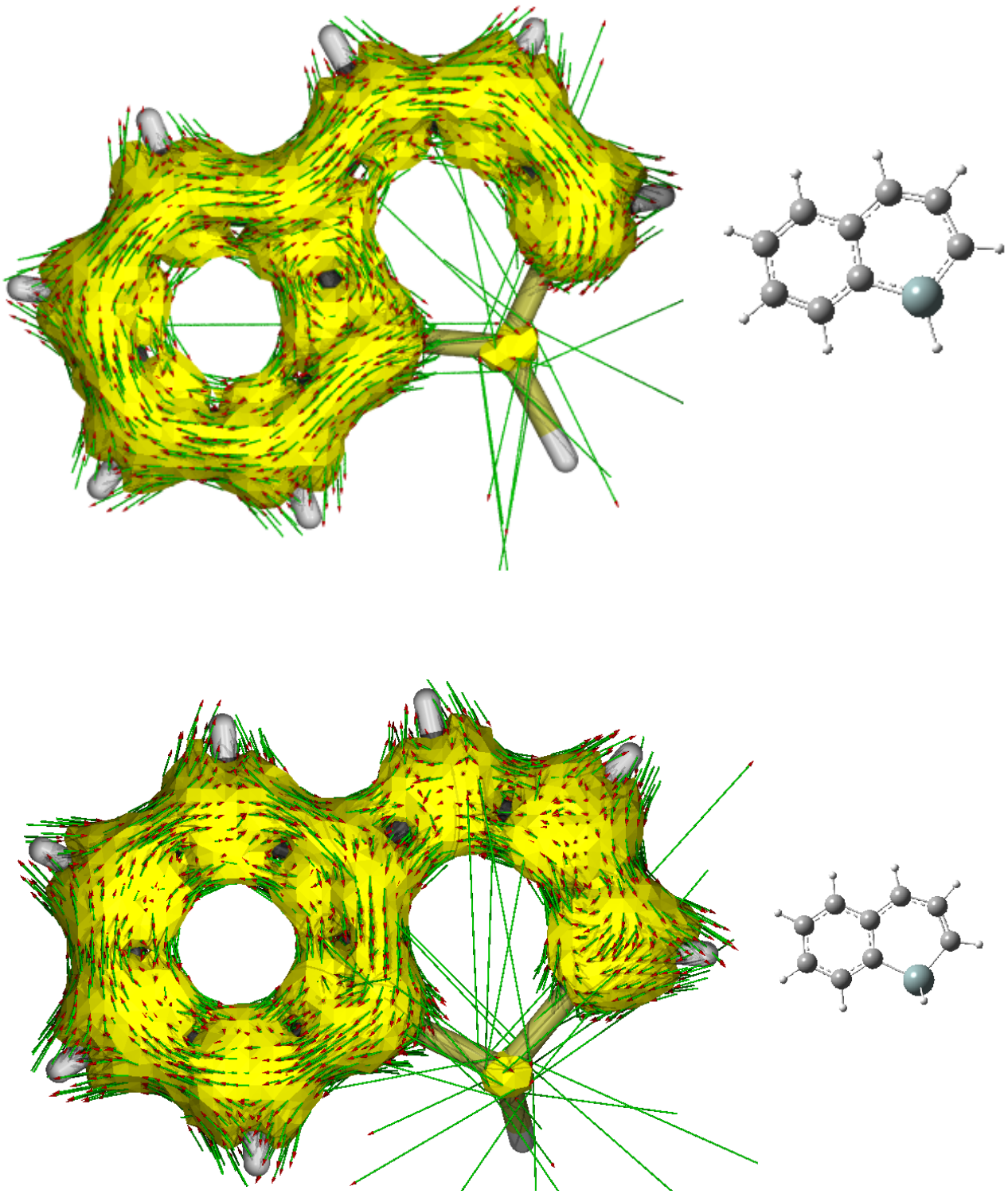


Figure S6. AICD plots of S_0 (top) and T_1 (bottom) 1-silanaphthalene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

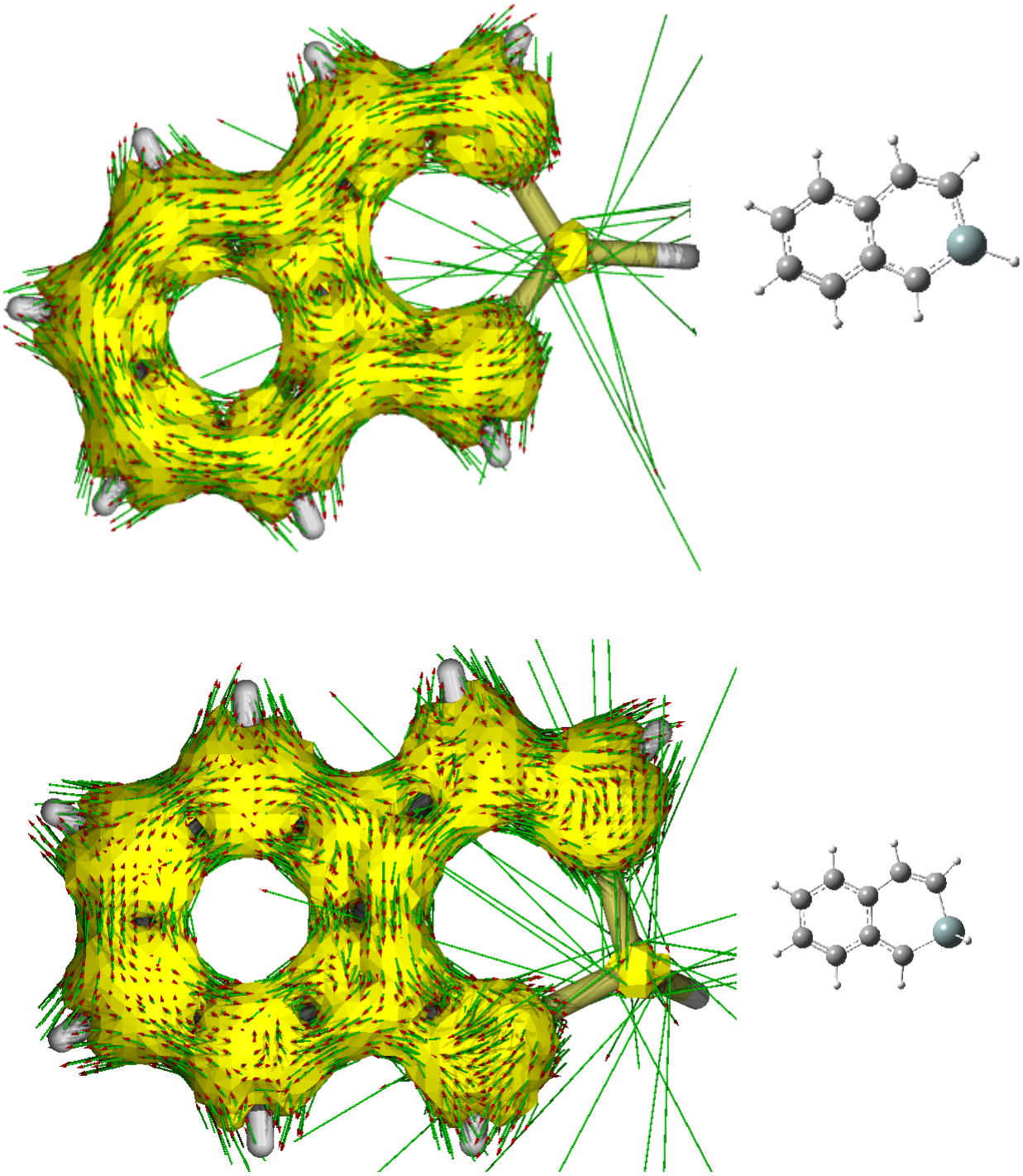


Figure S7. AICD plots of S_0 (top) and T_1 (bottom) 2-silanaphthalene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

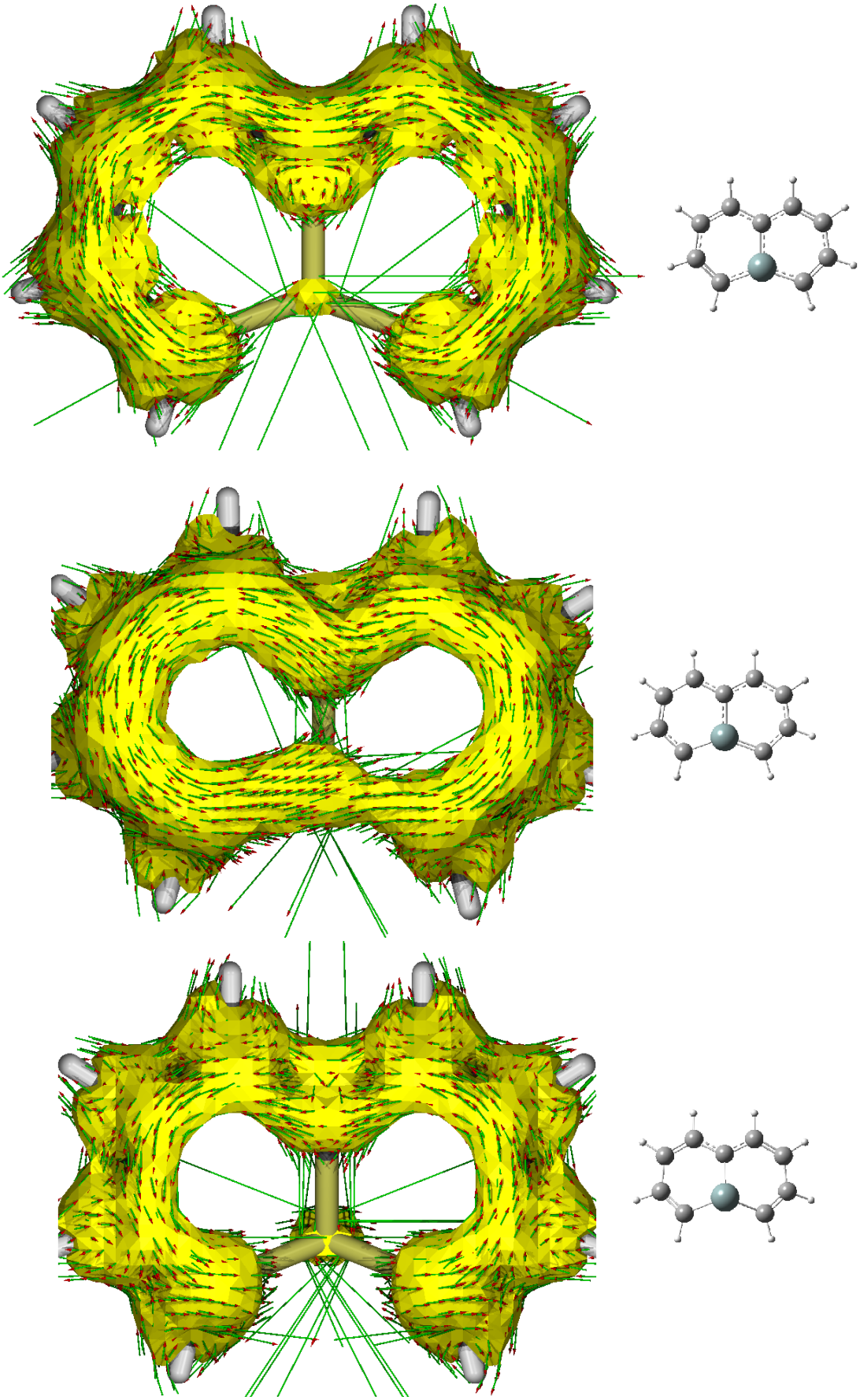


Figure S8. AICD plots of S_0 (top), T_1 planar (middle) and T_1 nonplanar (bottom) 9-silanaphthalene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

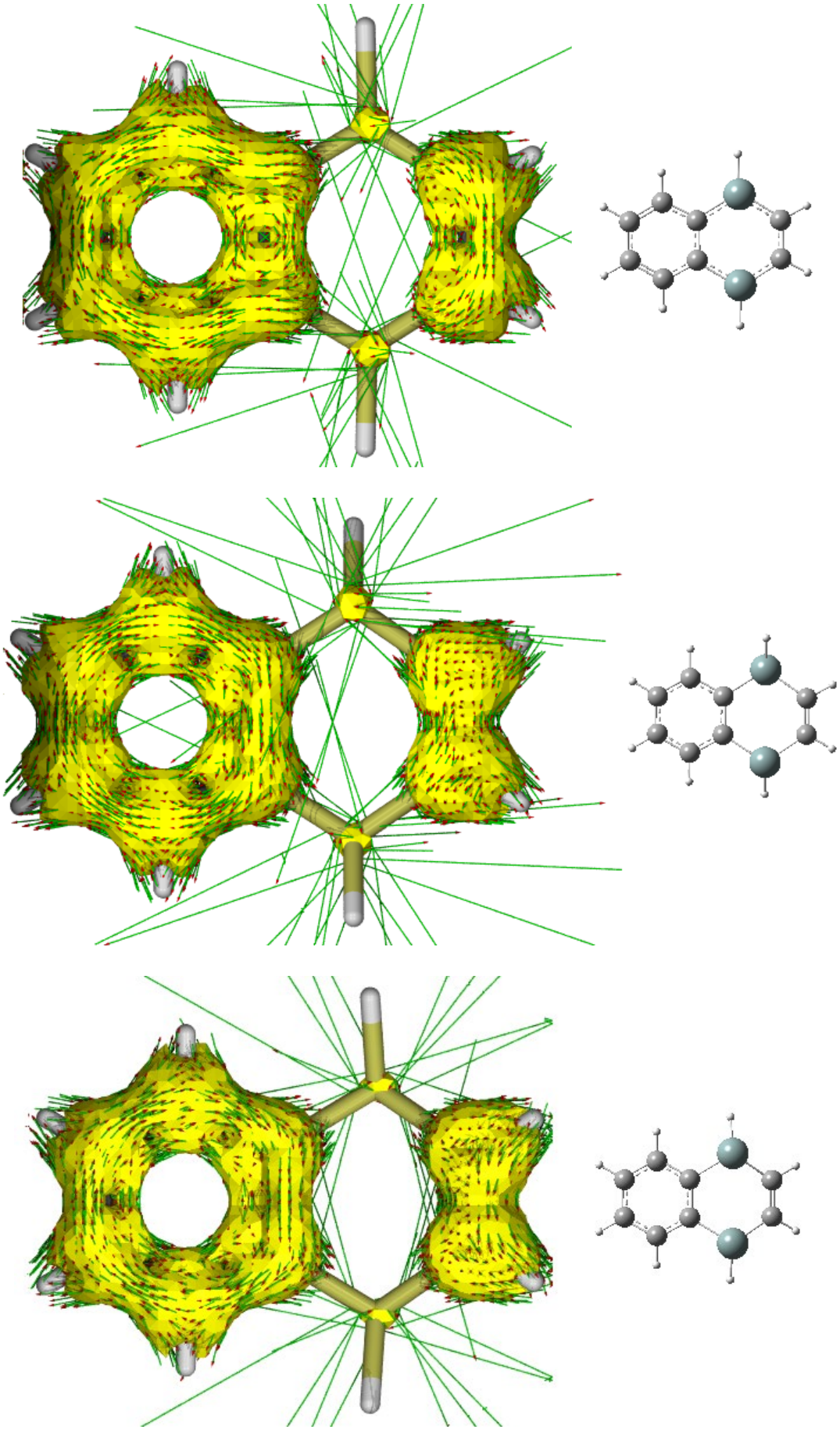


Figure S9. AICD plots of S_0 (top), T_1 opp (middle) and T_1 same (bottom) 1,4-disilanaphthalene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

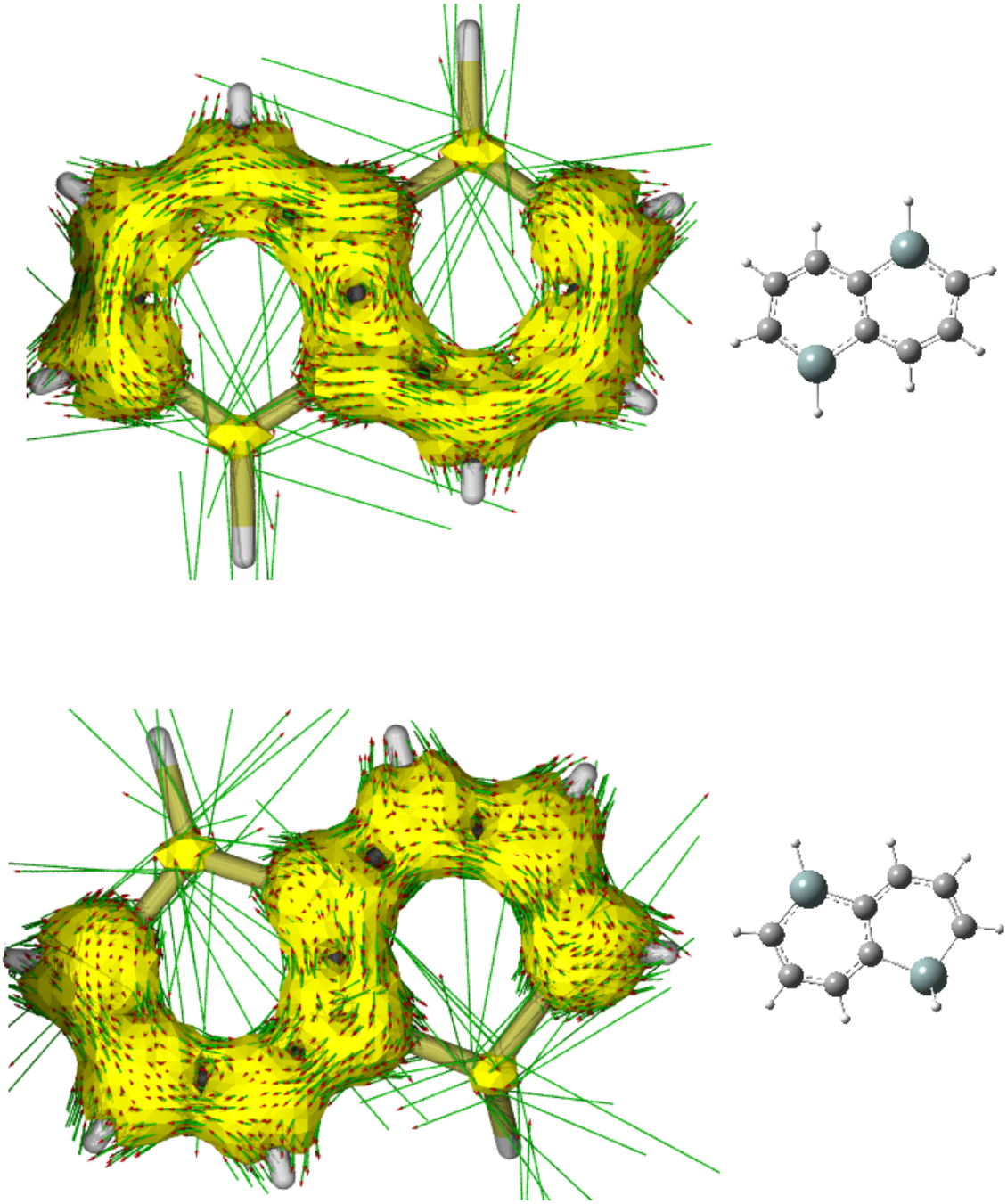


Figure S10. AICD plots of S_0 (top) and T_1 (bottom) 1,5-disilanaphthalene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

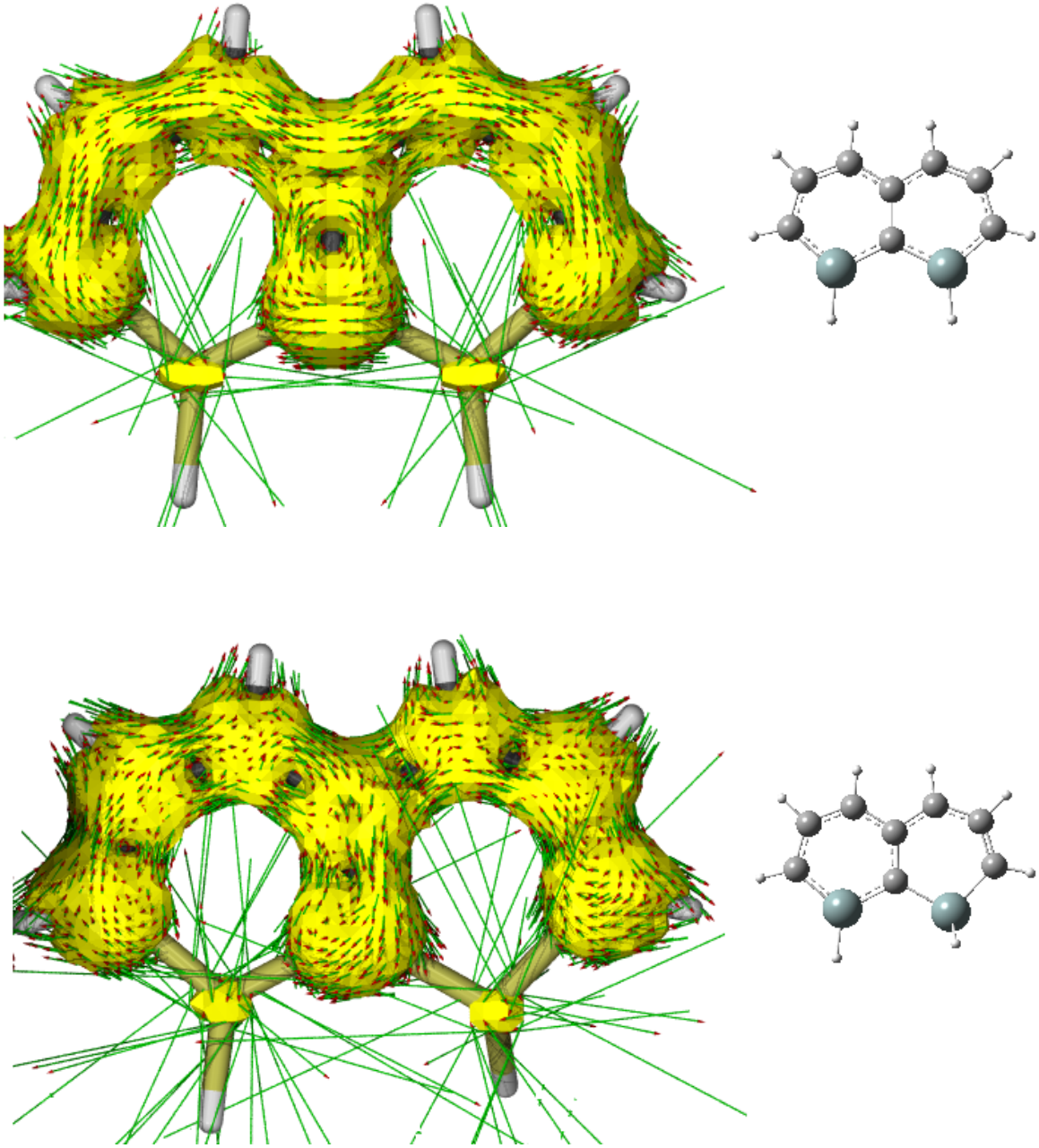


Figure S11. AICD plots of S_0 (top) and T_1 (bottom) 1,8-disilanaphthalene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

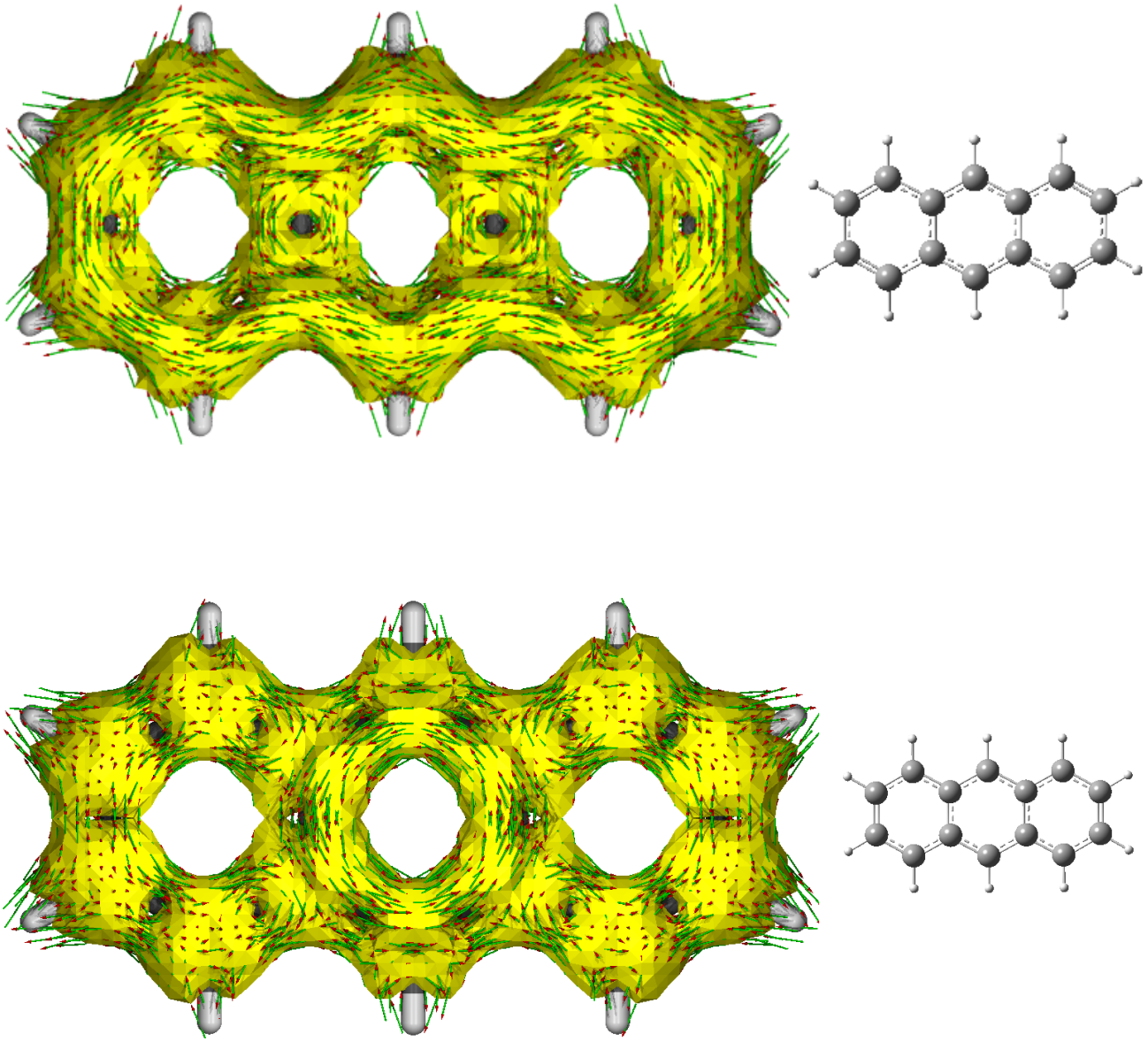
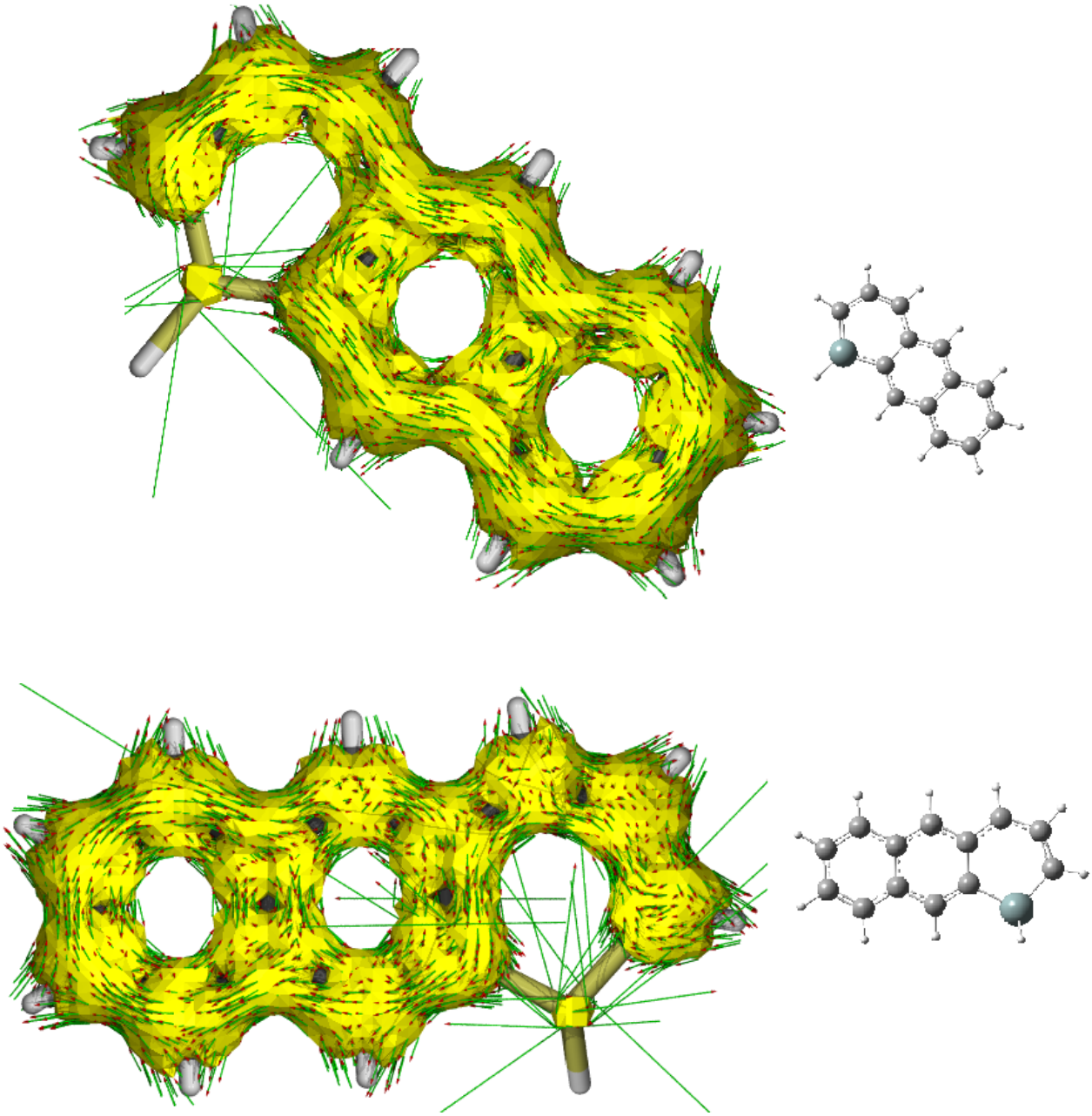


Figure S12. AICD plots of S_0 (top) and T_1 (bottom) anthracene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.



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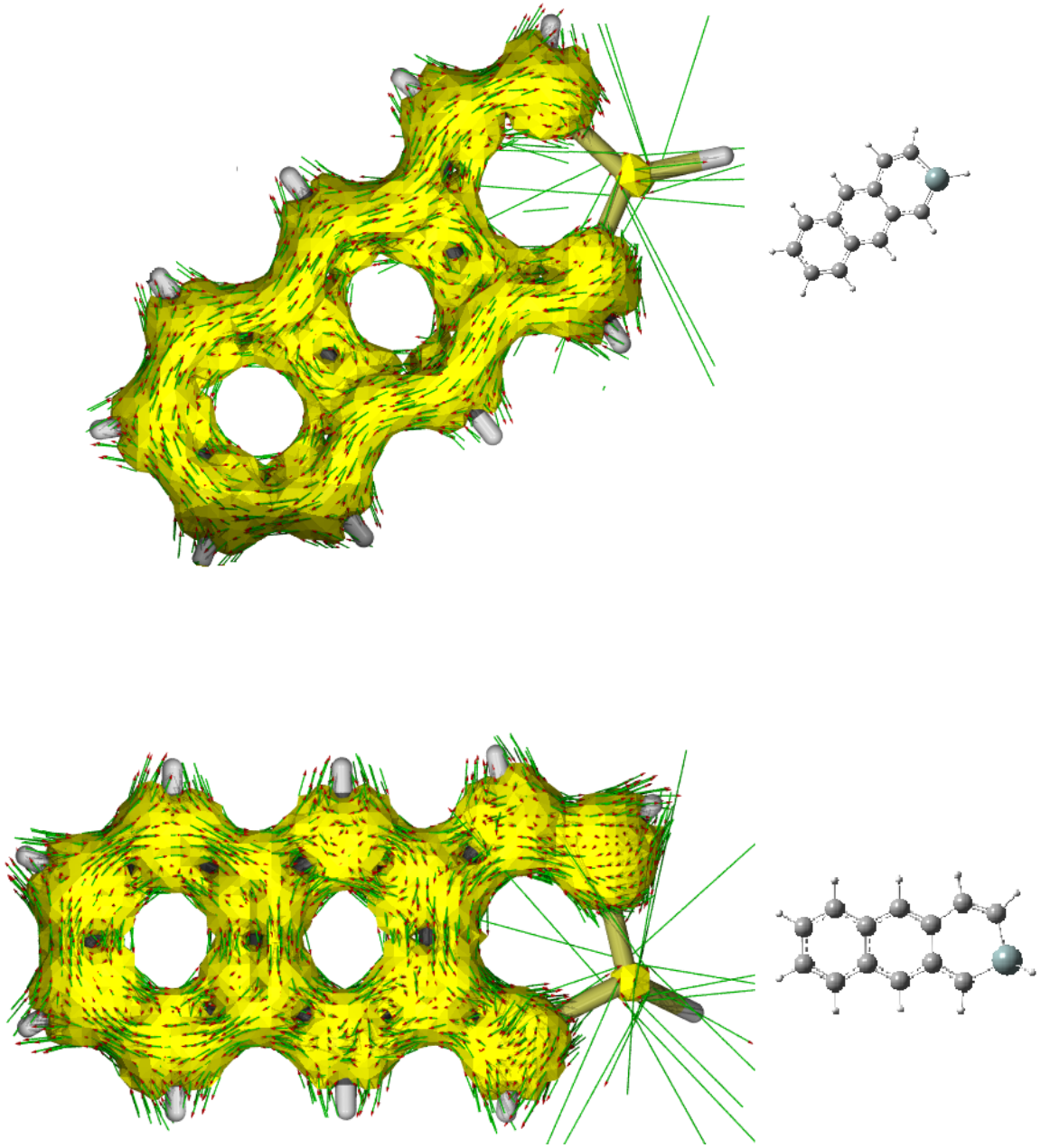

Figure S14. AICD plots of S_0 (top) and T_1 (bottom) 2-silaanthracene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

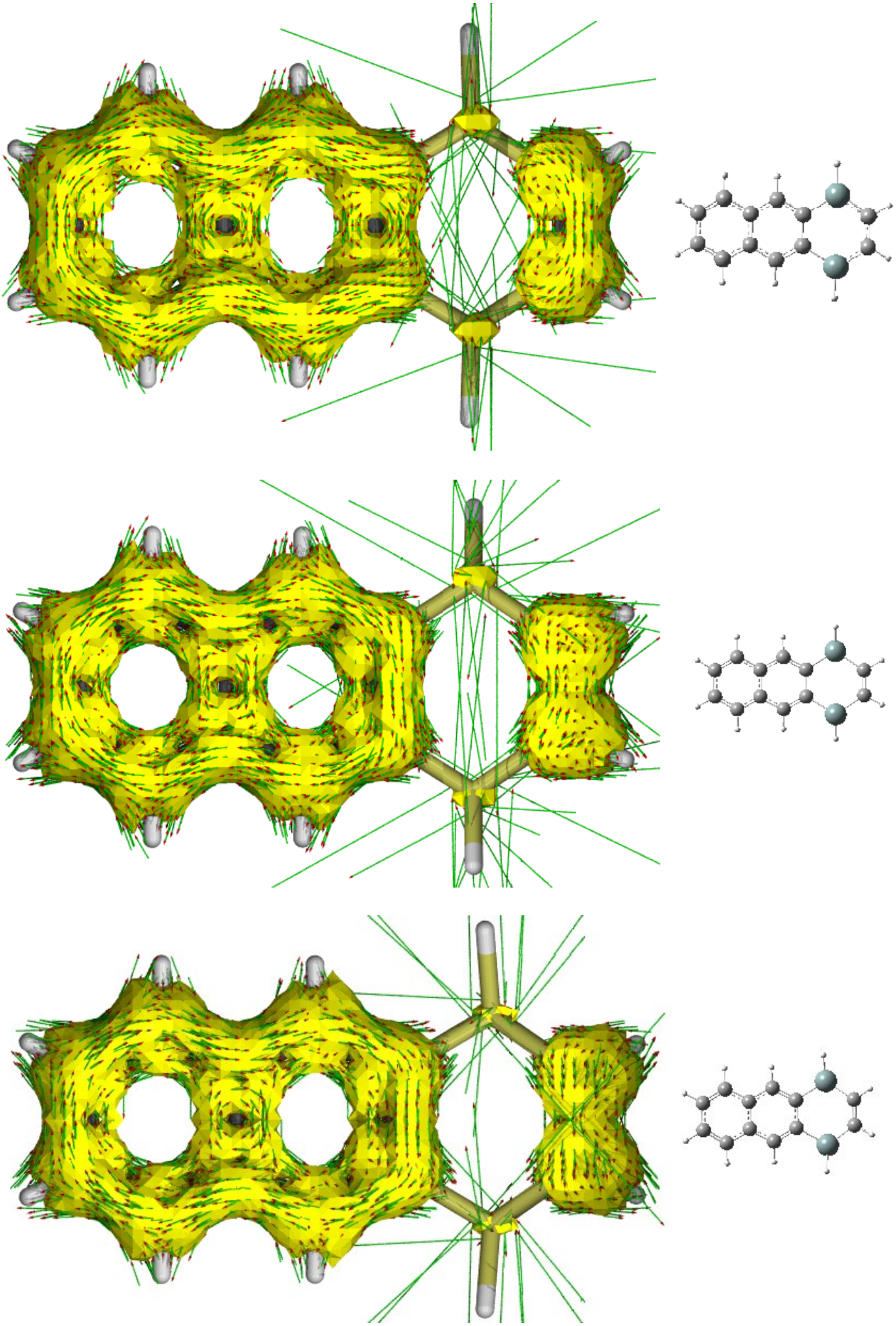

Figure S15. AICD plots of S_0 (top), T_1 opp (middle) and T_1 same (bottom) 1,4-disilaanthracene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

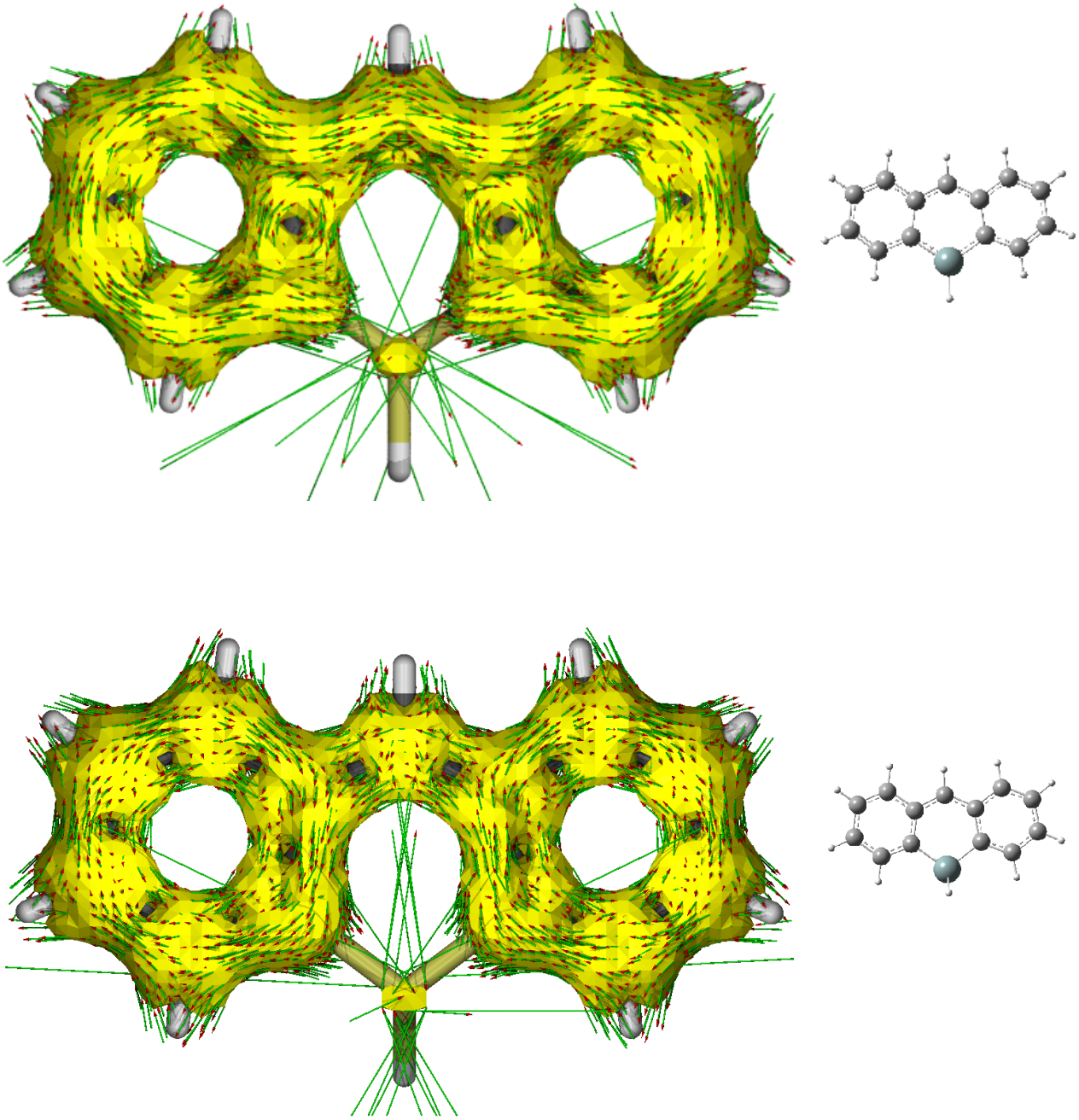

Figure S16. AICD plots of S_0 (top) and T_1 (bottom) 9-silaanthracene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

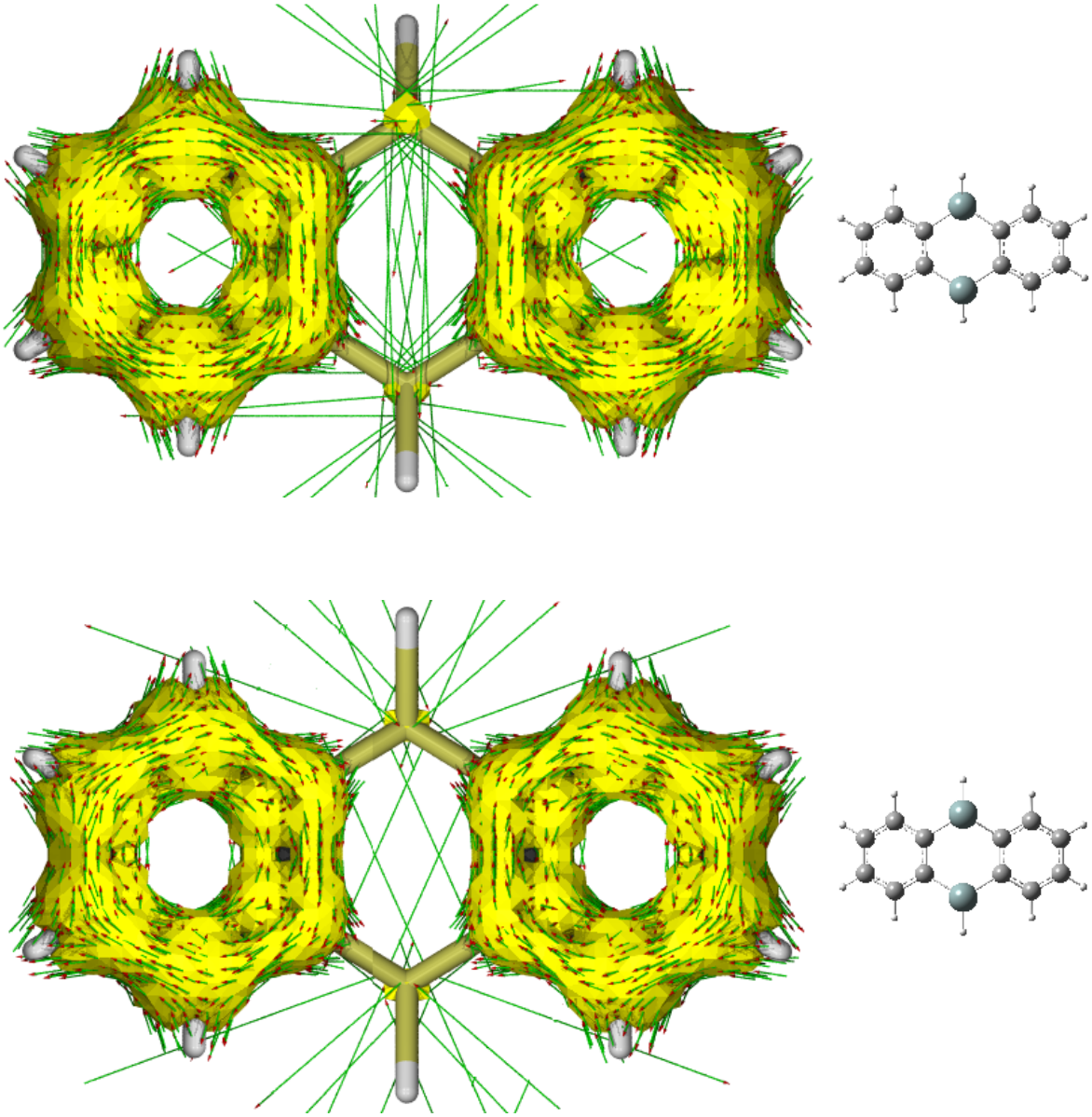

Figure S17. AICD plots of T_1 opp (top) and T_1 same (bottom) 9,10-disilaanthracene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic. For the S_0 state, no one axis was perpendicular to the molecular plane.

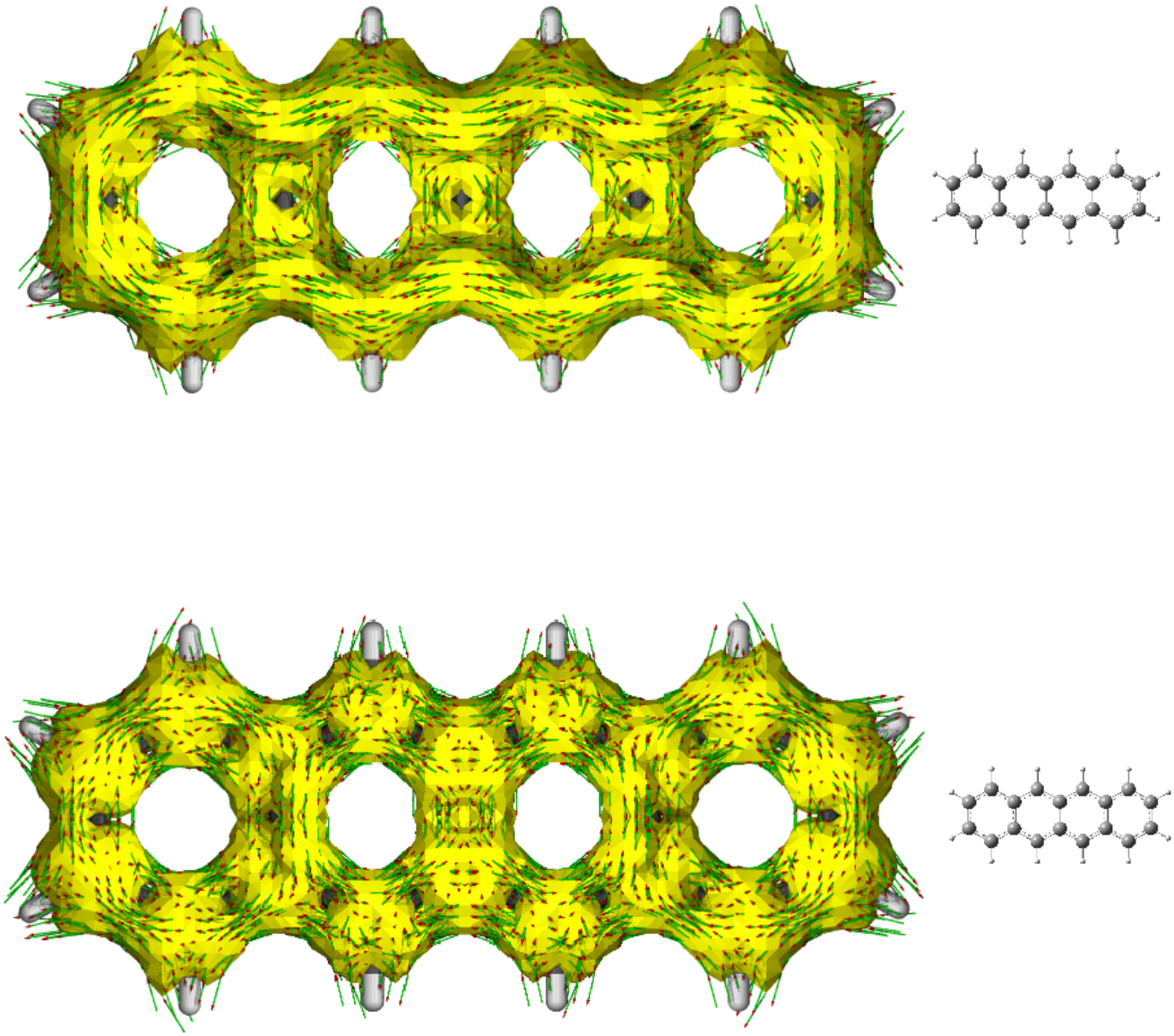

Figure S18. AICD plots of S_0 (top) and T_1 (bottom) tetracene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

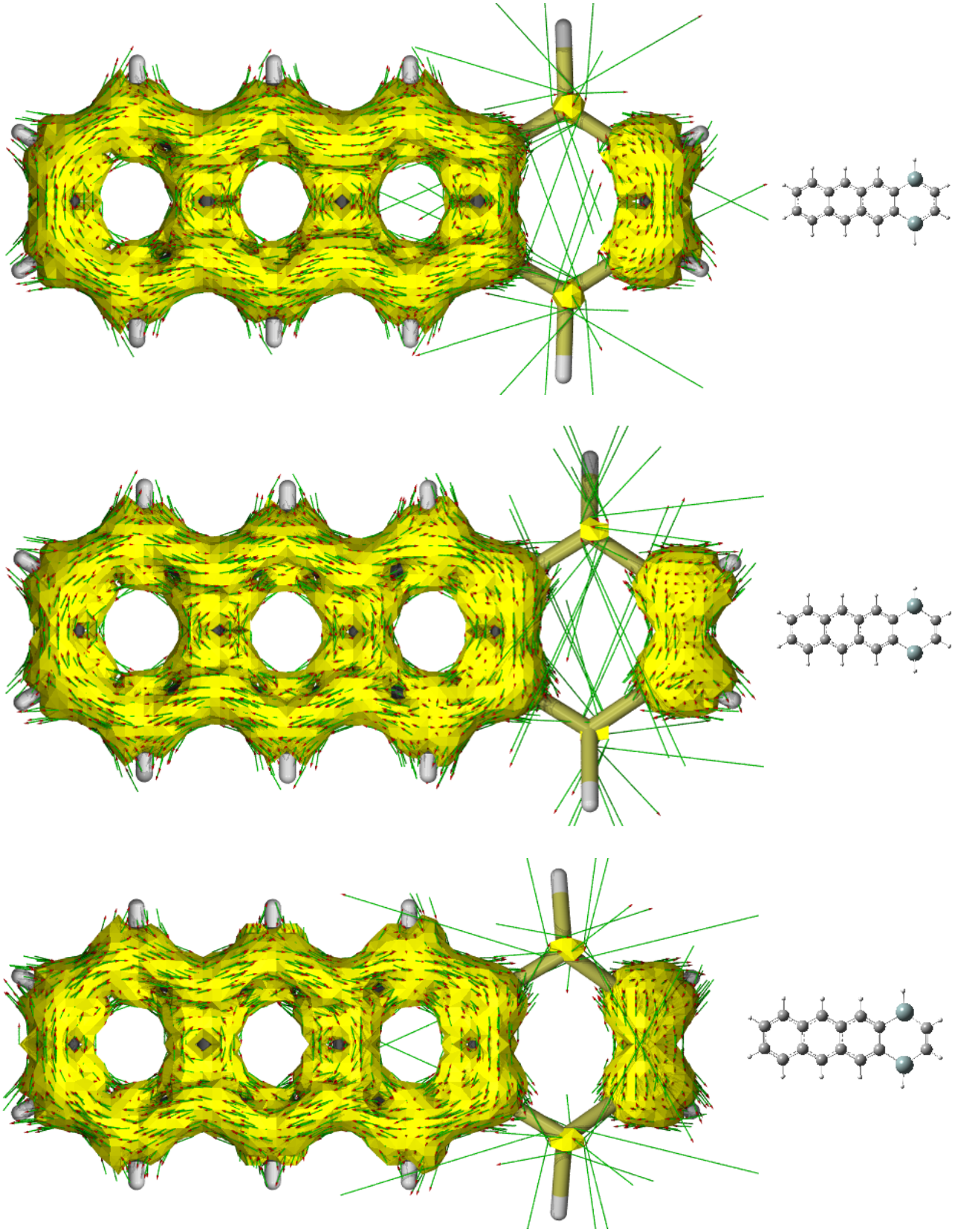

Figure S19. AICD plots of S_0 (top), T_1 opp (middle) and T1 same (bottom) 1,4-disilatetracene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

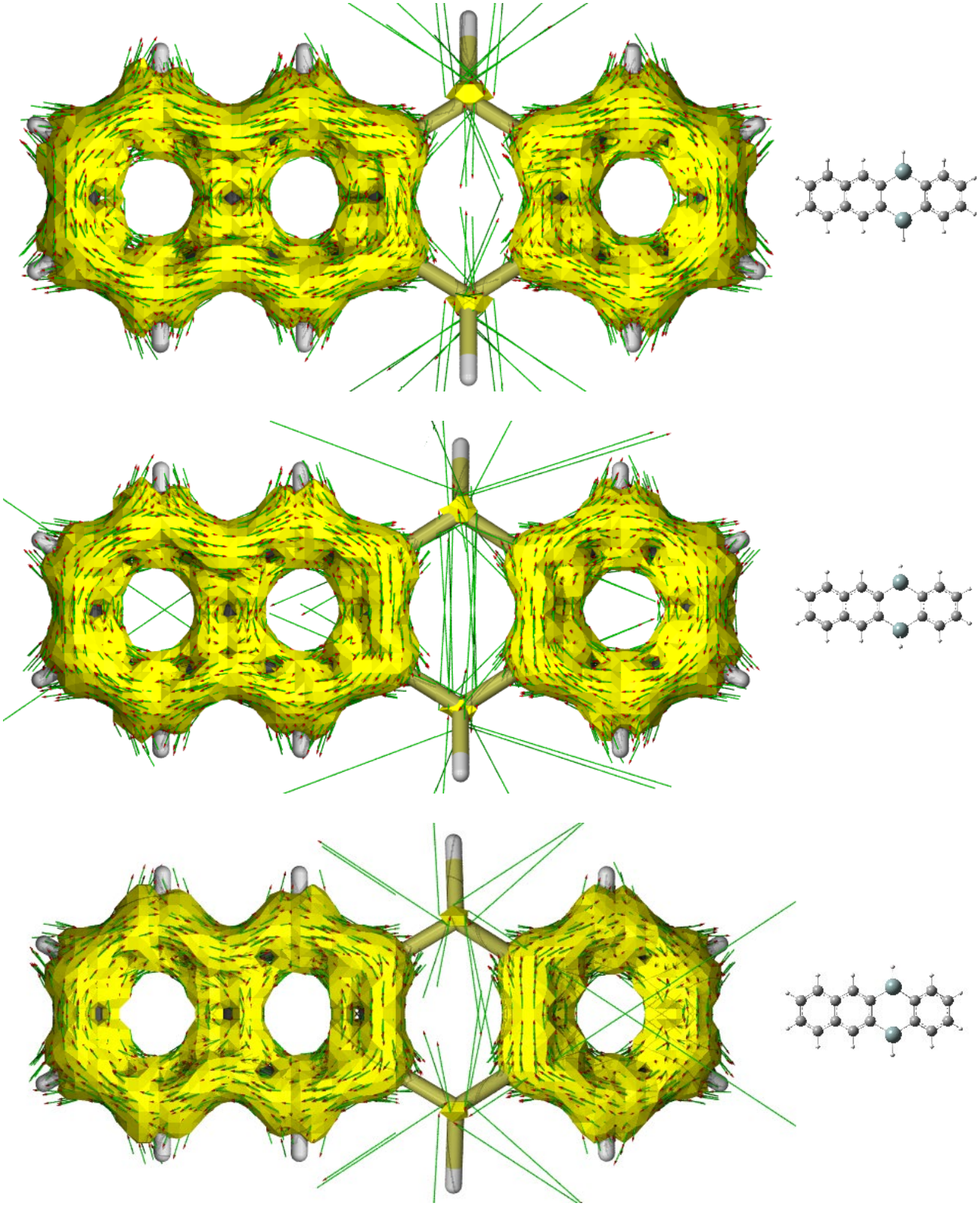

Figure S20. AICD plots of S_0 (top), T_1 opp (middle) and T1 same (bottom) 5,12-disilatetracene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

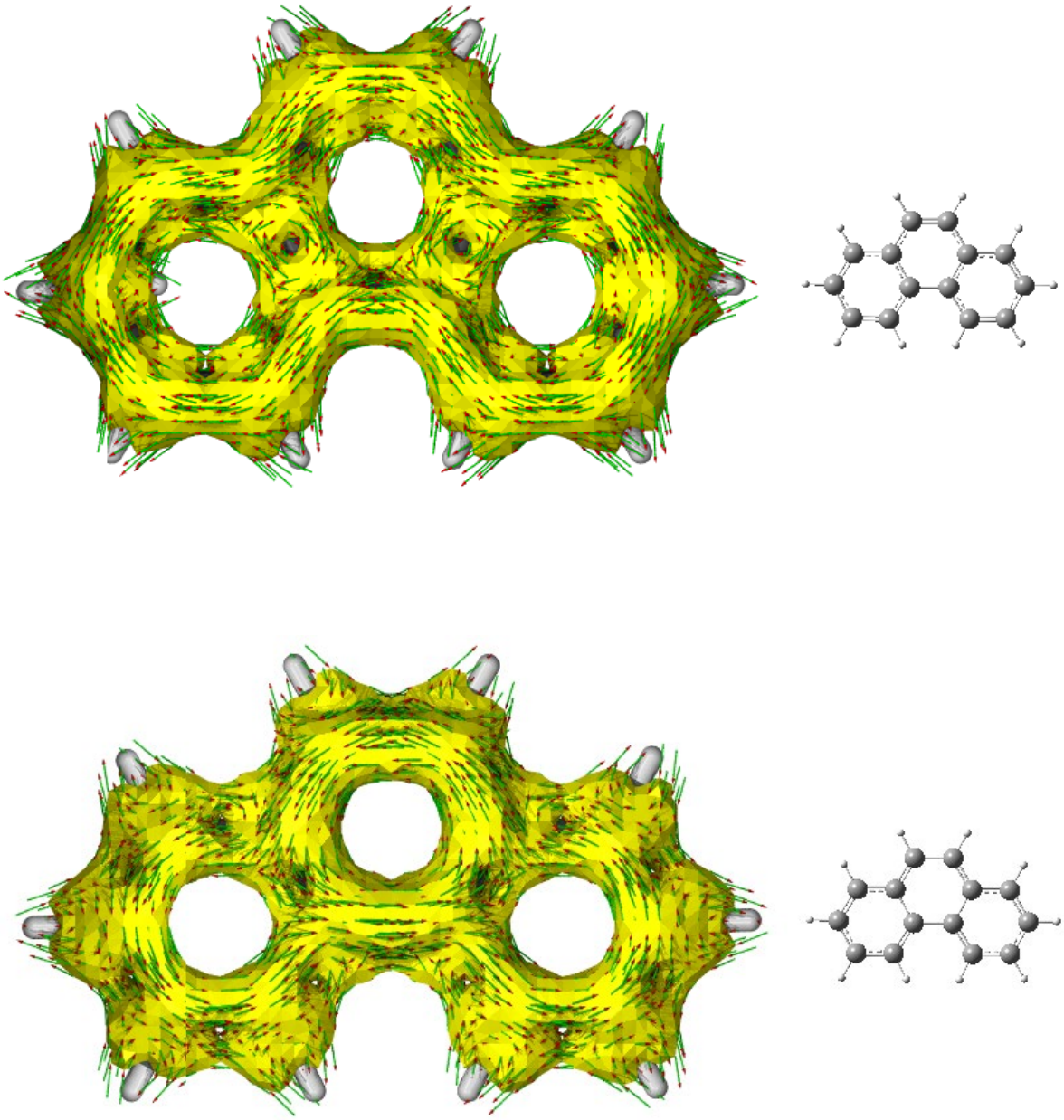

Figure S21. AICD plots of S_0 (top) and T_1 (bottom) phenantrene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

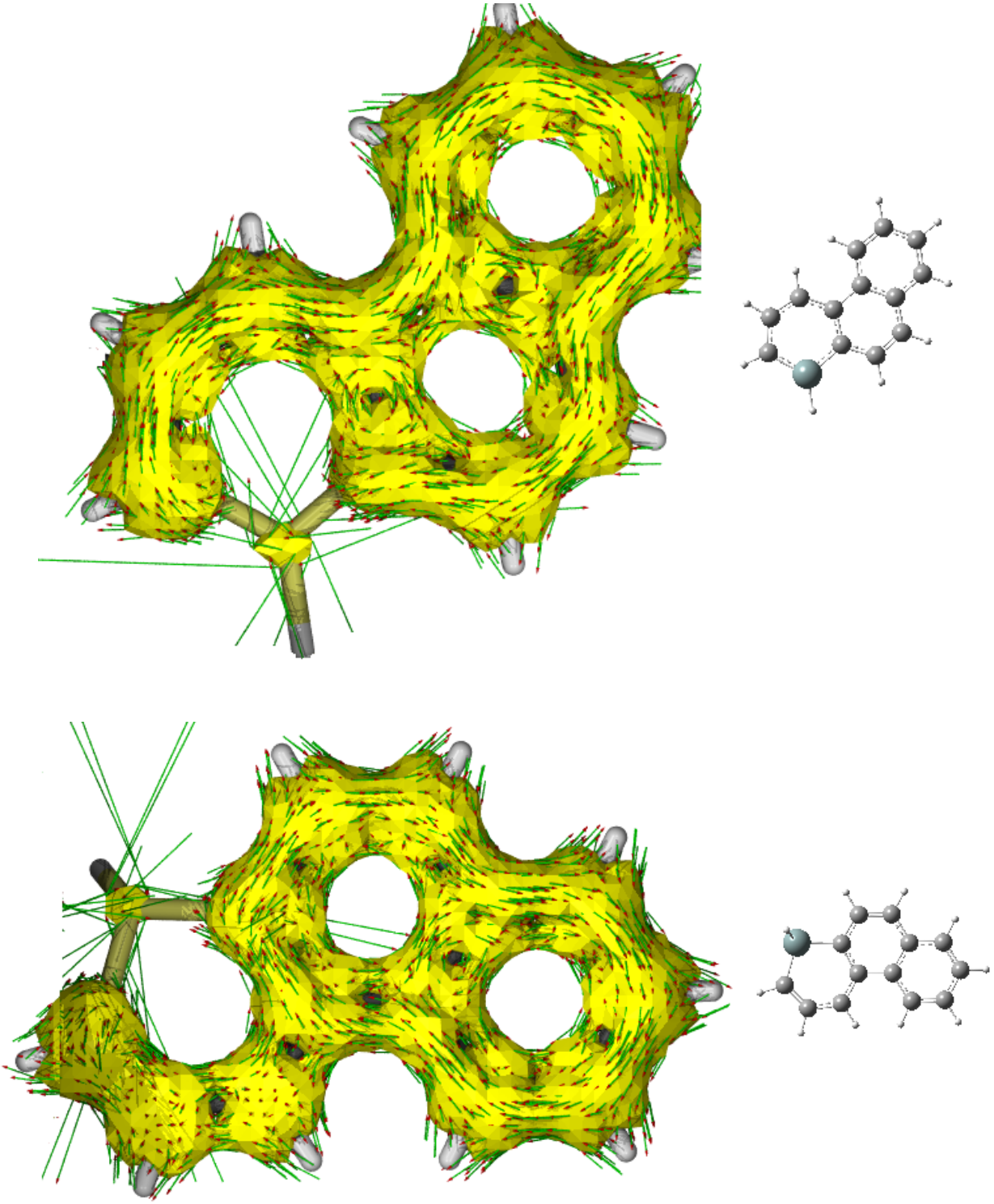

Figure S22. AICD plots of S_0 (top) and T_1 (bottom) 1-silaphenantrene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

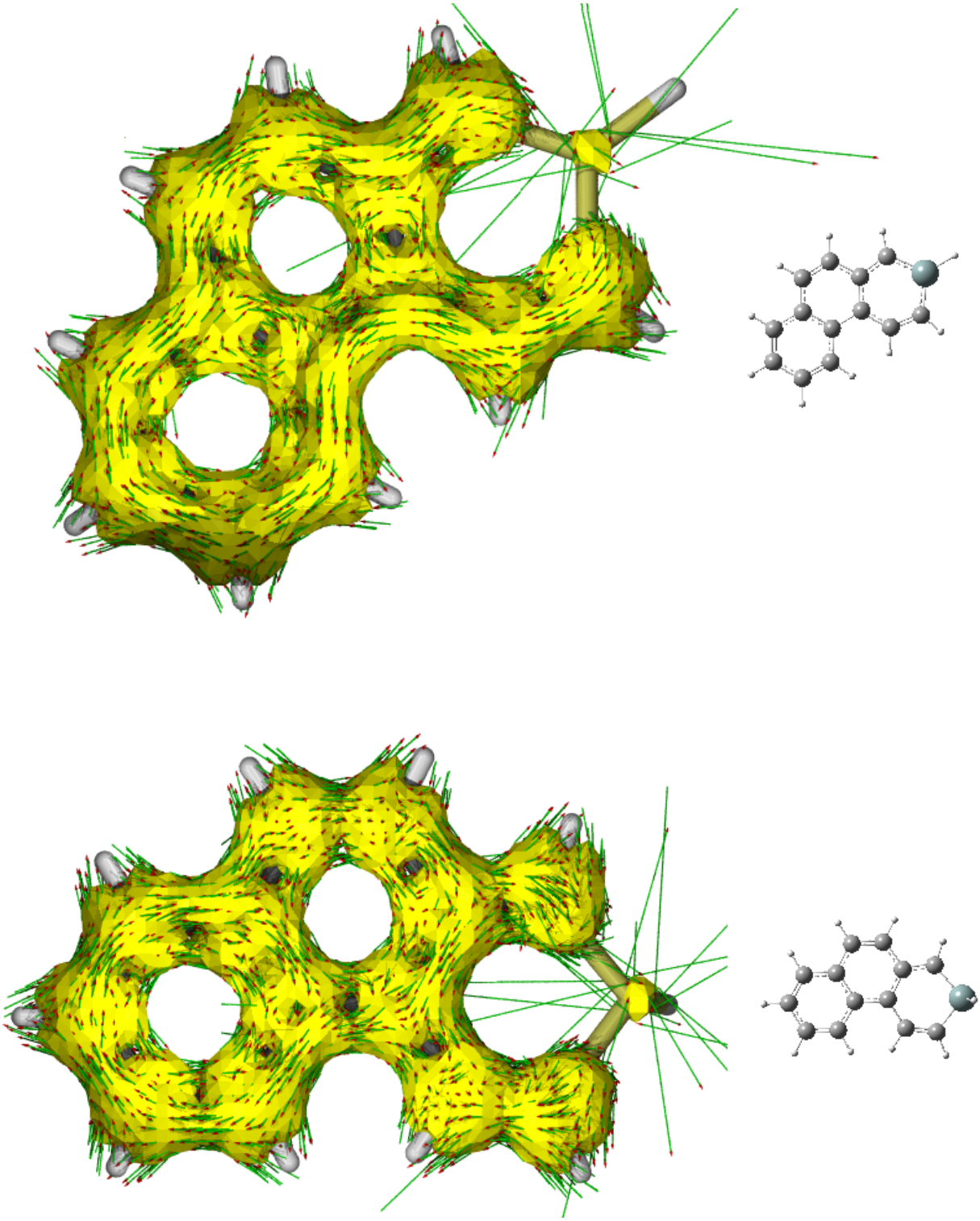

Figure S23. AICD plots of S_0 (top) and T_1 (bottom) 2-silaphenantrene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

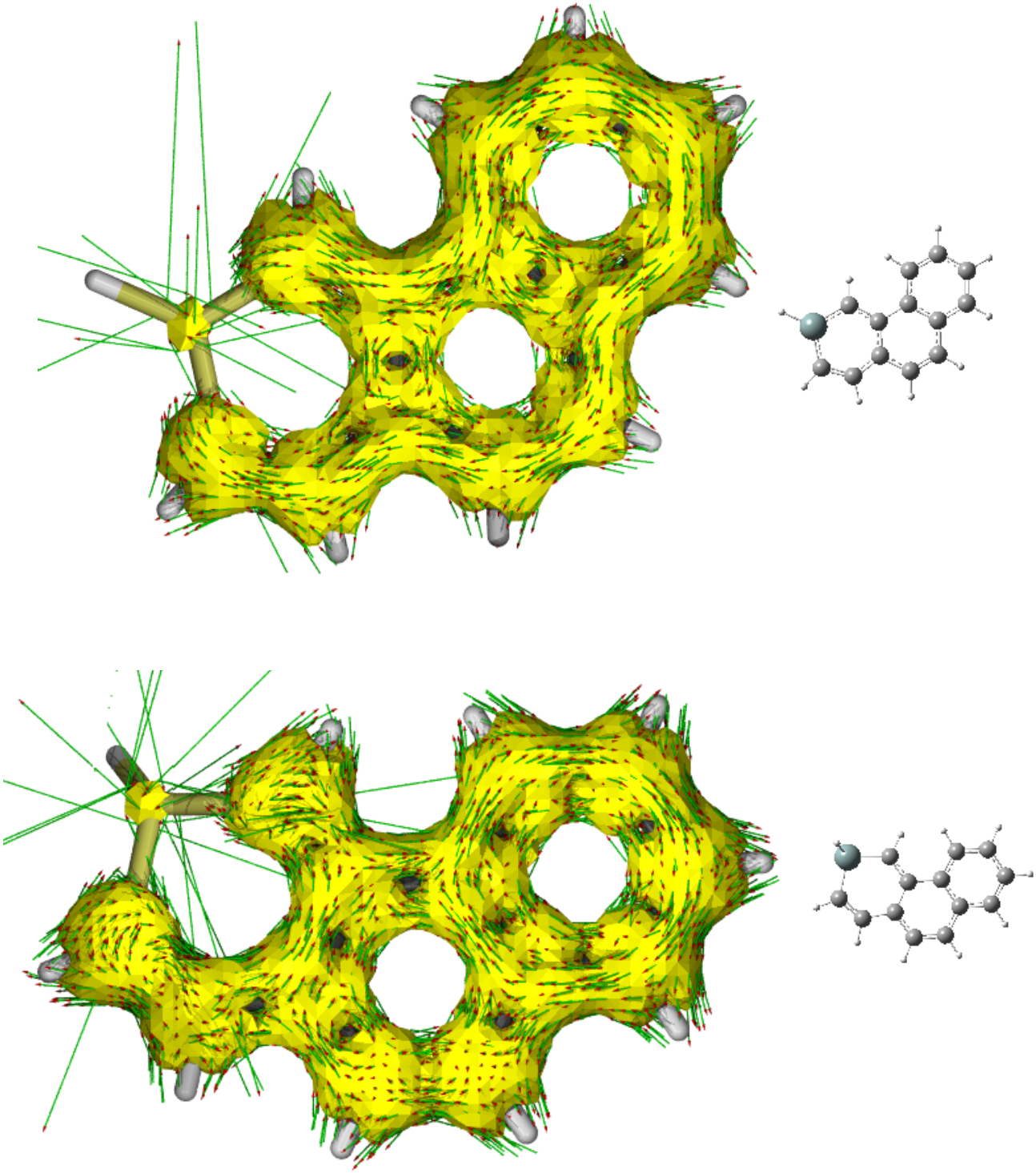

Figure S24. AICD plots of S_0 (top) and T_1 (bottom) 3-silaphenantrene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

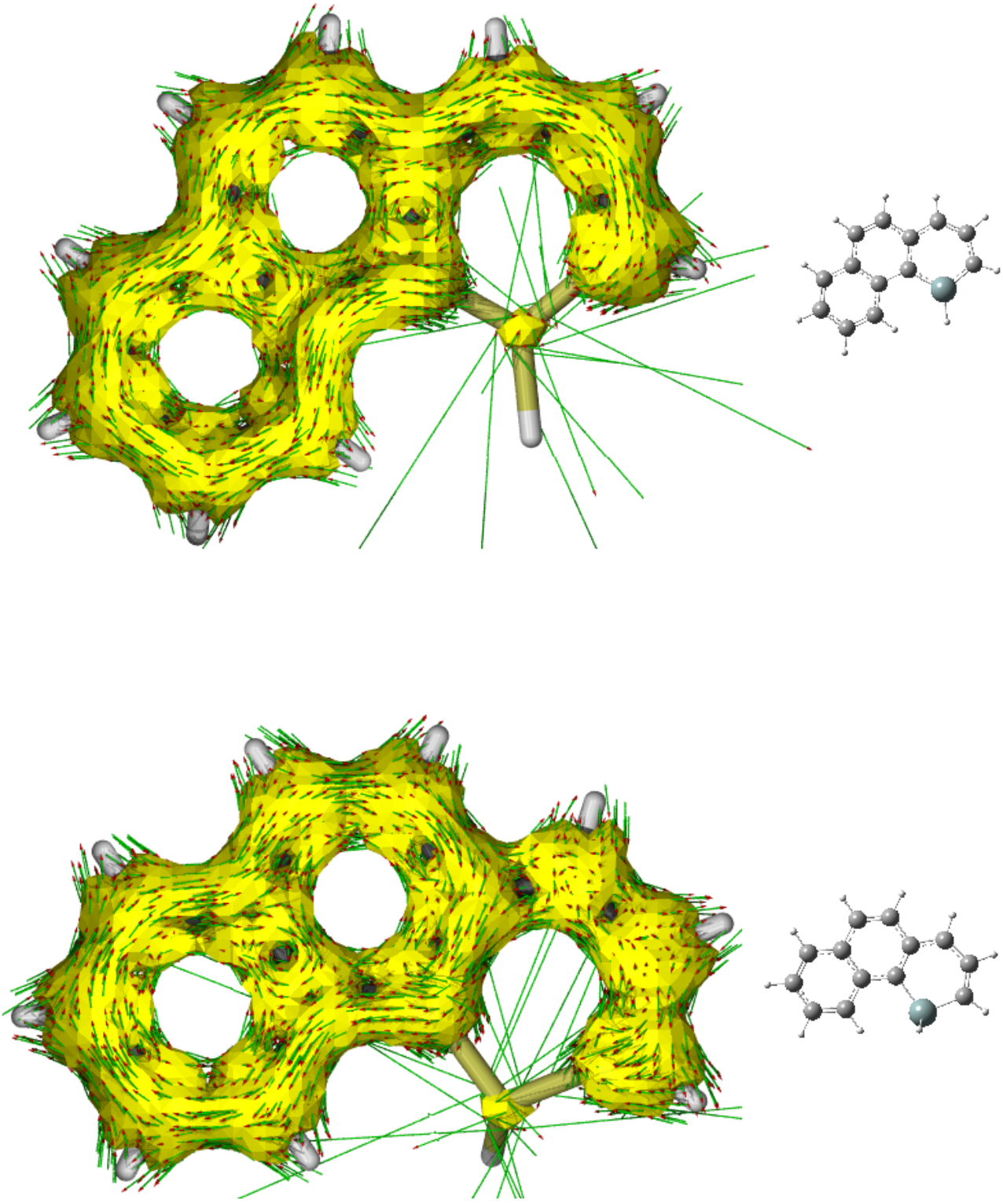

Figure S25. AICD plots of S_0 (top) and T_1 (bottom) 4-silaphenantrene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

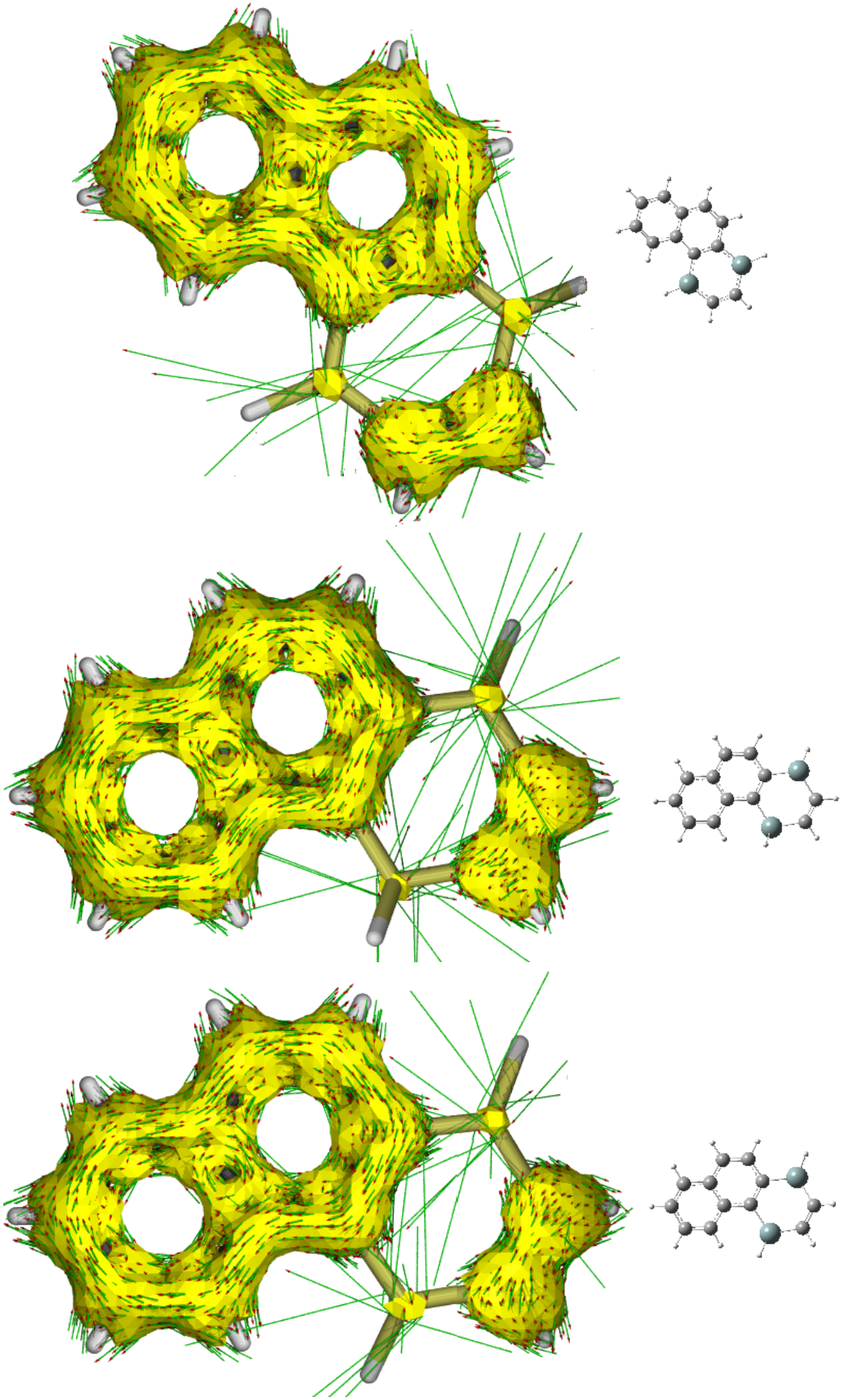

Figure S26. AICD plots of S_0 (top), T_1 opp (middle) and T1 same (bottom) 1,4-disilaphenantrene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

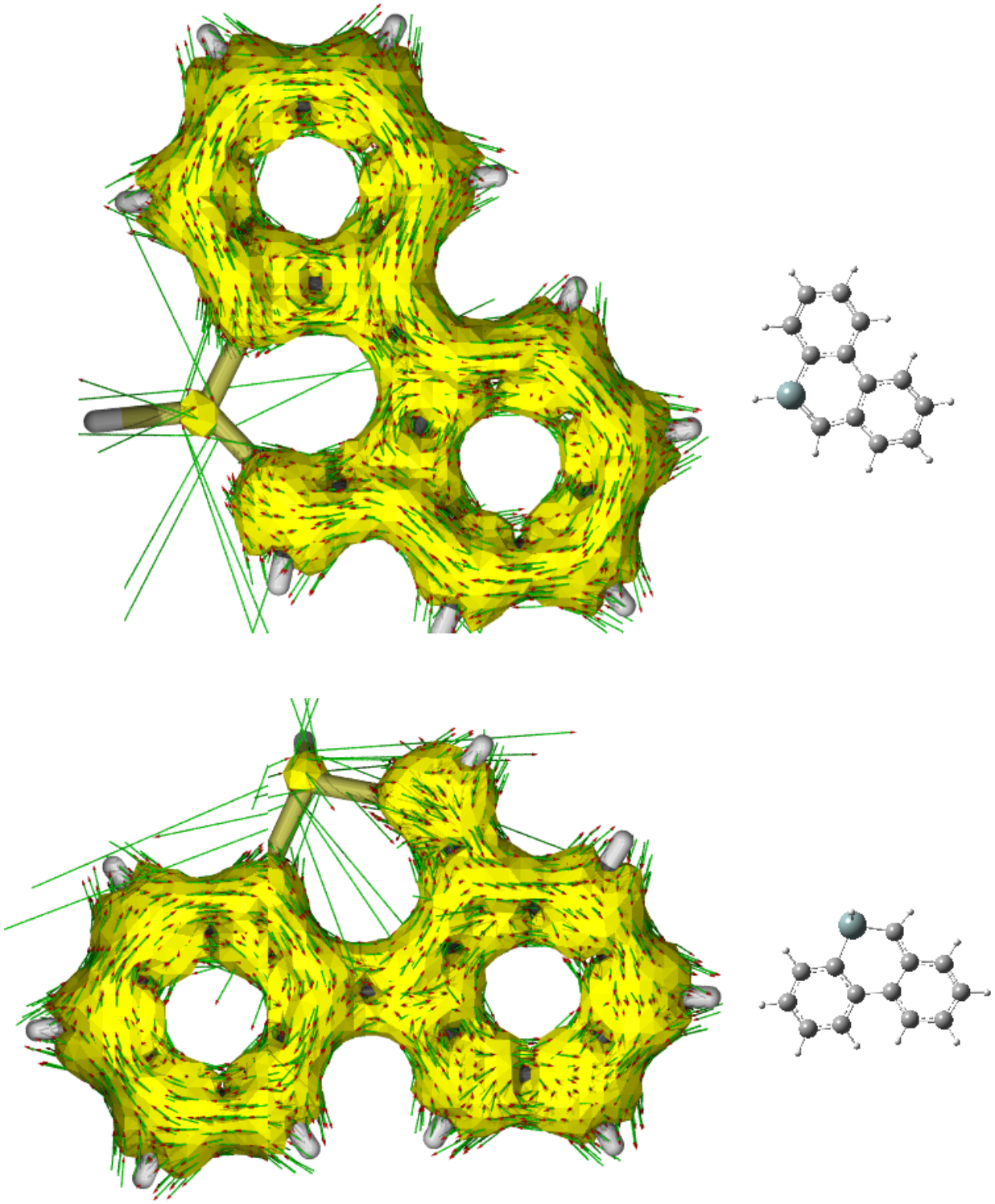

Figure S27. AICD plots of S_0 (top) and T_1 (bottom) 9-silaphenantrene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

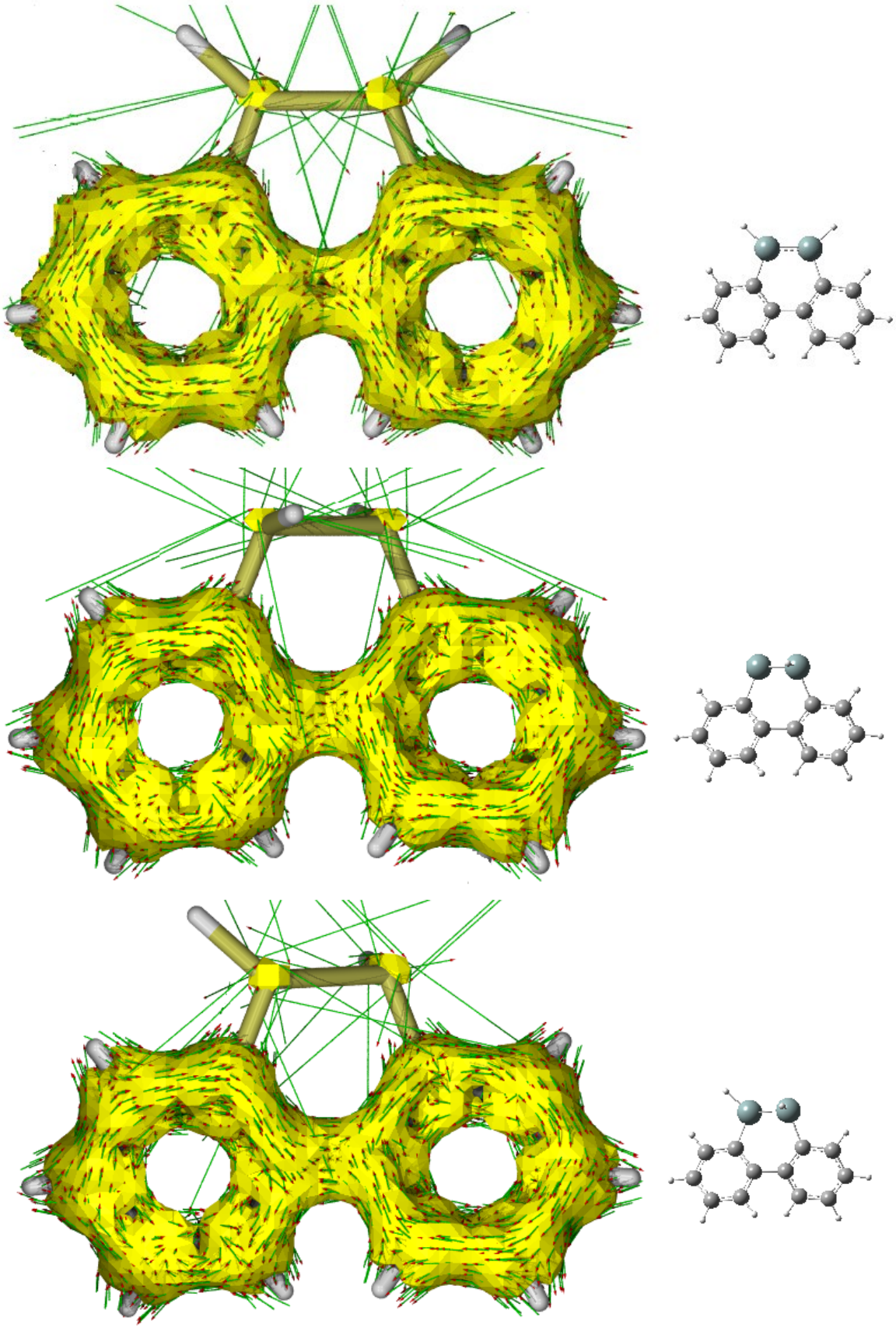

Figure S28. AICD plots of S_0 (top), T_1 opp (middle) and T1 same (bottom) 9,10-disilaphenantrene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

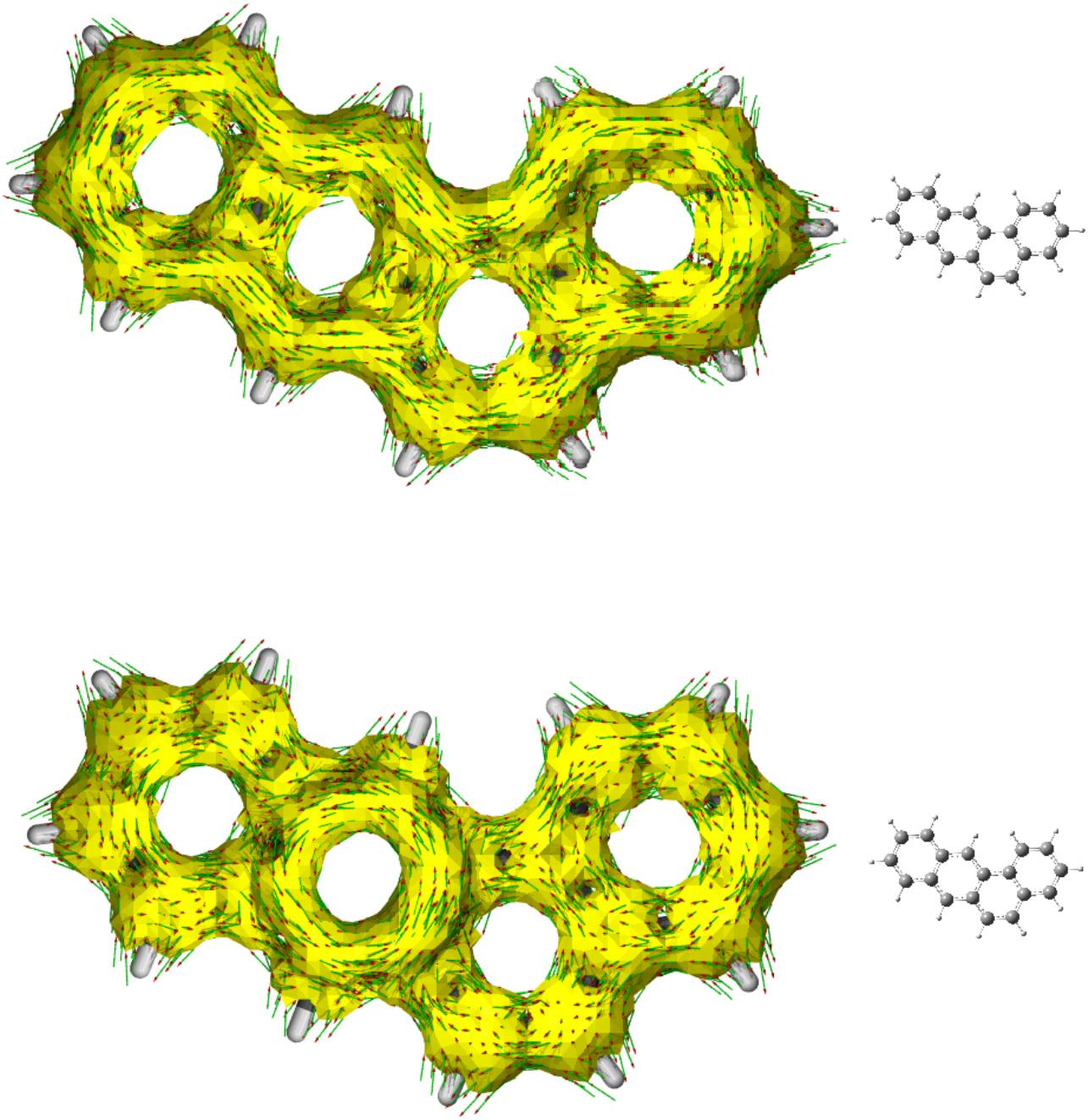

Figure S29. AICD plots of S_0 (top) and T_1 (bottom) benz[*a*]antracene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

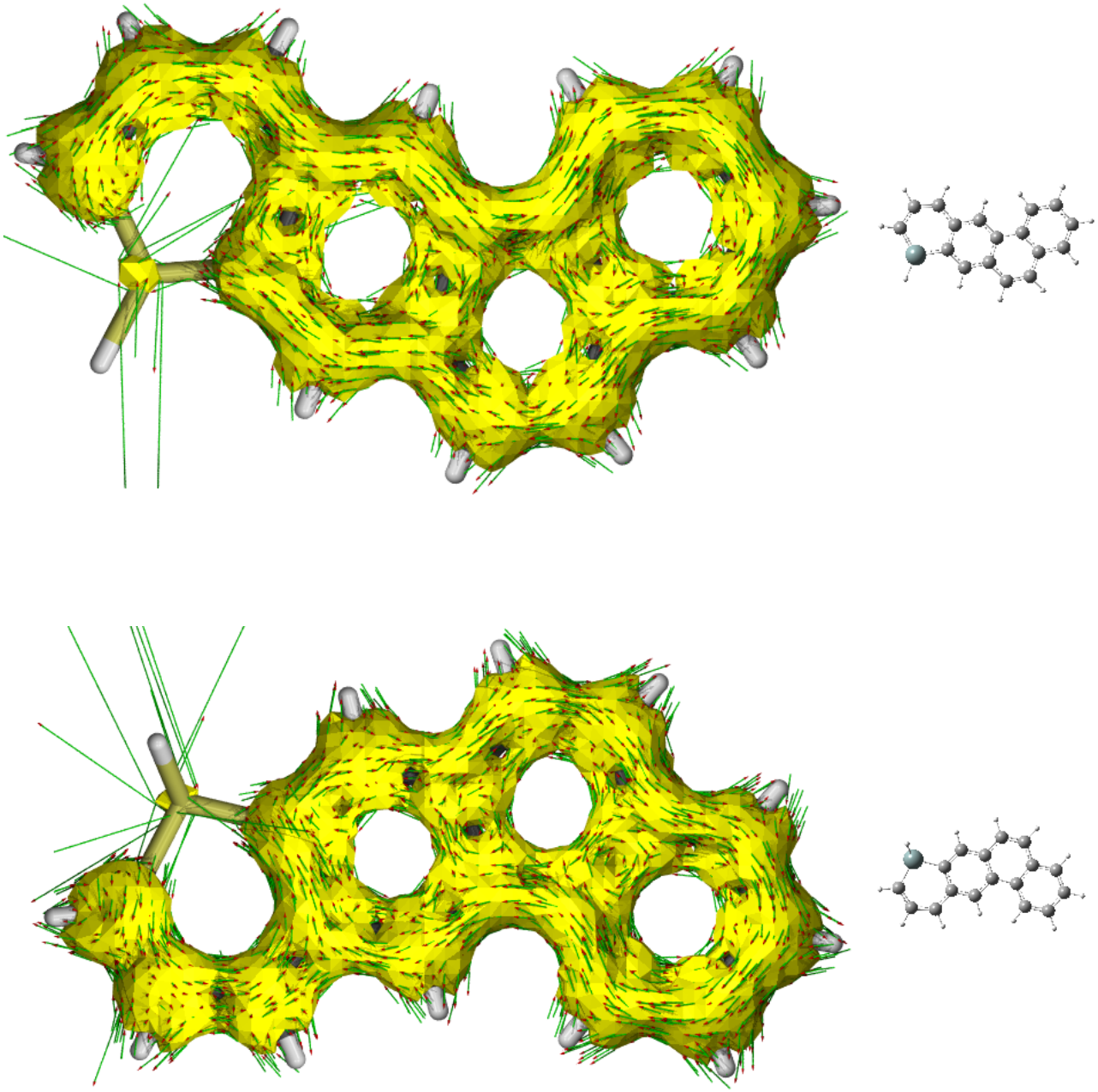

Figure S30. AICD plots of S_0 (top) and T_1 (bottom) 8-silabenz[*a*]antracene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

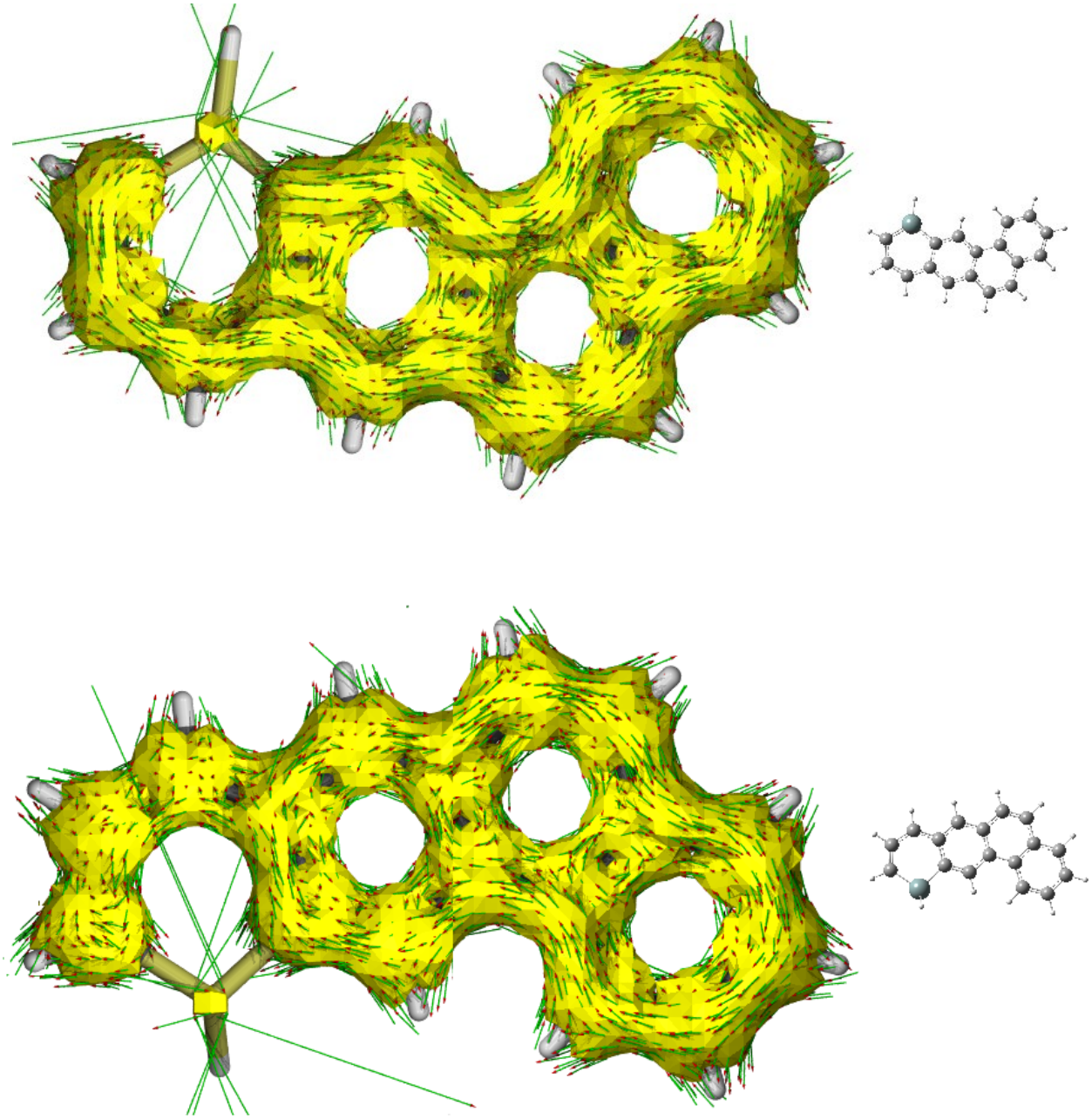

Figure S31. AICD plots of S_0 (top) and T_1 (bottom) 11-silabenz[*a*]antracene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

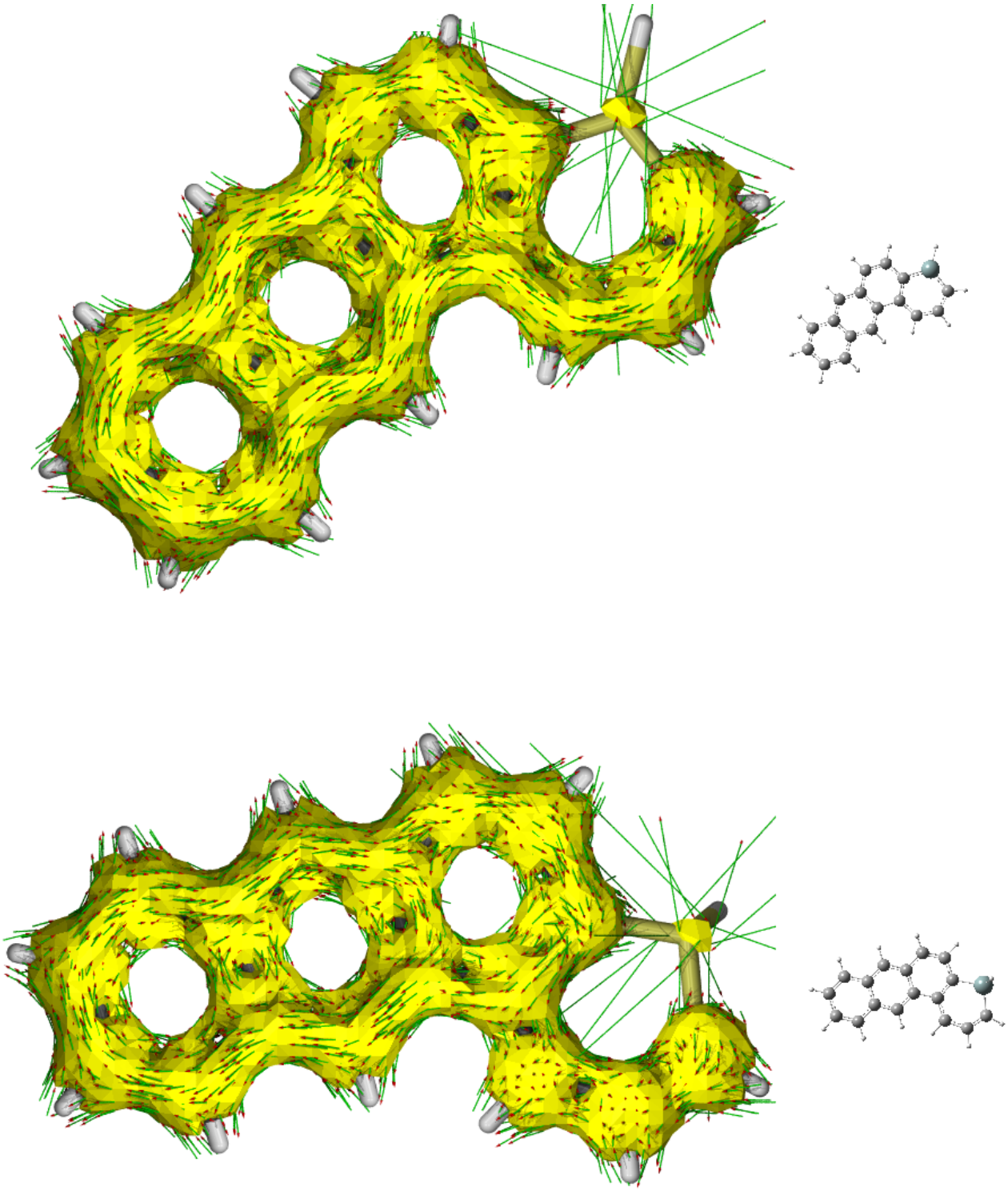

Figure S32. AICD plots of S_0 (top) and T_1 (bottom) 4-silabenz[*a*]antracene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

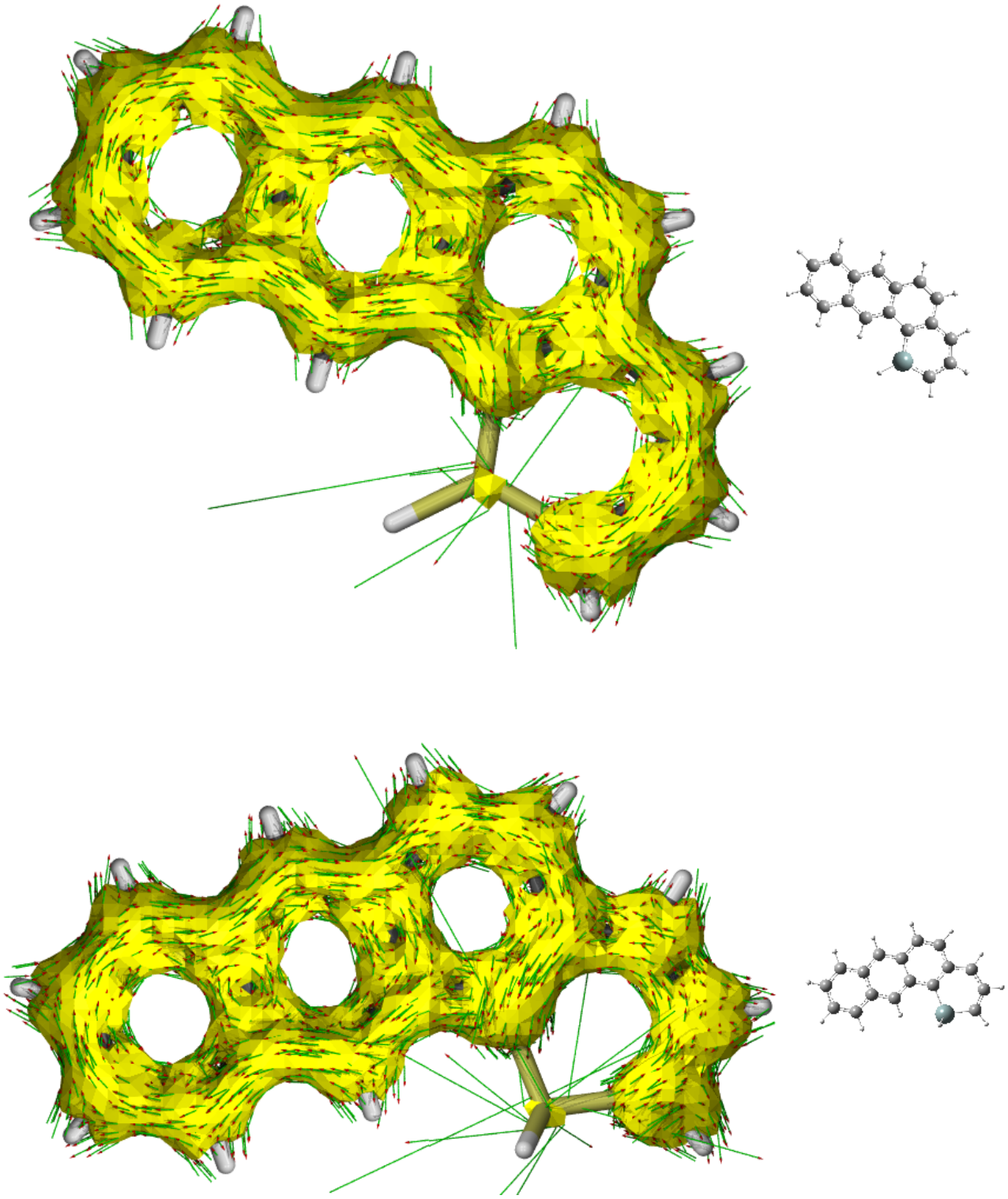

Figure S33. AICD plots of S_0 (top) and T_1 (bottom) 1-silabenz[*a*]antracene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

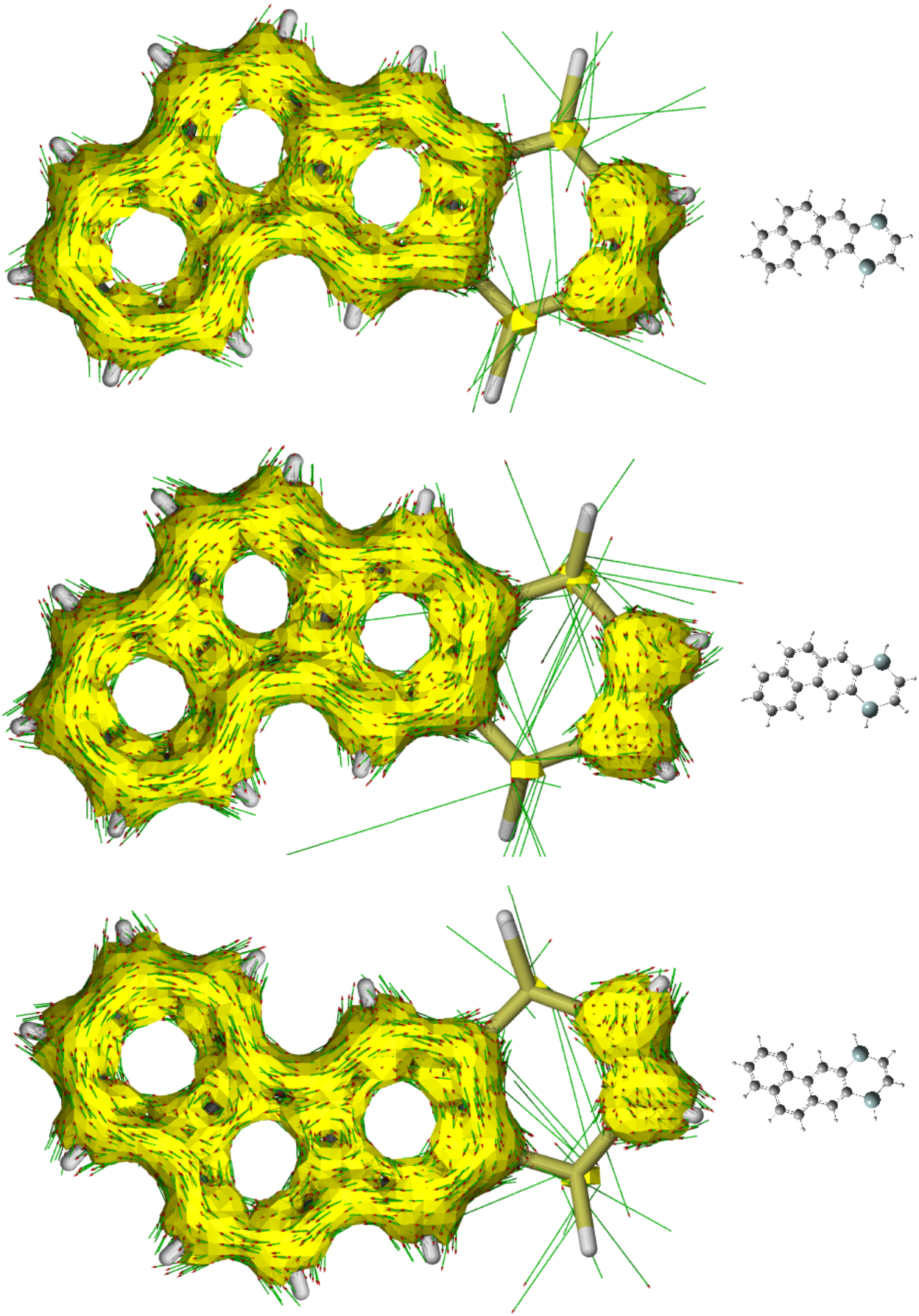

Figure S34. AICD plots of S_0 (top), T_1 opp (middle) and T1 same (bottom) 8,11-disilabenz[*a*]antracene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

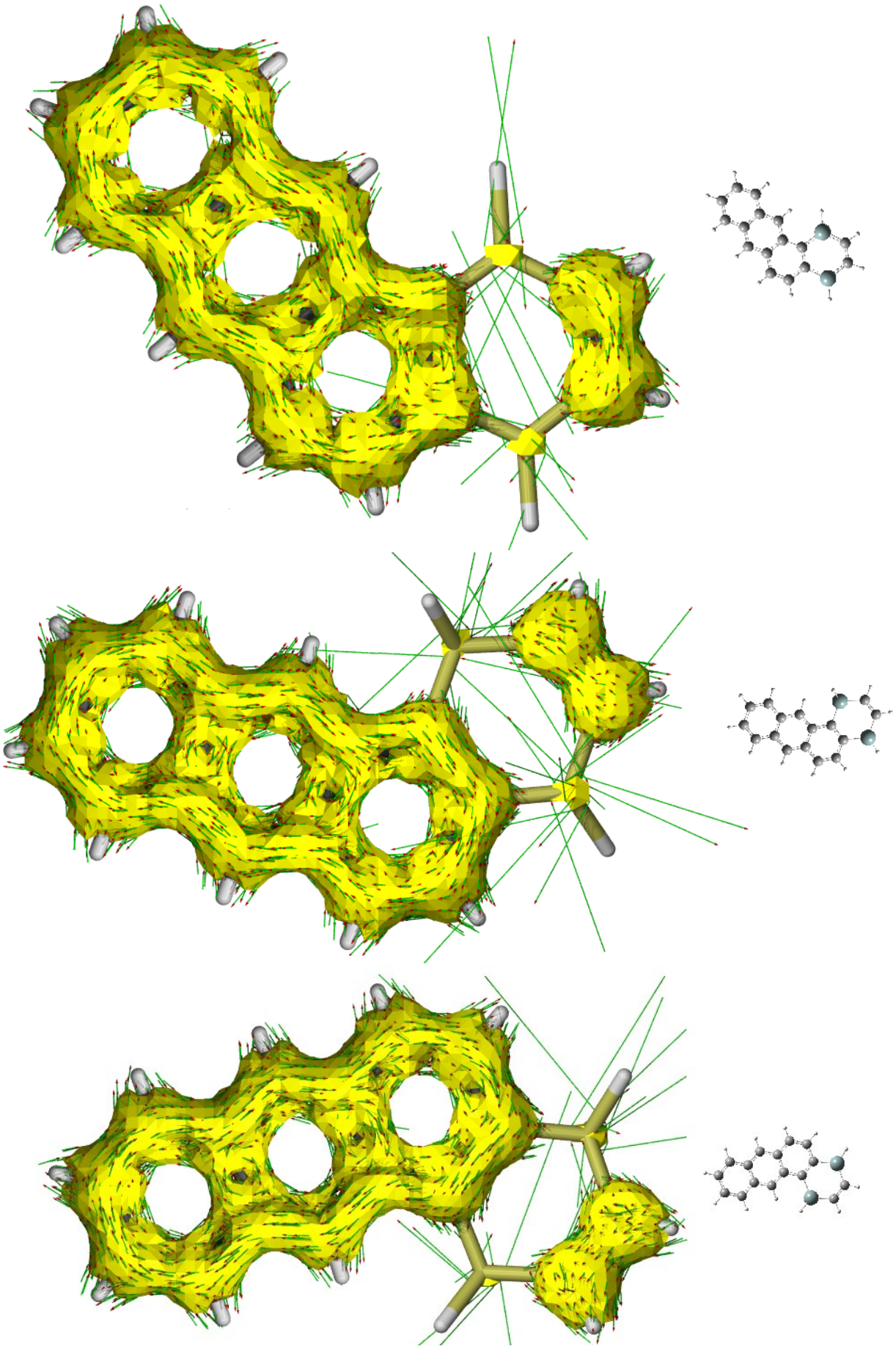

Figure S35. AICD plots of S_0 (top), T_1 opp (middle) and T1 same (bottom) 1,4-disilabenz[*a*]antracene at an isovalue of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

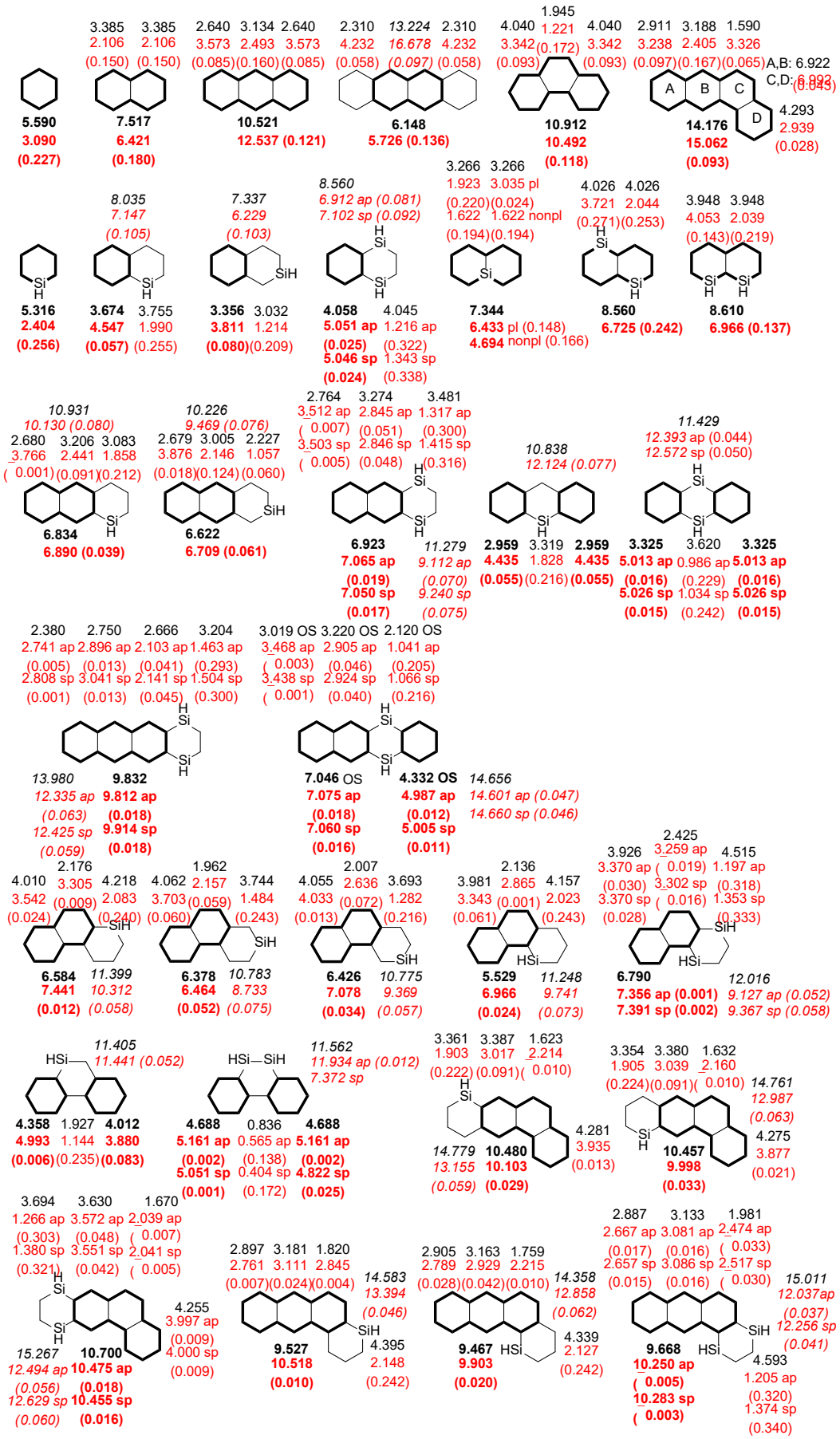

Figure S36. The $EDDB_H$, for global (anti)aromaticity, and $EDDB_F$, for (semi)local (anti)aromaticity, data are in electrons. Black font colour is used for the ground state and red font colour for the triplet state. Bold is used for (sub)units marked with the thick bonds, italic for global (anti)aromaticity and normal font for individual rings. Values in parentheses are $EDDB_{(\alpha-\beta)}$/EDDB. The ap/sp corresponds to the Si–H bonds spatial orientation in disilicon-substituted molecules: antiperiplanar/sinperiplanar.

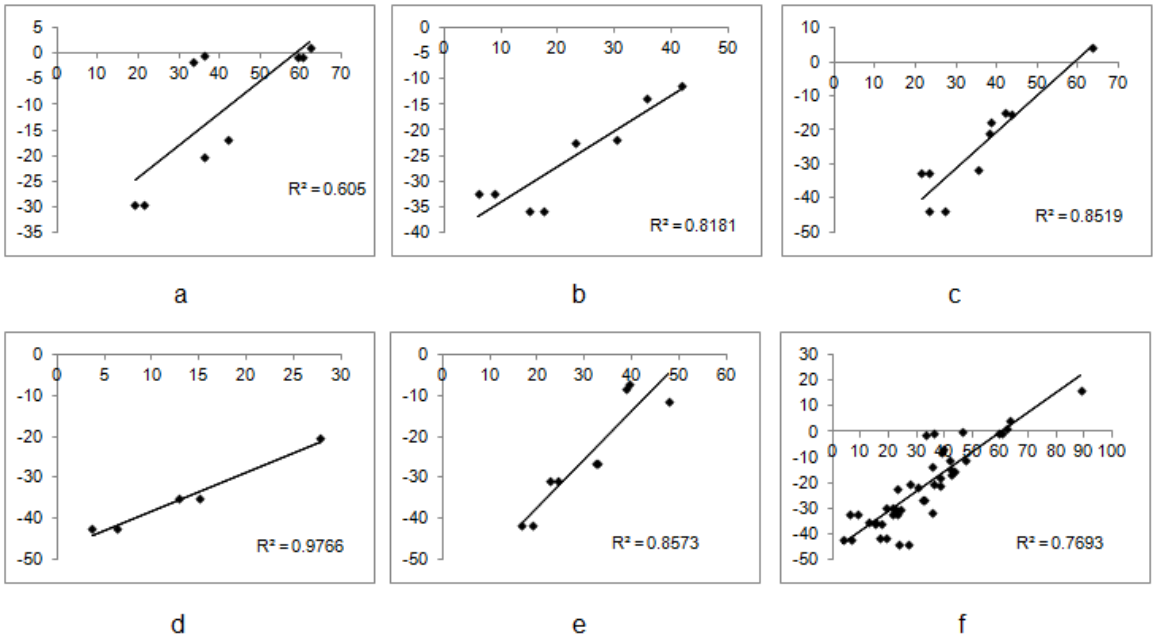

Figure S37. Correlations between ISE (y-axis) and S_0-T_1 energy gaps (x-axis), both in kcal/mol, for naphthalene and silanaphthalenes (a), anthracene and silaanthracenes (b), phenantrene and silaphenantrenes (c), tetracene and silatetracenes (d), benz[*a*]anthracene and silabenz[*a*]anthracenes (e) and all studied compounds (f).

Comparison of B3LYP and *ω*B97x results

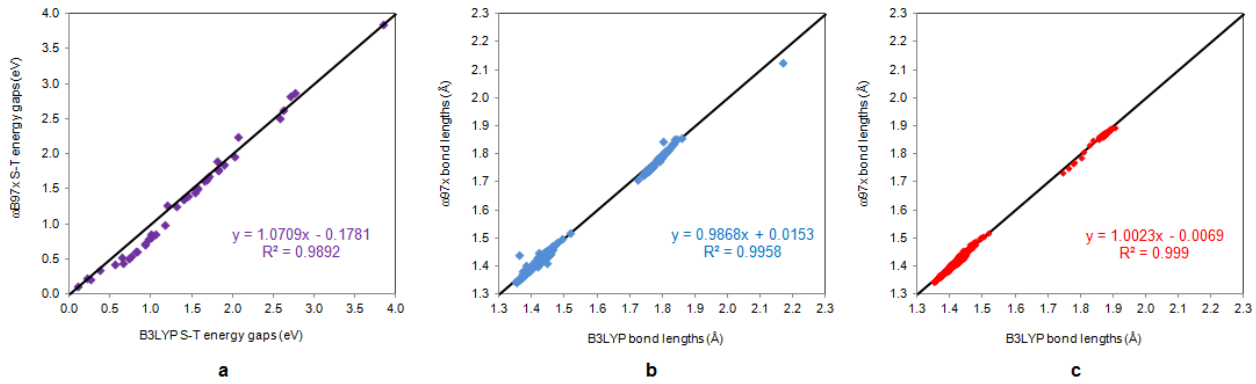

Figure S38. Correlation between B3LYP and ωB97x methods: S_0-T_1 energy gaps (**a**), C-C, C-Si and Si-Si bond lengths for singlet states (**b**) and triplet states (**c**) for all compounds studied.

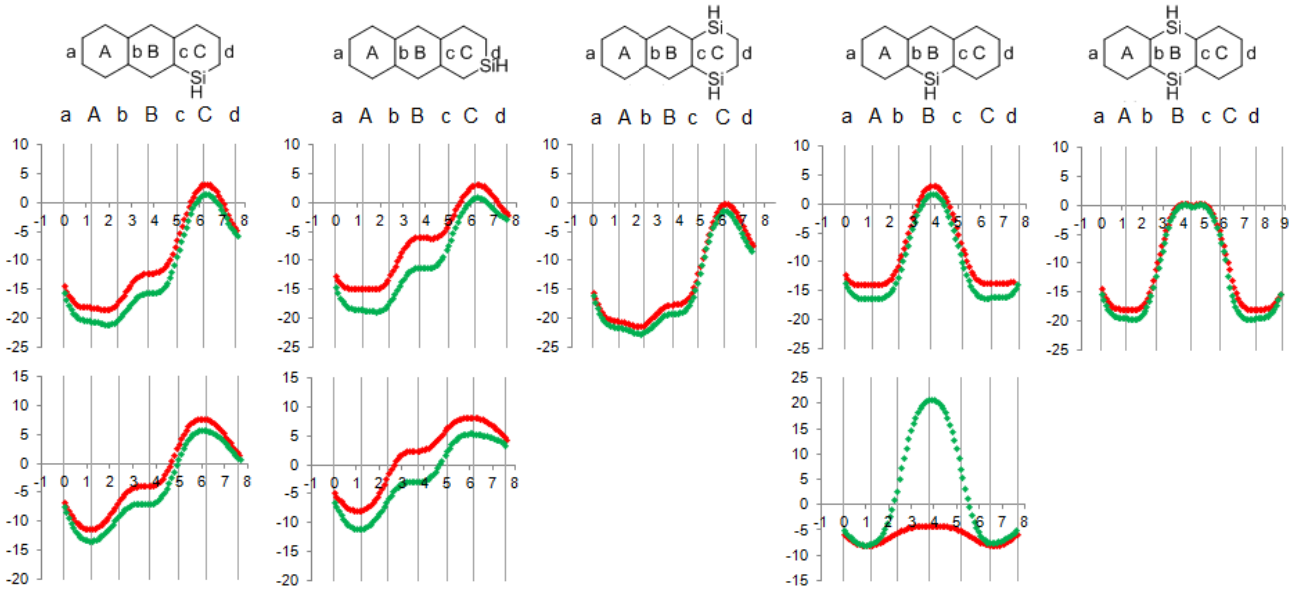

Figure S39. Comparison of NICS-*xy* scans obtained with B3LYP (shown in red) and ωB97x functionals (shown in green) for T_1 state of (di)silaanthracenes; x-axis: distance in Å, y-axis: NICS values in ppm. Upper row represents $NICS_{zz}$ data and lower row represents $NICS_{\pi zz}$ data (not obtained for sp disilicon-isomers, chosen for comparison, with both methods).

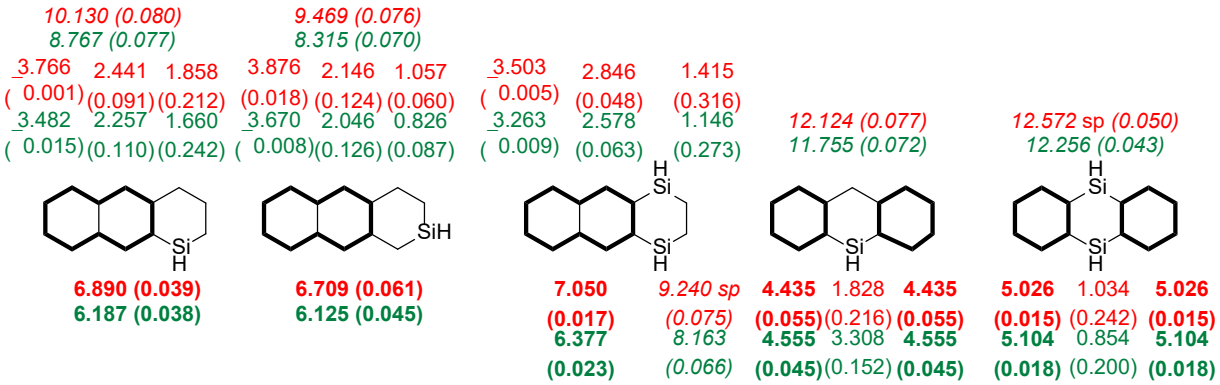

Figure S40. Comparison of B3LYP (shown in red) and ωB97x (shown in green) calculated EDDB data (in electrons) for T_1 state of (di)silaanthracenes. Bold is used for (sub)units marked with the thick bonds, italic for global (anti)aromaticity and normal font for individual rings. Values in parentheses are $EDDB_{(\alpha-\beta)}$/EDDB. The sp isomer is used in the case of disilicon-substituted compounds.

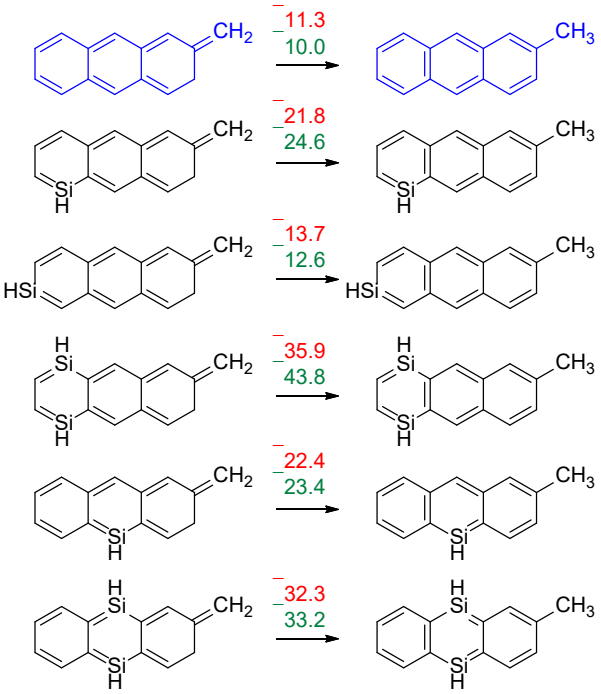

Figure S41. Comparison of ISE (in kcal/mol) calculated with B3LYP (shown in red) and ωB97x (shown in green) functionals for anthracene and T_1 (di)silaanthracenes.

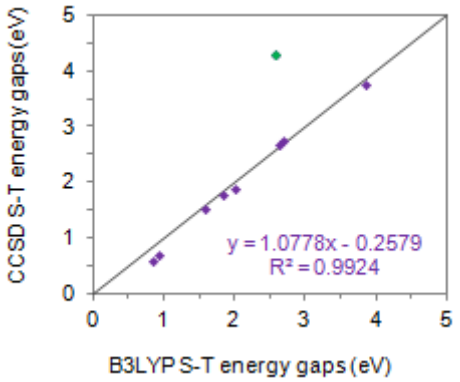

Figure S42. Correlation between B3LYP and CCSD S_0-T_1 energy gaps for benzene, silabenzene, naphthalene and selected silanaphthalenes (1-silanaphthalene, 2-silanaphthalene, 9-silanaphthalene, planar and nonplanar, 1,4-disilanaphthalene, ap- and sp-isomers) based on B3LYP geometries. Green dot, corresponding to the nonplanar 9-silanaphthalene is excluded from correlation.

Absolute energies and x, y, z coordinates of B3LYP/6-311+G(d,p) optimized structures

Benzene S_0

E = -232.3112416 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.394301	0.000000
2	6	0	1.207500	0.697151	0.000000
3	6	0	1.207500	-0.697151	0.000000
4	6	0	0.000000	-1.394301	0.000000
5	6	0	-1.207500	-0.697151	0.000000
6	6	0	-1.207500	0.697151	0.000000
7	1	0	0.000000	2.478574	0.000000
8	1	0	2.146508	1.239287	0.000000
9	1	0	2.146508	-1.239287	0.000000
10	1	0	0.000000	-2.478574	0.000000
11	1	0	-2.146508	-1.239287	0.000000
12	1	0	-2.146508	1.239287	0.000000

Benzene T_1

E = -232.1699199 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.207797	0.759712
2	6	0	0.000000	0.000000	1.441395
3	6	0	0.000000	-1.207797	0.759712
4	6	0	0.000000	-1.207797	-0.759712
5	6	0	0.000000	0.000000	-1.441395
6	6	0	0.000000	1.207797	-0.759712
7	1	0	0.000000	2.152534	1.287125
8	1	0	0.000000	0.000000	2.526694
9	1	0	0.000000	-2.152534	1.287125
10	1	0	0.000000	-2.152534	-1.287125
11	1	0	0.000000	0.000000	-2.526694
12	1	0	0.000000	2.152534	-1.287125

Silabenzene S_0

E = -483.6733009 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-1.244450	-1.015482

2	6	0	0.000000	-1.447606	0.367934
3	6	0	0.000000	1.447606	0.367934
4	6	0	0.000000	1.244450	-1.015482
5	6	0	0.000000	0.000000	-1.659999
6	1	0	0.000000	-2.123393	-1.657035
7	1	0	0.000000	-2.465445	0.741762
8	1	0	0.000000	0.000000	2.862981
9	1	0	0.000000	2.465445	0.741762
10	1	0	0.000000	2.123393	-1.657035
11	1	0	0.000000	0.000000	-2.744635
12	14	0	0.000000	0.000000	1.388769

Silabenzene T_1

E = -483.5991289 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.111228	1.014421	-1.269039
2	6	0	-0.111228	-0.339798	-1.466899
3	6	0	-0.111228	-0.339798	1.466899
4	6	0	-0.111228	1.014421	1.269039
5	6	0	-0.077111	1.663631	0.000000
6	1	0	-0.177084	1.670750	-2.135619
7	1	0	-0.180405	-0.710029	-2.485392
8	1	0	-0.180405	-0.710029	2.485392
9	1	0	-0.177084	1.670750	2.135619
10	1	0	-0.087859	2.748313	0.000000
11	14	0	0.167395	-1.483450	0.000000
12	1	0	1.591458	-1.978721	0.000000

Naphthalene S_0

E = -385.9888708 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	2.430634	0.707529
2	6	0	0.000000	1.243886	1.400697
3	6	0	0.000000	0.000000	0.715970

4	6	0	0.000000	0.000000	-0.715970
5	6	0	0.000000	1.243886	-1.400697
6	6	0	0.000000	2.430634	-0.707529
7	1	0	0.000000	-1.243119	2.485975
8	1	0	0.000000	3.373020	1.243931
9	1	0	0.000000	1.243119	2.485975
10	6	0	0.000000	-1.243886	1.400697
11	6	0	0.000000	-1.243886	-1.400697
12	1	0	0.000000	1.243119	-2.485975
13	1	0	0.000000	3.373020	-1.243931
14	6	0	0.000000	-2.430634	-0.707529
15	6	0	0.000000	-2.430634	0.707529
16	1	0	0.000000	-1.243119	-2.485975
17	1	0	0.000000	-3.373020	-1.243931
18	1	0	0.000000	-3.373020	1.243931

Naphthalene T_1

E = -385.8896466 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-2.484690	-0.680690
2	6	0	0.000000	-1.236673	-1.399394
3	6	0	0.000000	0.000000	-0.724072
4	6	0	0.000000	0.000000	0.724072
5	6	0	0.000000	-1.236673	1.399394
6	6	0	0.000000	-2.484690	0.680690
7	1	0	0.000000	1.245668	-2.483664
8	1	0	0.000000	-3.415172	-1.236225
9	1	0	0.000000	-1.245668	-2.483664
10	6	0	0.000000	1.236673	-1.399394
11	6	0	0.000000	1.236673	1.399394
12	1	0	0.000000	-1.245668	2.483664
13	1	0	0.000000	-3.415172	1.236225
14	6	0	0.000000	2.484690	0.680690
15	6	0	0.000000	2.484690	-0.680690
16	1	0	0.000000	1.245668	2.483664
17	1	0	0.000000	3.415172	1.236225
18	1	0	0.000000	3.415172	-1.236225

1-Silanaphthalene S_0

E = -637.3495888 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.259878	1.577091	0.000000
2	6	0	0.896271	1.764239	0.000000
3	6	0	0.000000	0.664598	0.000000
4	6	0	0.529770	-0.673529	0.000000
5	6	0	1.946559	-0.821563	0.000000

6	6	0	2.786135	0.266372	0.000000
7	1	0	-2.485647	2.115747	0.000000
8	1	0	2.929405	2.429667	0.000000
9	1	0	0.496769	2.773881	0.000000
10	6	0	-0.288893	-1.844436	0.000000
11	1	0	2.359519	-1.825086	0.000000
12	1	0	3.860654	0.119678	0.000000
13	6	0	-1.670104	-1.887158	0.000000
14	6	0	-2.543297	-0.771165	0.000000
15	1	0	0.238279	-2.793000	0.000000
16	1	0	-2.124260	-2.875414	0.000000
17	1	0	-3.611550	-0.953047	0.000000
18	14	0	-1.797220	0.811491	0.000000

1-Silanaphthalene T_1

E = -637.2918095 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.649608	-0.794738	-0.056256
2	6	0	-1.380875	-1.385636	-0.077492
3	6	0	-0.213805	-0.623990	-0.034078
4	6	0	-0.322176	0.799269	0.023840
5	6	0	-1.611116	1.375222	0.058064
6	6	0	-2.758541	0.591839	0.016505
7	1	0	1.685793	-2.200403	1.275221
8	1	0	-3.538537	-1.413920	-0.096766
9	1	0	-1.310958	-2.468358	-0.129847
10	6	0	0.821875	1.675213	0.044756
11	1	0	-1.699828	2.455032	0.123803
12	1	0	-3.735005	1.062620	0.040552
13	6	0	2.186021	1.303629	-0.034283
14	6	0	2.672394	0.022580	-0.122763
15	1	0	0.605732	2.737548	0.097108
16	1	0	2.895941	2.129364	-0.045352
17	1	0	3.746110	-0.113210	-0.208424
18	14	0	1.491838	-1.426358	0.002425

2-Silanaphthalene S_0

E = -637.349855 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.255686	1.715320	0.000000
2	6	0	0.891378	1.871443	0.000000
3	6	0	0.000000	0.757549	0.000000
4	6	0	0.584314	-0.562746	0.000000
5	6	0	2.000689	-0.677304	0.000000
6	6	0	2.824227	0.422721	0.000000
7	1	0	-1.734935	2.022737	0.000000

8	1	0	2.899452	2.588162	0.000000
9	1	0	0.460399	2.867056	0.000000
10	6	0	-1.406506	0.988650	0.000000
11	6	0	-0.179911	-1.773371	0.000000
12	1	0	2.431080	-1.673674	0.000000
13	1	0	3.901115	0.301087	0.000000
14	6	0	-1.550860	-1.897538	0.000000
15	1	0	0.412378	-2.687020	0.000000
16	1	0	-1.979419	-2.893667	0.000000
17	1	0	-3.967253	-0.306122	0.000000
18	14	0	-2.495494	-0.377636	0.000000

2-Silanaphthalene T_1

E = -637.2826632 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.759139	-0.781152	0.030254
2	6	0	-1.536973	-1.426050	-0.019942
3	6	0	-0.299841	-0.712114	-0.039546
4	6	0	-0.363558	0.732827	-0.010989
5	6	0	-1.613499	1.347243	0.039627
6	6	0	-2.805823	0.616226	0.063256
7	1	0	0.835922	-2.500866	-0.225955
8	1	0	-3.676779	-1.358361	0.046221
9	1	0	-1.497272	-2.509883	-0.043121
10	6	0	0.913555	-1.420073	-0.138328
11	6	0	0.821803	1.597549	-0.060016
12	1	0	-1.658200	2.431552	0.055586
13	1	0	-3.757275	1.133316	0.103350
14	6	0	2.118740	1.223824	-0.071763
15	1	0	0.586776	2.661689	-0.074682
16	1	0	2.869516	2.008757	-0.095116
17	1	0	3.276228	-0.882099	1.312004
18	14	0	2.583535	-0.575271	0.011885

9-Silanaphthalene S_0

E = -637.3451694 a.u

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-2.662157	0.510913
2	6	0	0.000000	-1.682598	1.491100
3	6	0	0.000000	0.000000	-0.901775
4	6	0	0.000000	-1.256441	-1.559873
5	6	0	0.000000	-2.472394	-0.900269
6	1	0	0.000000	1.987334	2.531115
7	1	0	0.000000	-3.698714	0.842470
8	1	0	0.000000	-1.987334	2.531115
9	6	0	0.000000	1.682598	1.491100
10	6	0	0.000000	1.256441	-1.559873

11	1	0	0.000000	-1.269760	-2.649285
12	1	0	0.000000	-3.372278	-1.505946
13	6	0	0.000000	2.472394	-0.900269
14	6	0	0.000000	2.662157	0.510913
15	1	0	0.000000	1.269760	-2.649285
16	1	0	0.000000	3.372278	-1.505946
17	1	0	0.000000	3.698714	0.842470
18	14	0	0.000000	0.000000	0.890821

9-Silanaphthalene T_1 nonplanar

E = -637.250487 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.234756	-0.578150	2.595063
2	6	0	0.135829	-1.479449	1.654641
3	6	0	0.048171	0.957197	0.000000
4	6	0	-0.234756	1.564939	1.238398
5	6	0	-0.308794	0.872575	2.434131
6	1	0	0.140157	-2.533015	-1.918293
7	1	0	-0.525001	-0.938949	3.580689
8	1	0	0.140157	-2.533015	1.918293
9	6	0	0.135829	-1.479449	-1.654641
10	6	0	-0.234756	1.564939	-1.238398
11	1	0	-0.484044	2.625986	1.252993
12	1	0	-0.553939	1.436107	3.328294
13	6	0	-0.308794	0.872575	-2.434131
14	6	0	-0.234756	-0.578150	-2.595063
15	1	0	-0.484044	2.625986	-1.252993
16	1	0	-0.553939	1.436107	-3.328294
17	1	0	-0.525001	-0.938949	-3.580689
18	14	0	0.733310	-0.820174	0.000000

9-Silanaphthalene T_1 planar

E = -637.2488878 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.739436	0.447172	0.000000
2	6	0	1.733712	1.461605	0.000000
3	6	0	-0.030236	-0.927473	0.000000
4	6	0	1.192334	-1.593447	0.000000
5	6	0	2.503268	-0.907576	0.000000
6	1	0	-1.893848	2.577994	0.000000
7	1	0	3.777381	0.767994	0.000000
8	1	0	2.043804	2.499870	0.000000
9	6	0	-1.620729	1.530222	0.000000
10	6	0	-1.317424	-1.542479	0.000000
11	1	0	1.218583	-2.680603	0.000000
12	1	0	3.370809	-1.559721	0.000000

13	6	0	-2.529229	-0.832819	0.000000
14	6	0	-2.673930	0.556089	0.000000
15	1	0	-1.365894	-2.629807	0.000000
16	1	0	-3.442205	-1.418787	0.000000
17	1	0	-3.691834	0.937350	0.000000
18	14	0	0.000000	0.882711	0.000000

1,4-Disilanaphthalene S_0

E = -888.7132631 a.u

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.704918	2.892427
2	6	0	0.000000	1.395362	1.699871
3	6	0	0.000000	0.720693	0.449955
4	6	0	0.000000	-0.720693	0.449955
5	6	0	0.000000	-1.395362	1.699871
6	6	0	0.000000	-0.704918	2.892427
7	1	0	0.000000	1.244977	3.832690
8	1	0	0.000000	2.481185	1.716145
9	1	0	0.000000	-2.481185	1.716145
10	1	0	0.000000	-1.244977	3.832690
11	6	0	0.000000	-0.707679	-2.599456
12	6	0	0.000000	0.707679	-2.599456
13	1	0	0.000000	-1.215213	-3.561474
14	1	0	0.000000	1.215213	-3.561474
15	1	0	0.000000	3.129956	-1.076769
16	1	0	0.000000	-3.129956	-1.076769
17	14	0	0.000000	1.657478	-1.111955
18	14	0	0.000000	-1.657478	-1.111955

1,4-Disilanaphthalene T_1 ap

E = -888.678987 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.003629	0.696055	2.911138
2	6	0	-0.000461	1.386274	1.699997
3	6	0	0.000461	0.711843	0.468646
4	6	0	-0.000461	-0.711843	0.468646
5	6	0	0.000461	-1.386274	1.699997
6	6	0	-0.003629	-0.696055	2.911138
7	1	0	0.006775	1.243383	3.847263
8	1	0	-0.012944	2.472448	1.717129
9	1	0	0.012944	-2.472448	1.717129
10	1	0	-0.006775	-1.243383	3.847263
11	6	0	0.009227	-0.676783	-2.640983
12	6	0	-0.009227	0.676783	-2.640983
13	1	0	0.025271	-1.193598	-3.601709
14	1	0	-0.025271	1.193598	-3.601709

15	14	0	-0.137142	1.724591	-1.105982
16	1	0	0.779451	2.899159	-1.111727
17	14	0	0.137142	-1.724591	-1.105982
18	1	0	-0.779451	-2.899159	-1.111727

1,4-Disilanaphthalene T_1 sp

E = -888.6826009 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.145732	2.895119	0.696499
2	6	0	-0.030639	1.689985	1.389563
3	6	0	0.092334	0.468974	0.710544
4	6	0	0.092334	0.468974	-0.710544
5	6	0	-0.030639	1.689985	-1.389563
6	6	0	-0.145732	2.895119	-0.696499
7	1	0	-0.236183	3.827557	1.242749
8	1	0	-0.041573	1.704820	2.475497
9	1	0	-0.041573	1.704820	-2.475497
10	1	0	-0.236183	3.827557	-1.242749
11	6	0	-0.332469	-2.585273	-0.676592
12	6	0	-0.332469	-2.585273	0.676592
13	1	0	-0.670104	-3.475047	-1.208252
14	1	0	-0.670104	-3.475047	1.208252
15	14	0	0.271322	-1.130632	-1.676067
16	1	0	-0.351617	-1.041311	-3.026205
17	14	0	0.271322	-1.130632	1.676067
18	1	0	-0.351617	-1.041311	3.026205

1,5-Disilanaphthalene S_0

E = -888.7101564 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.627047	0.691995	0.000000
2	6	0	1.396969	1.329477	0.000000
3	6	0	0.110945	0.713368	0.000000
4	6	0	-0.110945	-0.713368	0.000000
5	6	0	2.829499	-0.707289	0.000000
6	1	0	-1.368219	3.189426	0.000000
7	1	0	3.507493	1.330430	0.000000
8	1	0	1.416537	2.415562	0.000000
9	6	0	-1.396969	-1.329477	0.000000
10	1	0	1.368219	-3.189426	0.000000
11	1	0	3.846633	-1.081982	0.000000
12	6	0	-2.627047	-0.691995	0.000000
13	6	0	-2.829499	0.707289	0.000000
14	1	0	-1.416537	-2.415562	0.000000
15	1	0	-3.507493	-1.330430	0.000000
16	1	0	-3.846633	1.081982	0.000000

17	14	0	1.396969	-1.714423	0.000000
18	14	0	-1.396969	1.714423	0.000000

1,5-Disilanaphthalene T_1

E = -888.6565556 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.360270	1.361229	0.006343
2	6	0	-0.965812	1.620045	0.033042
3	6	0	0.079268	0.698321	0.035330
4	6	0	-0.105856	-0.731753	0.019169
5	6	0	-2.940497	0.101576	-0.025756
6	1	0	-3.012019	2.231865	0.013660
7	1	0	-0.692479	2.672119	0.055494
8	6	0	0.962227	-1.666836	-0.000770
9	1	0	-4.021490	0.019361	-0.045128
10	6	0	2.362555	-1.381207	-0.017483
11	6	0	2.933705	-0.141268	0.019001
12	1	0	0.696597	-2.720103	-0.009866
13	1	0	3.013148	-2.253939	-0.055279
14	1	0	4.017441	-0.073584	0.014371
15	14	0	-1.822033	-1.278757	-0.004753
16	1	0	-2.226284	-2.693269	-0.118620
17	14	0	1.846914	1.375373	0.063557
18	1	0	2.084837	2.304273	-1.091143

1,8-Disilanaphthalene S_0

E = -888.7164044 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-2.903393	-0.176369
2	6	0	0.000000	0.000000	-0.527788
3	6	0	0.000000	0.000000	0.922919
4	6	0	0.000000	-1.217950	1.675019
5	6	0	0.000000	-2.511652	1.183693
6	1	0	0.000000	1.728164	-2.807680
7	1	0	0.000000	-3.960387	-0.413238
8	1	0	0.000000	-1.728164	-2.807680
9	6	0	0.000000	1.217950	1.675019
10	1	0	0.000000	-1.105699	2.754199
11	1	0	0.000000	-3.304946	1.928222
12	6	0	0.000000	2.511652	1.183693
13	6	0	0.000000	2.903393	-0.176369
14	1	0	0.000000	1.105699	2.754199
15	1	0	0.000000	3.304946	1.928222
16	1	0	0.000000	3.960387	-0.413238
17	14	0	0.000000	1.595773	-1.338640
18	14	0	0.000000	-1.595773	-1.338640

1,8-Disilanaphthalene T_1

E = -888.6588691 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.916326	0.074369	-0.039805
2	6	0	0.000159	0.526279	-0.011240
3	6	0	0.030346	-0.912115	-0.000461
4	6	0	-1.176469	-1.701993	0.006775
5	6	0	-2.515638	-1.235113	0.001920
6	1	0	-3.981640	0.284772	-0.052107
7	6	0	1.239474	-1.656289	0.025655
8	1	0	-1.038713	-2.778068	0.019976
9	1	0	-3.278948	-2.011739	0.021665
10	6	0	2.552316	-1.160790	0.020354
11	6	0	2.920992	0.182146	-0.003640
12	1	0	1.135836	-2.735853	0.063367
13	1	0	3.343213	-1.907620	0.038613
14	1	0	3.973801	0.439572	-0.010228
15	14	0	1.565180	1.336455	-0.025665
16	1	0	1.733546	2.801300	-0.044660
17	14	0	-1.630726	1.437528	-0.056019
18	1	0	-1.778578	2.372908	1.109606

Anthracene S_0

E = -539.6602468 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	3.656102	-0.712388
2	6	0	0.000000	2.477219	-1.405274
3	6	0	0.000000	1.222066	-0.721430
4	6	0	0.000000	1.222066	0.721430
5	6	0	0.000000	2.477219	1.405274
6	6	0	0.000000	3.656102	0.712388
7	6	0	0.000000	0.000000	-1.401924
8	6	0	0.000000	0.000000	1.401924
9	6	0	0.000000	-1.222066	0.721430
10	6	0	0.000000	-1.222066	-0.721430
11	6	0	0.000000	-2.477219	-1.405274
12	1	0	0.000000	-2.476755	-2.490366
13	6	0	0.000000	-3.656102	-0.712388
14	6	0	0.000000	-3.656102	0.712388
15	6	0	0.000000	-2.477219	1.405274
16	1	0	0.000000	0.000000	-2.487846
17	1	0	0.000000	4.600534	-1.244964
18	1	0	0.000000	2.476755	-2.490366
19	1	0	0.000000	2.476755	2.490366
20	1	0	0.000000	4.600534	1.244964

21	1	0	0.000000	0.000000	2.487846
22	1	0	0.000000	-4.600534	-1.244964
23	1	0	0.000000	-4.600534	1.244964
24	1	0	0.000000	-2.476755	2.490366

Anthracene T_1

E = -539.5937577 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	3.700560	-0.690630
2	6	0	0.000000	2.476963	-1.394247
3	6	0	0.000000	1.253011	-0.719567
4	6	0	0.000000	1.253011	0.719567
5	6	0	0.000000	2.476963	1.394247
6	6	0	0.000000	3.700560	0.690630
7	6	0	0.000000	0.000000	-1.405484
8	6	0	0.000000	0.000000	1.405484
9	6	0	0.000000	-1.253011	0.719567
10	6	0	0.000000	-1.253011	-0.719567
11	6	0	0.000000	-2.476963	-1.394247
12	1	0	0.000000	-2.481282	-2.479271
13	6	0	0.000000	-3.700560	-0.690630
14	6	0	0.000000	-3.700560	0.690630
15	6	0	0.000000	-2.476963	1.394247
16	1	0	0.000000	0.000000	-2.490667
17	1	0	0.000000	4.635051	-1.239671
18	1	0	0.000000	2.481282	-2.479271
19	1	0	0.000000	2.481282	2.479271
20	1	0	0.000000	4.635051	1.239671
21	1	0	0.000000	0.000000	2.490667
22	1	0	0.000000	-4.635051	-1.239671
23	1	0	0.000000	-4.635051	1.239671
24	1	0	0.000000	-2.481282	2.479271

1-Silaanthracene S_0

E = -791.0216632 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.851587	2.231835	0.000000
2	6	0	2.526478	0.894937	0.000000
3	6	0	1.205844	0.328481	0.000000
4	6	0	0.000000	1.138072	0.000000
5	6	0	1.938583	3.326475	0.000000
6	6	0	1.056436	-1.066183	0.000000
7	6	0	-1.249023	0.512814	0.000000
8	6	0	-1.385944	-0.881915	0.000000
9	6	0	-0.195000	-1.691277	0.000000
10	6	0	-0.338402	-3.113138	0.000000
11	1	0	0.557159	-3.725671	0.000000
12	6	0	-1.576735	-3.694325	0.000000
13	6	0	-2.753730	-2.892077	0.000000
14	6	0	-2.658803	-1.527122	0.000000
15	1	0	1.948478	-1.685583	0.000000
16	1	0	3.912117	2.472644	0.000000
17	1	0	3.344943	0.182356	0.000000
18	1	0	-0.896581	3.874396	0.000000
19	1	0	2.343167	4.331542	0.000000
20	1	0	-2.152823	1.116398	0.000000
21	1	0	-1.669975	-4.774579	0.000000
22	1	0	-3.725868	-3.371825	0.000000

23	1	0	-3.553437	-0.912814	0.000000
24	14	0	0.240362	2.935262	0.000000

1-Silaanthracene T_1

E = -790.9733221 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.434556	1.234805	0.046245
2	6	0	2.080814	1.669770	-0.009399
3	6	0	0.906826	0.853676	-0.026673
4	6	0	0.964331	-0.598689	-0.023858
5	6	0	3.872929	-0.062258	0.032430
6	6	0	-0.346764	1.470682	-0.011190
7	6	0	-0.211394	-1.310702	-0.012515
8	6	0	-1.497609	-0.688725	-0.001852
9	6	0	-1.559292	0.738349	-0.003556
10	6	0	-2.828357	1.367351	0.007128
11	1	0	-2.877793	2.451245	0.008437
12	6	0	-3.986773	0.617411	0.015627
13	6	0	-3.923259	-0.790044	0.014761
14	6	0	-2.697543	-1.429598	0.006010
15	1	0	-0.398446	2.555359	0.012434
16	1	0	4.175253	2.030965	0.102038
17	1	0	1.915024	2.742412	-0.014018
18	1	0	4.942086	-0.244410	0.078281
19	1	0	-0.184376	-2.397778	-0.017581
20	1	0	-4.951838	1.111317	0.023673
21	1	0	-4.838793	-1.370358	0.022510
22	1	0	-2.646604	-2.513550	0.006378
23	14	0	2.631528	-1.449647	-0.098342
24	1	0	2.773311	-2.502324	0.955674

2-Silaanthracene S_0

E = -791.0218976 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.978428	1.969066	0.000000
2	6	0	-2.513615	0.681103	0.000000
3	6	0	-1.139467	0.244230	0.000000
4	6	0	0.000000	1.152395	0.000000
5	6	0	-0.146749	2.578608	0.000000
6	6	0	-0.901270	-1.134583	0.000000
7	6	0	1.285592	0.586188	0.000000
8	6	0	1.512481	-0.793040	0.000000
9	6	0	0.384173	-1.686083	0.000000
10	6	0	0.616823	-3.093992	0.000000
11	1	0	-0.237806	-3.762890	0.000000
12	6	0	1.890533	-3.594622	0.000000
13	6	0	3.008469	-2.712169	0.000000
14	6	0	2.825971	-1.356110	0.000000
15	1	0	-1.754300	-1.806891	0.000000
16	1	0	-4.050474	2.133169	0.000000
17	1	0	-3.244177	-0.126054	0.000000
18	1	0	0.766803	3.163527	0.000000
19	1	0	-2.058080	4.714629	0.000000
20	1	0	2.141220	1.254440	0.000000
21	1	0	2.056221	-4.665942	0.000000
22	1	0	4.011253	-3.124812	0.000000
23	1	0	3.679387	-0.686031	0.000000
24	14	0	-1.741223	3.275779	0.000000

2-Silaanthracene T_1

E = -790.9651309 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.363756	1.183553	0.032607
2	6	0	2.072014	1.596582	0.015370
3	6	0	0.869279	0.764454	0.002257
4	6	0	0.910812	-0.701616	0.004905
5	6	0	2.105228	-1.425768	-0.048003
6	6	0	-0.349521	1.395304	-0.002424
7	6	0	-0.332907	-1.386754	0.026206
8	6	0	-1.582268	-0.729182	0.011533
9	6	0	-1.602038	0.700487	-0.003507
10	6	0	-2.835967	1.370549	-0.014347
11	1	0	-2.847807	2.455561	-0.026048
12	6	0	-4.029759	0.661747	-0.008858
13	6	0	-4.015280	-0.743582	0.008078
14	6	0	-2.814197	-1.428367	0.017905
15	1	0	-0.376046	2.481202	-0.005558
16	1	0	4.133330	1.949824	0.069848
17	1	0	1.865886	2.666017	0.042973
18	1	0	2.013309	-2.508974	-0.063945
19	1	0	-0.316022	-2.471926	0.044128
20	1	0	-4.974930	1.192120	-0.017250
21	1	0	-4.950728	-1.291465	0.012885
22	1	0	-2.802741	-2.513144	0.030381
23	14	0	3.783383	-0.602738	-0.093197
24	1	0	4.733474	-1.065327	0.967011

9-Silaanthracene S_0

E = -791.0199591 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-3.890633	0.361793
2	6	0	0.000000	-2.803601	1.196610
3	6	0	0.000000	-1.472894	0.685005
4	6	0	0.000000	-1.267291	-0.749139
5	6	0	0.000000	-2.438217	-1.577595
6	6	0	0.000000	-3.698524	-1.046025
7	6	0	0.000000	0.000000	-1.363369
8	6	0	0.000000	1.267291	-0.749139
9	6	0	0.000000	1.472894	0.685005
10	6	0	0.000000	2.803601	1.196610
11	1	0	0.000000	2.954964	2.271771
12	6	0	0.000000	3.890633	0.361793
13	6	0	0.000000	3.698524	-1.046025
14	6	0	0.000000	2.438217	-1.577595
15	1	0	0.000000	0.000000	3.164009
16	1	0	0.000000	-4.895089	0.769372
17	1	0	0.000000	-2.954964	2.271771
18	1	0	0.000000	-2.303329	-2.654355
19	1	0	0.000000	-4.561658	-1.702807
20	1	0	0.000000	0.000000	-2.449245
21	1	0	0.000000	4.895089	0.769372
22	1	0	0.000000	4.561658	-1.702807
23	1	0	0.000000	2.303329	-2.654355
24	14	0	0.000000	0.000000	1.689264

9-Silaanthracene T_1

E = -790.9833689 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.324949	-0.079277	3.907654
2	6	0	1.170449	-0.031858	2.792490
3	6	0	0.670645	0.029358	1.492845
4	6	0	-0.745819	0.045542	1.293089
5	6	0	-1.580945	-0.002869	2.434295
6	6	0	-1.055507	-0.062041	3.719272
7	6	0	-1.363065	0.085643	0.000000
8	6	0	-0.745819	0.045542	-1.293089
9	6	0	0.670645	0.029358	-1.492845
10	6	0	1.170449	-0.031858	-2.792490
11	1	0	2.244868	-0.039088	-2.952419
12	6	0	0.324949	-0.079277	-3.907654
13	6	0	-1.055507	-0.062041	-3.719272
14	6	0	-1.580945	-0.002869	-2.434295
15	1	0	2.871482	-0.894656	0.000000
16	1	0	0.743001	-0.123609	4.906735
17	1	0	2.244868	-0.039088	2.952419
18	1	0	-2.657193	-0.004910	2.294126
19	1	0	-1.723079	-0.096936	4.573076
20	1	0	-2.448812	0.107572	0.000000
21	1	0	0.743001	-0.123609	-4.906735
22	1	0	-1.723079	-0.096936	-4.573076
23	1	0	-2.657193	-0.004910	-2.294126
24	14	0	1.795377	0.144002	0.000000

1,4-Disilaanthracene S_0

E = -1042.3864452 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.711648	4.186623
2	6	0	0.000000	1.405049	3.006202
3	6	0	0.000000	0.718962	1.755437
4	6	0	0.000000	-0.718962	1.755437
5	6	0	0.000000	-1.405049	3.006202
6	6	0	0.000000	-0.711648	4.186623
7	6	0	0.000000	1.397197	0.526761
8	6	0	0.000000	-1.397197	0.526761
9	6	0	0.000000	-0.728089	-0.700654
10	6	0	0.000000	0.728089	-0.700654
11	1	0	0.000000	3.135364	-2.234106
12	6	0	0.000000	0.711459	-3.753334
13	6	0	0.000000	-0.711459	-3.753334
14	1	0	0.000000	2.484024	0.545757
15	1	0	0.000000	1.244133	5.130979
16	1	0	0.000000	2.490139	3.005081
17	1	0	0.000000	-2.490139	3.005081
18	1	0	0.000000	-1.244133	5.130979
19	1	0	0.000000	-2.484024	0.545757
20	1	0	0.000000	1.216690	-4.716361
21	1	0	0.000000	-1.216690	-4.716361
22	1	0	0.000000	-3.135364	-2.234106
23	14	0	0.000000	-1.662292	-2.275540
24	14	0	0.000000	1.662292	-2.275540

1,4-Disilaanthracene T_1 ap

E = -1042.3587569 a.u.

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-4.198236	0.706028	0.023837
2	6	0	-3.009183	1.400507	0.047230
3	6	0	-1.770236	0.713557	0.024407
4	6	0	-1.770232	-0.713554	-0.024408
5	6	0	-3.009175	-1.400511	-0.047223
6	6	0	-4.198232	-0.706039	-0.023823
7	6	0	-0.522096	1.391276	0.035576
8	6	0	-0.522088	-1.391266	-0.035584
9	6	0	0.689826	-0.724066	-0.018046
10	6	0	0.689821	0.724082	0.018031
11	6	0	3.799864	0.677454	-0.004378
12	6	0	3.799872	-0.677463	0.004426
13	1	0	-0.542339	2.478549	0.043329
14	1	0	-5.140638	1.241625	0.041824
15	1	0	-3.007673	2.485012	0.082226
16	1	0	-3.007660	-2.485016	-0.082220
17	1	0	-5.140632	-1.241641	-0.041803
18	1	0	-0.542326	-2.478539	-0.043337
19	1	0	4.759911	1.195280	-0.017960
20	1	0	4.759922	-1.195279	0.018055
21	14	0	2.265366	-1.720005	0.141900
22	1	0	2.275843	-2.932803	-0.721298
23	14	0	2.265370	1.720001	-0.141922
24	1	0	2.275855	2.932838	0.721219

1,4-Disilaanthracene T_1 sp

E = -1042.3623113 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.114970	4.187338	0.706502
2	6	0	0.056527	2.999771	1.401055
3	6	0	-0.004905	1.761811	0.714296
4	6	0	-0.004905	1.761811	-0.714296
5	6	0	0.056527	2.999771	-1.401055
6	6	0	0.114970	4.187338	-0.706502
7	6	0	-0.064782	0.515793	1.394593
8	6	0	-0.064782	0.515793	-1.394593
9	6	0	-0.130287	-0.690814	-0.722767
10	6	0	-0.130287	-0.690814	0.722767
11	6	0	0.400914	-3.726222	0.677564
12	6	0	0.400914	-3.726222	-0.677564
13	1	0	-0.052039	0.534134	2.481546
14	1	0	0.162688	5.128474	1.242531
15	1	0	0.057012	2.998331	2.486150
16	1	0	0.057012	2.998331	-2.486150
17	1	0	0.162688	5.128474	-1.242531
18	1	0	-0.052039	0.534134	-2.481546
19	1	0	0.761436	-4.607753	1.207873
20	1	0	0.761436	-4.607753	-1.207873
21	14	0	-0.250526	-2.296269	-1.675927
22	1	0	0.343635	-2.191482	-3.036913
23	14	0	-0.250526	-2.296269	1.675927
24	1	0	0.343635	-2.191482	3.036913

9,10-Disilaanthracene S_0

E = -1042.3838826 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.006806	0.708946	-3.985658
2	6	0	-0.006806	1.398683	-2.799226
3	6	0	-0.000787	0.724362	-1.541213
4	6	0	0.000787	-0.724362	-1.541213
5	6	0	0.006806	-1.398683	-2.799226
6	6	0	0.006806	-0.708946	-3.985658
7	6	0	0.000787	-0.724362	1.541213
8	6	0	-0.000787	0.724362	1.541213
9	6	0	-0.006806	1.398683	2.799226
10	1	0	-0.012542	2.484506	2.815636
11	6	0	-0.006806	0.708946	3.985658
12	6	0	0.006806	-0.708946	3.985658
13	6	0	0.006806	-1.398683	2.799226
14	1	0	-0.079809	3.123286	0.000000
15	1	0	-0.015819	1.247010	-4.926942
16	1	0	-0.012542	2.484506	-2.815636
17	1	0	0.012542	-2.484506	-2.815636
18	1	0	0.015819	-1.247010	-4.926942
19	1	0	0.079809	-3.123286	0.000000
20	1	0	-0.015819	1.247010	4.926942
21	1	0	0.015819	-1.247010	4.926942
22	1	0	0.012542	-2.484506	2.815636
23	14	0	0.062331	1.655763	0.000000
24	14	0	-0.062331	-1.655763	0.000000

9,10-Disilaanthracene T_1 ap

E = -1042.3698498 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.009417	0.696578	-4.013726
2	6	0	-0.009417	1.387195	-2.803661
3	6	0	-0.004880	0.711304	-1.572329
4	6	0	0.004880	-0.711304	-1.572329
5	6	0	0.009417	-1.387195	-2.803661
6	6	0	0.009417	-0.696578	-4.013726
7	6	0	0.004880	-0.711304	1.572329
8	6	0	-0.004880	0.711304	1.572329
9	6	0	-0.009417	1.387195	2.803661
10	1	0	-0.004551	2.473417	2.820319
11	6	0	-0.009417	0.696578	4.013726
12	6	0	0.009417	-0.696578	4.013726
13	6	0	0.009417	-1.387195	2.803661
14	1	0	-0.700516	2.931121	0.000000
15	1	0	-0.018133	1.243326	-4.950160
16	1	0	-0.004551	2.473417	-2.820319
17	1	0	0.004551	-2.473417	-2.820319
18	1	0	0.018133	-1.243326	-4.950160
19	1	0	0.700516	-2.931121	0.000000
20	1	0	-0.018133	1.243326	4.950160
21	1	0	0.018133	-1.243326	4.950160
22	1	0	0.004551	-2.473417	2.820319
23	14	0	0.158864	1.714235	0.000000
24	14	0	-0.158864	-1.714235	0.000000

9,10-Disilaanthracene T_1 ap

E = -1042.3742961 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.905019	-0.696898	-0.490174
2	6	0	-2.736189	-1.390847	-0.181300

3	6	0	-1.549504	-0.711139	0.133685
4	6	0	-1.549504	0.711139	0.133685
5	6	0	-2.736189	1.390847	-0.181300
6	6	0	-3.905019	0.696898	-0.490174
7	6	0	1.549504	0.711139	0.133685
8	6	0	1.549504	-0.711139	0.133685
9	6	0	2.736189	-1.390847	-0.181300
10	1	0	2.749815	-2.476700	-0.191735
11	6	0	3.905019	-0.696898	-0.490174
12	6	0	3.905019	0.696898	-0.490174
13	6	0	2.736189	1.390847	-0.181300
14	1	0	0.000000	-3.042526	0.040706
15	1	0	-4.811151	-1.242177	-0.730264
16	1	0	-2.749815	-2.476700	-0.191735
17	1	0	-2.749815	2.476700	-0.191735
18	1	0	-4.811151	1.242177	-0.730264
19	1	0	0.000000	3.042526	0.040706
20	1	0	4.811151	-1.242177	-0.730264
21	1	0	4.811151	1.242177	-0.730264
22	1	0	2.749815	2.476700	-0.191735
23	14	0	0.000000	-1.657679	0.589769
24	14	0	0.000000	1.657679	0.589769

Tetracene S_0

E = -693.3291848 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-4.882672	-0.714729
2	6	0	0.000000	-3.707214	-1.407609
3	6	0	0.000000	-2.447136	-0.724875
4	6	0	0.000000	-2.447136	0.724875
5	6	0	0.000000	-3.707214	1.407609
6	6	0	0.000000	-4.882672	0.714729
7	6	0	0.000000	-1.233900	-1.404851
8	6	0	0.000000	-1.233900	1.404851
9	6	0	0.000000	0.000000	0.725082
10	6	0	0.000000	0.000000	-0.725082
11	6	0	0.000000	1.233900	-1.404851
12	1	0	0.000000	1.234305	-2.490713
13	6	0	0.000000	2.447136	-0.724875
14	6	0	0.000000	2.447136	0.724875
15	6	0	0.000000	1.233900	1.404851
16	1	0	0.000000	-1.234305	-2.490713
17	1	0	0.000000	-5.827993	-1.245598
18	1	0	0.000000	-3.707160	-2.492672
19	1	0	0.000000	-3.707160	2.492672
20	1	0	0.000000	-5.827993	1.245598
21	1	0	0.000000	-1.234305	2.490713
22	1	0	0.000000	1.234305	2.490713
23	6	0	0.000000	3.707214	1.407609
24	1	0	0.000000	3.707160	2.492672
25	6	0	0.000000	3.707214	-1.407609
26	1	0	0.000000	3.707160	-2.492672
27	6	0	0.000000	4.882672	-0.714729
28	1	0	0.000000	5.827993	-1.245598
29	6	0	0.000000	4.882672	0.714729
30	1	0	0.000000	5.827993	1.245598

Tetracene T_1

E = -693.2849498 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-4.919284	-0.697776
2	6	0	0.000000	-3.711776	-1.395660
3	6	0	0.000000	-2.483205	-0.716420
4	6	0	0.000000	-2.483205	0.716420
5	6	0	0.000000	-3.711776	1.395660
6	6	0	0.000000	-4.919284	0.697776
7	6	0	0.000000	-1.229453	-1.403546
8	6	0	0.000000	-1.229453	1.403546
9	6	0	0.000000	0.000000	0.729919
10	6	0	0.000000	0.000000	-0.729919
11	6	0	0.000000	1.229453	-1.403546
12	1	0	0.000000	1.233518	-2.489148
13	6	0	0.000000	2.483205	-0.716420
14	6	0	0.000000	2.483205	0.716420
15	6	0	0.000000	1.229453	1.403546
16	1	0	0.000000	-1.233518	-2.489148
17	1	0	0.000000	-5.857240	-1.241115
18	1	0	0.000000	-3.712932	-2.480818
19	1	0	0.000000	-3.712932	2.480818
20	1	0	0.000000	-5.857240	1.241115
21	1	0	0.000000	-1.233518	2.489148
22	1	0	0.000000	1.233518	2.489148
23	6	0	0.000000	3.711776	1.395660
24	1	0	0.000000	3.712932	2.480818
25	6	0	0.000000	3.711776	-1.395660
26	1	0	0.000000	3.712932	-2.480818
27	6	0	0.000000	4.919284	-0.697776
28	1	0	0.000000	5.857240	-1.241115
29	6	0	0.000000	4.919284	0.697776
30	1	0	0.000000	5.857240	1.241115

1,4-Disilatetracene S_0

E = -1196.0560361 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-0.713330	-4.936814
2	6	0	0.000000	-0.732094	-1.882146
3	6	0	0.000000	0.732094	-1.882146
4	6	0	0.000000	0.713330	-4.936814
5	6	0	0.000000	-1.400374	-0.663626
6	6	0	0.000000	1.400374	-0.663626
7	6	0	0.000000	0.722816	0.577000
8	6	0	0.000000	-0.722816	0.577000
9	6	0	0.000000	-1.404839	1.806482
10	1	0	0.000000	-2.490669	1.806250
11	6	0	0.000000	-0.724349	3.021667
12	6	0	0.000000	0.724349	3.021667
13	6	0	0.000000	1.404839	1.806482
14	1	0	0.000000	-2.487171	-0.644510
15	1	0	0.000000	-1.217474	-5.900305
16	1	0	0.000000	-3.137676	-3.418843
17	1	0	0.000000	3.137676	-3.418843
18	1	0	0.000000	1.217474	-5.900305
19	1	0	0.000000	2.487171	-0.644510
20	1	0	0.000000	2.490669	1.806250
21	6	0	0.000000	1.407505	4.280357
22	1	0	0.000000	2.492488	4.280171
23	6	0	0.000000	-1.407505	4.280357
24	1	0	0.000000	-2.492488	4.280171
25	6	0	0.000000	-0.714280	5.456283
26	1	0	0.000000	-1.245082	6.401575
27	6	0	0.000000	0.714280	5.456283
28	1	0	0.000000	1.245082	6.401575
29	14	0	0.000000	1.664629	-3.462826
30	14	0	0.000000	-1.664629	-3.462826

1,4-Disilatetracene T_1 ap

E = -1196.0320801 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.636059	-0.235218	-4.986556
2	6	0	-0.673893	-0.281808	-1.876250
3	6	0	0.673893	0.281808	-1.876250
4	6	0	0.636059	0.235218	-4.986556
5	6	0	-1.286797	-0.542457	-0.669364
6	6	0	1.286797	0.542457	-0.669364
7	6	0	0.660820	0.286909	0.588826
8	6	0	-0.660820	-0.286909	0.588826
9	6	0	-1.286797	-0.557911	1.805581
10	1	0	-2.284305	-0.986984	1.805285
11	6	0	-0.660928	-0.286947	3.032540
12	6	0	0.660928	0.286947	3.032540
13	6	0	1.286797	0.557911	1.805581
14	1	0	-2.298055	-0.941918	-0.649328
15	1	0	-1.126938	-0.405201	-5.945551
16	1	0	2.548078	1.648620	-3.461463
17	1	0	1.126938	0.405201	-5.945551
18	1	0	2.298055	0.941918	-0.649328
19	1	0	2.284305	0.986984	1.805285
20	6	0	1.288311	0.558875	4.283683
21	1	0	2.283944	0.990096	4.283456
22	6	0	-1.288311	-0.558875	4.283683
23	1	0	-2.283944	-0.990096	4.283456
24	6	0	-0.651987	-0.282976	5.465253
25	1	0	-1.141239	-0.495332	6.409092
26	6	0	0.651987	0.282976	5.465253
27	1	0	1.141239	0.495332	6.409092
28	14	0	1.655109	0.459288	-3.450270
29	14	0	-1.655109	-0.459288	-3.450270
30	1	0	-2.548078	-1.648620	-3.461463

1,4-Disilatetracene T_1 sp

E = -1196.0354272 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.426790	-4.908165	0.678254
2	6	0	-0.126776	-1.877094	0.728632
3	6	0	-0.126776	-1.877094	-0.728632
4	6	0	0.426790	-4.908165	-0.678254
5	6	0	-0.086067	-0.674455	1.398802
6	6	0	-0.086067	-0.674455	-1.398802
7	6	0	-0.051891	0.582635	-0.720598
8	6	0	-0.051891	0.582635	0.720598
9	6	0	-0.015396	1.799560	1.402477
10	1	0	-0.014436	1.799296	2.488345
11	6	0	0.020204	3.025207	0.720695
12	6	0	0.020204	3.025207	-0.720695
13	6	0	-0.015396	1.799560	-1.402477
14	1	0	-0.072204	-0.656008	2.485745
15	1	0	0.783421	-5.791744	1.207688
16	1	0	0.783421	-5.791744	-1.207688
17	1	0	-0.072204	-0.656008	-2.485745
18	1	0	-0.014436	1.799296	-2.488345
19	6	0	0.057936	4.276292	-1.404606
20	1	0	0.057934	4.275783	-2.489603
21	6	0	0.057936	4.276292	1.404606
22	1	0	0.057934	4.275783	2.489603
23	6	0	0.093156	5.456798	0.711060
24	1	0	0.121359	6.400385	1.244128
25	6	0	0.093156	5.456798	-0.711060
26	1	0	0.121359	6.400385	-1.244128
27	14	0	-0.224118	-3.481194	-1.675644
28	14	0	-0.224118	-3.481194	1.675644
29	1	0	0.353829	-3.375667	3.042681
30	1	0	0.353829	-3.375667	-3.042681

5,12-Disilatetracene S_0 open-shell

E = -1196.0573467 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.700870	-0.056549	-5.144224
2	6	0	1.390385	-0.096067	-3.946921
3	6	0	0.715267	-0.044127	-2.702859
4	6	0	-0.715267	0.044127	-2.702859
5	6	0	-1.390385	0.096067	-3.946921
6	6	0	-0.700870	0.056549	-5.144224
7	6	0	-0.723502	0.043445	0.414705
8	6	0	0.723502	-0.043445	0.414705
9	6	0	1.392843	-0.096697	1.636299
10	1	0	2.477990	-0.161447	1.654856
11	6	0	0.715267	-0.058905	2.871084
12	6	0	-0.715267	0.058905	2.871084
13	6	0	-1.392843	0.096697	1.636299
14	1	0	3.012963	-0.562989	-1.151292
15	1	0	1.240257	-0.108177	-6.083512
16	1	0	2.474204	-0.166419	-3.962548
17	1	0	-2.474204	0.166419	-3.962548
18	1	0	-1.240257	0.108177	-6.083512
19	1	0	-3.012963	0.562989	-1.151292
20	1	0	-2.477990	0.161447	1.654856
21	6	0	-1.398667	0.119073	4.118101
22	1	0	-2.480084	0.208552	4.116920
23	6	0	1.398667	-0.119073	4.118101
24	1	0	2.480084	-0.208552	4.116920
25	6	0	0.707322	-0.060280	5.301688
26	1	0	1.239279	-0.104742	6.245315
27	6	0	-0.707322	0.060280	5.301688
28	1	0	-1.239279	0.104742	6.245315
29	14	0	-1.689020	-0.107326	-1.150498
30	14	0	1.689020	0.107326	-1.150498

5,12-Disilatetracene T_1 ap

E = -1196.0492495 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.692481	-0.078758	-5.162184
2	6	0	-1.379962	-0.147048	-3.952670
3	6	0	-0.707706	-0.075056	-2.721060
4	6	0	0.707706	0.075056	-2.721060
5	6	0	1.379962	0.147048	-3.952670
6	6	0	0.692481	0.078758	-5.162184
7	6	0	0.718001	0.089821	0.425003
8	6	0	-0.718001	-0.089821	0.425003
9	6	0	-1.381424	-0.177194	1.636744
10	1	0	-2.462199	-0.295806	1.656582
11	6	0	-0.707706	-0.097958	2.883619
12	6	0	0.707706	0.097958	2.883619
13	6	0	1.381424	0.177194	1.636744
14	1	0	-1.235250	-0.142535	-6.098794
15	1	0	-2.461245	-0.250543	-3.969275
16	1	0	2.461245	0.250543	-3.969275
17	1	0	1.235250	0.142535	-6.098794
18	1	0	2.462199	0.295806	1.656582
19	6	0	1.388099	0.192492	4.123384
20	1	0	2.463134	0.339967	4.121927
21	6	0	-1.388099	-0.192492	4.123384
22	1	0	-2.463134	-0.339967	4.121927
23	6	0	-0.700043	-0.097151	5.312077
24	1	0	-1.230776	-0.170727	6.254550
25	6	0	0.700043	0.097151	5.312077
26	1	0	1.230776	0.170727	6.254550
27	14	0	1.716500	-0.003168	-1.148526
28	14	0	-1.716500	0.003168	-1.148526
29	1	0	2.886937	0.916882	-1.155103
30	1	0	-2.886937	-0.916882	-1.155103

5,12-Disilatetracene T_1 sp

E = -1196.0534756 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.721992	-4.981720	0.697186
2	6	0	-0.320992	-3.841772	1.390858
3	6	0	0.085858	-2.682356	0.711631
4	6	0	0.085858	-2.682356	-0.711631
5	6	0	-0.320992	-3.841772	-1.390858
6	6	0	-0.721992	-4.981720	-0.697186
7	6	0	0.349380	0.404547	-0.722827
8	6	0	0.349380	0.404547	0.722827
9	6	0	0.150249	1.596638	1.395661
10	1	0	0.139148	1.613820	2.482550
11	6	0	-0.053890	2.825602	0.714733
12	6	0	-0.053890	2.825602	-0.714733
13	6	0	0.150249	1.596638	-1.395661
14	1	0	-1.033851	-5.865780	1.242358
15	1	0	-0.331541	-3.854845	2.476725
16	1	0	-0.331541	-3.854845	-2.476725
17	1	0	-1.033851	-5.865780	-1.242358
18	1	0	0.139148	1.613820	-2.482550
19	6	0	-0.259268	4.049084	-1.401202
20	1	0	-0.259477	4.047591	-2.486319
21	6	0	-0.259268	4.049084	1.401202
22	1	0	-0.259477	4.047591	2.486319
23	6	0	-0.455848	5.221021	0.706956
24	1	0	-0.612588	6.150383	1.242763
25	6	0	-0.455848	5.221021	-0.706956
26	1	0	-0.612588	6.150383	-1.242763
27	14	0	0.666263	-1.178716	-1.660574
28	14	0	0.666263	-1.178716	1.660574
29	1	0	0.129651	-1.135410	-3.049026
30	1	0	0.129651	-1.135410	3.049026

Phenantrene S_0

E = -539.6684063 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-3.556732	-0.296817
2	6	0	0.000000	-2.834692	0.877201
3	6	0	0.000000	-1.421382	0.865240
4	6	0	0.000000	-0.728223	-0.379156
5	6	0	0.000000	-1.497811	-1.564549
6	6	0	0.000000	-2.878091	-1.528060
7	6	0	0.000000	-0.678589	2.091990
8	6	0	0.000000	0.728223	-0.379156
9	6	0	0.000000	1.421382	0.865240
10	6	0	0.000000	0.678589	2.091990
11	6	0	0.000000	2.834692	0.877201
12	1	0	0.000000	3.345807	1.834509
13	6	0	0.000000	3.556732	-0.296817
14	6	0	0.000000	2.878091	-1.528060
15	6	0	0.000000	1.497811	-1.564549
16	1	0	0.000000	-1.228957	3.027126
17	1	0	0.000000	-4.640536	-0.273515
18	1	0	0.000000	-3.345807	1.834509
19	1	0	0.000000	-1.005214	-2.528278
20	1	0	0.000000	-3.440624	-2.454943
21	1	0	0.000000	1.228957	3.027126
22	1	0	0.000000	4.640536	-0.273515
23	1	0	0.000000	3.440624	-2.454943
24	1	0	0.000000	1.005214	-2.528278

Phenantrene T_1

E = -539.5670303 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-3.592992	-0.309963
2	6	0	0.000000	-2.880896	0.874940
3	6	0	0.000000	-1.446025	0.885735
4	6	0	0.000000	-0.745783	-0.384378
5	6	0	0.000000	-1.496539	-1.543969
6	6	0	0.000000	-2.911011	-1.528164
7	6	0	0.000000	-0.735258	2.075278
8	6	0	0.000000	0.745783	-0.384378
9	6	0	0.000000	1.446025	0.885735
10	6	0	0.000000	0.735258	2.075278
11	6	0	0.000000	2.880896	0.874940
12	1	0	0.000000	3.400016	1.827342
13	6	0	0.000000	3.592992	-0.309963
14	6	0	0.000000	2.911011	-1.528164
15	6	0	0.000000	1.496539	-1.543969
16	1	0	0.000000	-1.263583	3.021226
17	1	0	0.000000	-4.677105	-0.292476
18	1	0	0.000000	-3.400016	1.827342
19	1	0	0.000000	-1.004771	-2.508871
20	1	0	0.000000	-3.456452	-2.464084
21	1	0	0.000000	1.263583	3.021226
22	1	0	0.000000	4.677105	-0.292476
23	1	0	0.000000	3.456452	-2.464084
24	1	0	0.000000	1.004771	-2.508871

1-Silaphenantrene S_0

E = -791.0272395 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.761969	-2.696370	0.000000
2	6	0	1.403277	-2.921856	0.000000
3	6	0	0.482106	-1.848505	0.000000
4	6	0	0.959850	-0.504908	0.000000
5	6	0	2.361607	-0.312098	0.000000
6	6	0	3.242069	-1.375548	0.000000
7	6	0	-0.925223	-2.107866	0.000000
8	6	0	0.000000	0.603845	0.000000
9	6	0	-1.394549	0.281840	0.000000
10	6	0	-1.819973	-1.085116	0.000000
11	1	0	-4.021731	1.427283	0.000000
12	6	0	-1.722737	3.183174	0.000000
13	6	0	-0.316410	3.105082	0.000000
14	6	0	0.456335	1.949953	0.000000
15	1	0	-1.263265	-3.138706	0.000000
16	1	0	3.456441	-3.528833	0.000000
17	1	0	1.016236	-3.935597	0.000000
18	1	0	2.772357	0.687891	0.000000
19	1	0	4.309878	-1.187838	0.000000
20	1	0	-2.883453	-1.304001	0.000000
21	1	0	-2.190131	4.160520	0.000000
22	1	0	0.234400	4.043170	0.000000
23	1	0	1.524525	2.113946	0.000000
24	14	0	-2.563228	1.645171	0.000000

1-Silaphenantrene T_1

E = -790.965581 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.863361	-0.256984	0.022943
2	6	0	3.132826	0.903447	-0.041777
3	6	0	1.713180	0.877939	-0.045916
4	6	0	1.022940	-0.376488	0.008443
5	6	0	1.816201	-1.550790	0.081914
6	6	0	3.192521	-1.496107	0.088543
7	6	0	0.971200	2.082624	-0.098062
8	6	0	-0.433814	-0.389651	-0.003696
9	6	0	-1.125876	0.847455	-0.026914
10	6	0	-0.406826	2.056093	-0.079361
11	6	0	-3.516313	-0.887156	-0.146284
12	6	0	-2.543022	-1.847170	-0.107128
13	6	0	-1.137163	-1.636389	-0.017937
14	1	0	1.503493	3.026512	-0.150292
15	1	0	4.946879	-0.225294	0.026863
16	1	0	3.631607	1.865879	-0.088177
17	1	0	1.346281	-2.522885	0.137594
18	1	0	3.764693	-2.415346	0.144809
19	1	0	-0.950813	2.995618	-0.109972
20	1	0	-4.550344	-1.202064	-0.244199
21	1	0	-2.844708	-2.892058	-0.168703
22	1	0	-0.547011	-2.541938	-0.006001
23	14	0	-3.011244	0.894849	0.087155
24	1	0	-3.437957	1.422745	1.429294

2-Silaphenantrene S_0

E = -791.0262732 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.515543	-2.963180	0.000000
2	6	0	1.143057	-3.081989	0.000000
3	6	0	0.309420	-1.941553	0.000000
4	6	0	0.876895	-0.633715	0.000000
5	6	0	2.291579	-0.552764	0.000000
6	6	0	3.088554	-1.680722	0.000000
7	6	0	-1.113498	-2.089667	0.000000
8	6	0	0.000000	0.540154	0.000000
9	6	0	-1.423562	0.339662	0.000000
10	6	0	-1.930111	-1.009305	0.000000
11	6	0	-2.378482	1.389748	0.000000
12	1	0	-3.423112	1.097075	0.000000
13	6	0	-0.060102	3.068384	0.000000
14	6	0	0.579647	1.840636	0.000000
15	1	0	-1.529316	-3.092096	0.000000
16	1	0	3.145998	-3.844864	0.000000
17	1	0	0.677593	-4.062282	0.000000
18	1	0	2.786060	0.408510	0.000000
19	1	0	4.167316	-1.570633	0.000000
20	1	0	-3.006776	-1.140491	0.000000
21	1	0	-2.705745	4.244741	0.000000
22	1	0	0.556287	3.960438	0.000000
23	1	0	1.662124	1.882178	0.000000
24	14	0	-1.837433	3.054521	0.000000

2-Silaphenantrene T_1

E = -790.9565511 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.845864	-0.439737	0.099822
2	6	0	-3.193224	0.775092	0.033986
3	6	0	-1.787541	0.847524	-0.018242
4	6	0	-1.003887	-0.355180	-0.019740
5	6	0	-1.715489	-1.586479	0.068983
6	6	0	-3.092101	-1.627288	0.125082
7	6	0	-1.125167	2.114882	-0.065499
8	6	0	0.431379	-0.279344	-0.093562
9	6	0	1.068198	1.016345	-0.060742
10	6	0	0.226859	2.192111	-0.075606
11	6	0	2.453899	1.197963	-0.053873
12	1	0	2.804245	2.226081	-0.092945
13	6	0	2.542985	-1.673303	-0.230555
14	6	0	1.200953	-1.512028	-0.273406
15	1	0	-1.729503	3.015984	-0.076763
16	1	0	-4.928157	-0.479791	0.141988
17	1	0	-3.760131	1.700229	0.026316
18	1	0	-1.176596	-2.521950	0.119141
19	1	0	-3.596080	-2.584409	0.198161
20	1	0	0.719893	3.158065	-0.088725
21	1	0	2.933437	-2.671021	-0.409080
22	1	0	0.610578	-2.394539	-0.495749
23	14	0	3.643328	-0.225374	0.176142
24	1	0	4.149719	-0.316750	1.591773

3-Silaphenantrene S_0

E = -791.0280356 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.199256	-3.163438	0.000000
2	6	0	0.821793	-3.172158	0.000000
3	6	0	0.081527	-1.967326	0.000000
4	6	0	0.763671	-0.716717	0.000000
5	6	0	2.177278	-0.746686	0.000000
6	6	0	2.881151	-1.934595	0.000000
7	6	0	-1.348478	-1.994391	0.000000
8	6	0	0.000000	0.537360	0.000000
9	6	0	-1.434545	0.451660	0.000000
10	6	0	-2.060201	-0.839345	0.000000
11	6	0	-2.312312	1.575951	0.000000
12	1	0	-3.370770	1.321610	0.000000
13	6	0	-1.983771	2.917691	0.000000
14	6	0	0.668500	1.786608	0.000000
15	1	0	-1.852478	-2.954753	0.000000
16	1	0	2.754066	-4.094860	0.000000
17	1	0	0.279710	-4.112153	0.000000
18	1	0	2.739613	0.177084	0.000000
19	1	0	3.965149	-1.916443	0.000000
20	1	0	-3.144746	-0.873276	0.000000
21	1	0	-2.785644	3.647034	0.000000
22	1	0	0.350548	4.631894	0.000000
23	1	0	1.749979	1.796271	0.000000
24	14	0	-0.243475	3.283565	0.000000

3-Silaphenantrene T_1

E = -790.9607106 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.840839	-0.517012	0.012512
2	6	0	-3.221553	0.713577	0.008130
3	6	0	-1.810035	0.820827	0.001167
4	6	0	-1.006657	-0.358187	-0.014909
5	6	0	-1.674869	-1.598530	0.006333
6	6	0	-3.056185	-1.682238	0.017314
7	6	0	-1.180373	2.095824	0.023230
8	6	0	0.467337	-0.250168	-0.039540
9	6	0	1.041817	1.081762	0.006608
10	6	0	0.195875	2.200808	0.034403
11	6	0	2.480281	1.358749	-0.018287
12	1	0	2.715871	2.422773	-0.008378
13	6	0	3.502520	0.477909	-0.048530
14	6	0	1.268953	-1.377202	-0.155590
15	1	0	-1.797200	2.987547	0.037227
16	1	0	-4.922465	-0.587678	0.019221
17	1	0	-3.810317	1.624929	0.012726
18	1	0	-1.106794	-2.518881	0.025212
19	1	0	-3.533317	-2.655559	0.034596
20	1	0	0.649699	3.186193	0.055448
21	1	0	4.513960	0.873328	-0.059239
22	1	0	3.610738	-1.968364	1.276504
23	1	0	0.780841	-2.337600	-0.275483
24	14	0	3.135811	-1.344529	-0.008205

4-Silaphenantrene S_0

E = -791.0293035 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.791340	-3.325979	0.000000

2	6	0	-0.419672	-3.191406	0.000000
3	6	0	0.188044	-1.915457	0.000000
4	6	0	-0.622999	-0.744999	0.000000
5	6	0	-2.027451	-0.919825	0.000000
6	6	0	-2.600527	-2.174898	0.000000
7	6	0	1.612321	-1.772603	0.000000
8	6	0	0.000000	0.566314	0.000000
9	6	0	1.427548	0.669121	0.000000
10	6	0	2.197394	-0.548282	0.000000
11	6	0	2.151134	1.894685	0.000000
12	1	0	3.232447	1.804858	0.000000
13	6	0	1.622506	3.175116	0.000000
14	6	0	0.250146	3.490885	0.000000
15	1	0	2.222258	-2.670287	0.000000
16	1	0	-2.246084	-4.309912	0.000000
17	1	0	0.217403	-4.070068	0.000000
18	1	0	-2.674408	-0.049998	0.000000
19	1	0	-3.680245	-2.273846	0.000000
20	1	0	3.279039	-0.463709	0.000000
21	1	0	2.333972	3.997716	0.000000
22	1	0	-0.045894	4.533513	0.000000
23	1	0	-2.338863	2.289608	0.000000
24	14	0	-0.873018	2.142579	0.000000

4-Silaphenantrene T_1

E = -790.9685083 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.731728	-0.460819	-0.049833
2	6	0	-3.129260	0.776144	-0.015270
3	6	0	-1.719720	0.899180	0.006134
4	6	0	-0.903519	-0.282318	-0.011056
5	6	0	-1.567752	-1.542442	-0.042241
6	6	0	-2.938949	-1.630856	-0.063563
7	6	0	-1.079436	2.166671	0.044259
8	6	0	0.516863	-0.175572	-0.000018
9	6	0	1.120235	1.100095	0.025318
10	6	0	0.282783	2.262156	0.056326
11	6	0	2.541908	1.315519	0.006988
12	1	0	2.863911	2.351433	0.039820
13	6	0	3.560174	0.335564	-0.098180
14	6	0	3.359628	-1.018615	-0.161838
15	1	0	-1.691671	3.062404	0.065118
16	1	0	-4.812630	-0.541934	-0.063574
17	1	0	-3.731165	1.679055	-0.003398
18	1	0	-0.973843	-2.451050	-0.054757
19	1	0	-3.417593	-2.603343	-0.088672
20	1	0	0.756067	3.237991	0.092935
21	1	0	4.578141	0.717867	-0.155463
22	1	0	4.224717	-1.664480	-0.276261
23	14	0	1.632370	-1.703915	0.062592
24	1	0	1.483530	-2.401387	1.385810

9-Silaphenantrene S_0

E = -791.022846 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.661654	-2.548232	0.000000
2	6	0	1.301892	-2.753334	0.000000
3	6	0	0.362740	-1.685039	0.000000

4	6	0	0.861131	-0.331959	0.000000
5	6	0	2.269131	-0.174621	0.000000
6	6	0	3.152371	-1.235149	0.000000
7	6	0	-1.029494	-2.051038	0.000000
8	6	0	0.000000	0.872112	0.000000
9	6	0	-1.431271	0.821892	0.000000
10	6	0	-2.193620	2.012396	0.000000
11	1	0	-3.277441	1.944041	0.000000
12	6	0	-1.593614	3.253780	0.000000
13	6	0	-0.193390	3.321718	0.000000
14	6	0	0.571202	2.171497	0.000000
15	1	0	-1.251660	-3.112037	0.000000
16	1	0	3.342749	-3.391966	0.000000
17	1	0	0.910040	-3.764771	0.000000
18	1	0	2.696829	0.816701	0.000000
19	1	0	4.219708	-1.046491	0.000000
20	1	0	-3.690461	-0.956658	0.000000
21	1	0	-2.190613	4.158404	0.000000
22	1	0	0.301751	4.286573	0.000000
23	1	0	1.643844	2.295250	0.000000
24	14	0	-2.224081	-0.805227	0.000000

9-Silaphenantrene T_1

E = -790.9661729 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.634575	-0.554646	-0.046815
2	6	0	2.970845	0.622237	-0.316873
3	6	0	1.548236	0.736178	-0.229228
4	6	0	0.786413	-0.461778	0.054936
5	6	0	1.504229	-1.621223	0.370375
6	6	0	2.895972	-1.682849	0.330306
7	6	0	0.963748	2.009376	-0.402103
8	6	0	-0.704762	-0.522838	-0.015620
9	6	0	-1.536646	0.620624	0.110980
10	6	0	-2.929956	0.466809	0.087183
11	1	0	-3.561392	1.344824	0.186453
12	6	0	-3.527361	-0.778944	-0.075789
13	6	0	-2.715688	-1.897076	-0.247354
14	6	0	-1.331654	-1.766410	-0.221846
15	1	0	1.629049	2.812705	-0.706063
16	1	0	4.716267	-0.598995	-0.103429
17	1	0	3.530450	1.514914	-0.574753
18	1	0	0.967049	-2.512631	0.666391
19	1	0	3.399526	-2.607704	0.586877
20	1	0	-0.793968	2.865140	1.606801
21	1	0	-4.607317	-0.872550	-0.092397
22	1	0	-3.157333	-2.873631	-0.412508
23	1	0	-0.732138	-2.652419	-0.386082
24	14	0	-0.766993	2.325971	0.202843

1,4-Disilaphenantrene S_0

E = -1042.3914281 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.423753	2.789932	0.000000
2	6	0	-1.361318	-0.067957	0.000000
3	6	0	0.000000	0.378178	0.000000
4	6	0	-1.091648	3.244584	0.000000
5	6	0	-1.636214	-1.477407	0.000000

6	6	0	1.061548	-0.620336	0.000000
7	6	0	0.732494	-2.008048	0.000000
8	6	0	-0.640909	-2.404321	0.000000
9	6	0	1.764585	-2.974806	0.000000
10	1	0	1.491173	-4.024969	0.000000
11	6	0	3.090710	-2.601678	0.000000
12	6	0	3.425196	-1.235188	0.000000
13	6	0	2.434691	-0.275033	0.000000
14	1	0	-2.670304	-1.808799	0.000000
15	1	0	-3.222538	3.527618	0.000000
16	1	0	-4.142949	0.494496	0.000000
17	1	0	1.672328	2.742508	0.000000
18	1	0	-0.919049	4.319194	0.000000
19	1	0	-0.876233	-3.463597	0.000000
20	1	0	3.871934	-3.353136	0.000000
21	1	0	4.466512	-0.933292	0.000000
22	1	0	2.724392	0.768392	0.000000
23	14	0	-2.782647	1.060769	0.000000
24	14	0	0.316393	2.170950	0.000000

1,4-Disilaphenantrene T_1 ap

E = -1042.3544653 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.690083	-0.313954	-0.130124
2	6	0	0.892916	1.023195	0.020960
3	6	0	0.256797	-0.228451	0.038853
4	6	0	3.097173	-1.529370	-0.123660
5	6	0	0.104773	2.210578	-0.006399
6	6	0	-1.178506	-0.287126	0.012786
7	6	0	-1.946089	0.923334	-0.010665
8	6	0	-1.264675	2.165547	-0.023711
9	6	0	-3.362643	0.856454	-0.030060
10	1	0	-3.926069	1.783723	-0.046185
11	6	0	-4.013271	-0.353574	-0.031496
12	6	0	-3.266346	-1.553089	-0.015939
13	6	0	-1.892397	-1.518343	0.005344
14	1	0	0.601453	3.176387	-0.009531
15	1	0	4.774639	-0.259820	-0.232411
16	1	0	0.922183	-2.770447	1.091320
17	1	0	3.726608	-2.413362	-0.238307
18	1	0	-1.844499	3.082729	-0.048074
19	1	0	-5.096515	-0.392705	-0.046103
20	1	0	-3.781873	-2.506849	-0.020322
21	1	0	-1.342475	-2.452950	0.015648
22	14	0	2.746339	1.257383	0.156401
23	14	0	1.256370	-1.831152	-0.017211
24	1	0	3.221744	2.414865	-0.650011

1,4-Disilaphenantrene T_1 sp

E = -1042.3573176 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.663140	-0.302760	0.314134
2	6	0	0.893830	1.010927	-0.082627
3	6	0	0.252767	-0.236782	-0.093336
4	6	0	3.062309	-1.512807	0.319513
5	6	0	0.119396	2.200847	0.013111
6	6	0	-1.182266	-0.293097	-0.033563
7	6	0	-1.937922	0.922371	0.062928

8	6	0	-1.249262	2.160122	0.088482
9	6	0	-3.354246	0.866441	0.122115
10	1	0	-3.907291	1.796892	0.199234
11	6	0	-4.016912	-0.335904	0.080509
12	6	0	-3.282372	-1.538516	-0.023119
13	6	0	-1.908837	-1.515999	-0.076621
14	1	0	0.621997	3.163201	0.032002
15	1	0	4.704078	-0.217925	0.625300
16	1	0	0.730532	-2.979139	0.488803
17	1	0	3.630200	-2.387771	0.637869
18	1	0	-1.822845	3.078486	0.163199
19	1	0	-5.099634	-0.366482	0.124647
20	1	0	-3.807244	-2.486474	-0.061020
21	1	0	-1.371841	-2.452885	-0.155879
22	14	0	2.753696	1.219047	-0.248996
23	14	0	1.299508	-1.802571	-0.223272
24	1	0	3.219453	2.472379	0.408436

9,10-Disilaphenantrene S_0

E = -1042.4030675 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.052549	-3.579854	-0.928433
2	6	0	0.221736	-2.986689	0.292162
3	6	0	0.221736	-1.584981	0.466961
4	6	0	-0.023272	-0.746610	-0.663190
5	6	0	-0.348187	-1.387217	-1.879271
6	6	0	-0.363148	-2.765857	-2.018863
7	6	0	0.023272	0.746610	-0.663190
8	6	0	-0.221736	1.584981	0.466961
9	6	0	-0.221736	2.986689	0.292162
10	1	0	-0.420360	3.622050	1.149556
11	6	0	0.052549	3.579854	-0.928433
12	6	0	0.363148	2.765857	-2.018863
13	6	0	0.348187	1.387217	-1.879271
14	1	0	-0.054678	-4.659692	-1.025160
15	1	0	0.420360	-3.622050	1.149556
16	1	0	-0.628556	-0.785853	-2.733898
17	1	0	-0.628736	-3.205523	-2.973758
18	1	0	0.054678	4.659692	-1.025160
19	1	0	0.628736	3.205523	-2.973758
20	1	0	0.628556	0.785853	-2.733898
21	14	0	-0.500750	0.962076	2.197742
22	14	0	0.500750	-0.962076	2.197742
23	1	0	-0.425584	2.055266	3.198687
24	1	0	0.425584	-2.055266	3.198687

9,10-Disilaphenantrene T_1 ap

E = -1042.3598766 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.017758	-3.569171	-0.904553
2	6	0	-0.383605	-2.967394	0.284683
3	6	0	-0.387233	-1.572604	0.450665
4	6	0	0.017758	-0.751318	-0.636697
5	6	0	0.449890	-1.382755	-1.815782
6	6	0	0.453284	-2.767144	-1.954098
7	6	0	-0.017758	0.751318	-0.636697
8	6	0	0.387233	1.572604	0.450665
9	6	0	0.383605	2.967394	0.284683

10	1	0	0.694733	3.598599	1.111394
11	6	0	-0.017758	3.569171	-0.904553
12	6	0	-0.453284	2.767144	-1.954098
13	6	0	-0.449890	1.382755	-1.815782
14	1	0	-2.175026	-0.470706	2.357476
15	1	0	0.007964	-4.649054	-1.000793
16	1	0	-0.694733	-3.598599	1.111394
17	1	0	0.808671	-0.774664	-2.637663
18	1	0	0.802689	-3.213785	-2.878402
19	1	0	2.175026	0.470706	2.357476
20	1	0	-0.007964	4.649054	-1.000793
21	1	0	-0.802689	3.213785	-2.878402
22	1	0	-0.808671	0.774664	-2.637663
23	14	0	0.750056	0.882109	2.178763
24	14	0	-0.750056	-0.882109	2.178763

9,10-Disilaphenantrene T_1 sp

E = -1042.365695 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.589616	-0.853552	-0.120296
2	6	0	2.976233	0.329965	0.280221
3	6	0	1.579588	0.476778	0.310090
4	6	0	0.769693	-0.631571	-0.059361
5	6	0	1.410968	-1.803973	-0.497064
6	6	0	2.796454	-1.919950	-0.530530
7	6	0	-0.728788	-0.662240	0.027333
8	6	0	-1.581322	0.422551	-0.323469
9	6	0	-2.976883	0.237285	-0.262830
10	1	0	-3.630294	1.057352	-0.542834
11	6	0	-3.542380	-0.959562	0.159267
12	6	0	-2.706940	-2.004405	0.547080
13	6	0	-1.325374	-1.850111	0.480229
14	1	0	0.601557	2.418991	2.115102
15	1	0	4.670925	-0.931928	-0.131344
16	1	0	3.601657	1.170244	0.566802
17	1	0	0.808576	-2.639307	-0.833711
18	1	0	3.250754	-2.839817	-0.881736
19	1	0	-4.620182	-1.069925	0.201129
20	1	0	-3.126283	-2.936790	0.908424
21	1	0	-0.692396	-2.665693	0.808635
22	14	0	-0.926107	2.119959	-0.773692
23	14	0	0.898163	2.211442	0.658877
24	1	0	-2.038298	3.109974	-0.667071

Benz[*a*]anthracene S_0

E = -693.3422676 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.123325	-4.050504	0.000000
2	6	0	-2.225269	-2.684061	0.000000
3	6	0	-1.059918	-1.863258	0.000000
4	6	0	0.228539	-2.496778	0.000000
5	6	0	0.295260	-3.920525	0.000000
6	6	0	-0.847362	-4.676479	0.000000
7	6	0	-1.133448	-0.459041	0.000000
8	6	0	1.372085	-1.683861	0.000000
9	6	0	1.289770	-0.294191	0.000000
10	6	0	0.000000	0.347839	0.000000
11	6	0	-0.060672	1.811460	0.000000
12	6	0	1.151164	2.555644	0.000000

13	6	0	2.415631	1.865505	0.000000
14	6	0	2.481379	0.513920	0.000000
15	1	0	-2.120609	-0.012948	0.000000
16	1	0	-3.017891	-4.663003	0.000000
17	1	0	-3.199442	-2.206042	0.000000
18	1	0	1.270424	-4.396400	0.000000
19	1	0	-0.784190	-5.758809	0.000000
20	1	0	2.351834	-2.152103	0.000000
21	1	0	3.323160	2.460187	0.000000
22	1	0	3.441589	0.008892	0.000000
23	6	0	1.104648	3.964828	0.000000
24	1	0	2.039162	4.516461	0.000000
25	6	0	-1.274802	2.527488	0.000000
26	1	0	-2.217311	1.995283	0.000000
27	6	0	-0.100634	4.639773	0.000000
28	1	0	-0.120806	5.723571	0.000000
29	6	0	-1.298999	3.911167	0.000000
30	1	0	-2.250206	4.431360	0.000000

Benz[*a*]anthracene T_1

E = -693.2661336 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.852383	-4.231827	0.000000
2	6	0	-2.034846	-2.824701	0.000000
3	6	0	-0.945466	-1.953467	0.000000
4	6	0	0.383916	-2.504262	0.000000
5	6	0	0.541244	-3.895544	0.000000
6	6	0	-0.580265	-4.759228	0.000000
7	6	0	-1.103399	-0.531798	0.000000
8	6	0	1.480998	-1.603738	0.000000
9	6	0	1.311583	-0.172113	0.000000
10	6	0	0.000000	0.375960	0.000000
11	6	0	-0.161296	1.800438	0.000000
12	6	0	1.008305	2.647580	0.000000
13	6	0	2.286127	2.060418	0.000000
14	6	0	2.429059	0.680672	0.000000

15	1	0	-2.115826	-0.150183	0.000000
16	1	0	-2.718344	-4.883529	0.000000
17	1	0	-3.039896	-2.415799	0.000000
18	1	0	1.542375	-4.313497	0.000000
19	1	0	-0.429941	-5.832589	0.000000
20	1	0	2.490005	-2.002493	0.000000
21	1	0	3.162137	2.699862	0.000000
22	1	0	3.421033	0.241064	0.000000
23	6	0	0.845396	4.061379	0.000000
24	1	0	1.735925	4.681671	0.000000
25	6	0	-1.434389	2.438672	0.000000
26	1	0	-2.335904	1.840187	0.000000
27	6	0	-0.399476	4.632768	0.000000
28	1	0	-0.508527	5.711248	0.000000
29	6	0	-1.552747	3.806057	0.000000
30	1	0	-2.537197	4.260463	0.000000

1-Silabenz[*a*]anthracene S_0

E = -944.7031969 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.310575	-4.556623	0.000000
2	6	0	-0.331286	-3.598024	0.000000
3	6	0	-0.664170	-2.211690	0.000000
4	6	0	-2.050958	-1.837445	0.000000
5	6	0	-3.040862	-2.862366	0.000000
6	6	0	-2.682327	-4.184984	0.000000
7	6	0	0.316311	-1.205137	0.000000
8	6	0	-2.373118	-0.471468	0.000000
9	6	0	-1.393182	0.516721	0.000000
10	6	0	0.000000	0.151854	0.000000
11	6	0	1.018295	1.198190	0.000000
12	6	0	0.620855	2.570275	0.000000
13	6	0	-0.793947	2.875738	0.000000
14	6	0	-1.742274	1.911126	0.000000
15	1	0	1.355212	-1.517648	0.000000
16	1	0	-1.042881	-5.607257	0.000000

17	1	0	0.715779	-3.883178	0.000000
18	1	0	-4.087477	-2.575908	0.000000
19	1	0	-3.444314	-4.956136	0.000000
20	1	0	-3.418080	-0.175645	0.000000
21	1	0	-1.083226	3.921346	0.000000
22	1	0	-2.794352	2.177305	0.000000
23	6	0	1.515299	3.673030	0.000000
24	1	0	1.056095	4.655976	0.000000
25	1	0	3.443759	-0.395087	0.000000
26	6	0	2.902901	3.624065	0.000000
27	1	0	3.425167	4.578016	0.000000
28	6	0	3.673808	2.449614	0.000000
29	1	0	4.754515	2.532015	0.000000
30	14	0	2.795085	0.927782	0.000000

1-Silabenz[*a*]anthracene T_1

E = -944.6413574 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.469964	-1.502988	-0.034675
2	6	0	-3.125249	-1.760203	-0.020459
3	6	0	-2.175095	-0.694285	-0.010788
4	6	0	-2.659849	0.661842	-0.014140
5	6	0	-4.066287	0.887101	-0.028546
6	6	0	-4.946905	-0.163119	-0.038880
7	6	0	-0.794325	-0.925558	0.004942
8	6	0	-1.727746	1.712025	0.002026
9	6	0	-0.356352	1.478785	0.017192
10	6	0	0.144680	0.119938	0.010188
11	6	0	1.553475	-0.125496	0.008429
12	6	0	2.453822	0.959068	0.021616
13	6	0	1.927086	2.303202	0.046553
14	6	0	0.592353	2.550827	0.039962
15	1	0	-0.445962	-1.954379	0.012181
16	1	0	-5.180482	-2.321788	-0.042543
17	1	0	-2.760283	-2.781971	-0.017460
18	1	0	-4.429932	1.909391	-0.030903

19	1	0	-6.014971	0.022495	-0.049858
20	1	0	-2.088594	2.736335	0.003716
21	1	0	2.631919	3.128032	0.068977
22	1	0	0.222348	3.570856	0.053250
23	6	0	3.874858	0.816087	-0.010869
24	1	0	4.446264	1.738537	0.011907
25	1	0	1.943995	-2.535317	1.380350
26	6	0	4.621365	-0.390468	-0.117092
27	1	0	5.701646	-0.269816	-0.181448
28	6	0	4.095066	-1.650844	-0.169846
29	1	0	4.773571	-2.491025	-0.280966
30	14	0	2.253921	-1.886203	0.059937

4-Silabenz[*a*]anthracene S_0

E = -944.7010705 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.565807	-3.285546	0.000000
2	6	0	3.167581	-1.974278	0.000000
3	6	0	1.784238	-1.630422	0.000000
4	6	0	0.811811	-2.685336	0.000000
5	6	0	1.262583	-4.037569	0.000000
6	6	0	2.601284	-4.329634	0.000000
7	6	0	1.347461	-0.293926	0.000000
8	6	0	-0.546006	-2.336436	0.000000
9	6	0	-0.970112	-1.009376	0.000000
10	6	0	0.000000	0.058203	0.000000
11	6	0	-0.467425	1.457472	0.000000
12	6	0	-1.876290	1.693044	0.000000
13	6	0	-2.798370	0.589850	0.000000
14	6	0	-2.371961	-0.696306	0.000000
15	1	0	2.114293	0.469579	0.000000
16	1	0	4.621108	-3.534022	0.000000
17	1	0	3.903368	-1.176648	0.000000
18	1	0	0.525082	-4.833447	0.000000
19	1	0	2.933142	-5.361830	0.000000
20	1	0	-1.293189	-3.124303	0.000000

21	1	0	-3.863605	0.799974	0.000000
22	1	0	-3.083350	-1.515293	0.000000
23	1	0	-3.865269	3.753895	0.000000
24	6	0	0.467554	2.523070	0.000000
25	1	0	1.517510	2.266241	0.000000
26	6	0	-1.069063	4.499030	0.000000
27	1	0	-1.127533	5.580849	0.000000
28	6	0	0.197323	3.889143	0.000000
29	1	0	1.066591	4.543205	0.000000
30	14	0	-2.434760	3.396136	0.000000

4-Silabenz[*a*]anthracene T_1

E = -944.6381155 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.643407	-1.416867	0.081948
2	6	0	-3.311103	-1.734180	0.083003
3	6	0	-2.315391	-0.714183	0.031505
4	6	0	-2.738574	0.658604	-0.021460
5	6	0	-4.136213	0.949926	-0.020768
6	6	0	-5.061165	-0.057501	0.029312
7	6	0	-0.943173	-1.012770	0.030068
8	6	0	-1.758110	1.653490	-0.067432
9	6	0	-0.392242	1.350373	-0.064420
10	6	0	0.043003	-0.027743	-0.022298
11	6	0	1.483528	-0.320133	-0.023269
12	6	0	2.396684	0.764329	-0.016513
13	6	0	1.922840	2.092641	-0.062872
14	6	0	0.580122	2.388697	-0.095418
15	1	0	-0.671891	-2.059476	0.075777
16	1	0	-5.389633	-2.202301	0.121411
17	1	0	-2.993511	-2.771010	0.123135
18	1	0	-4.452322	1.987101	-0.060608
19	1	0	-6.120153	0.174639	0.029423
20	1	0	-2.061168	2.695510	-0.101770
21	1	0	2.640119	2.908031	-0.076034
22	1	0	0.243443	3.418911	-0.141660

23	6	0	1.935161	-1.667241	-0.064316
24	1	0	1.185489	-2.446185	-0.085683
25	6	0	4.418463	-1.386606	-0.141642
26	1	0	5.375293	-1.890097	-0.236135
27	6	0	3.281337	-2.141093	-0.147269
28	1	0	3.377765	-3.222130	-0.240782
29	14	0	4.254628	0.449414	0.144689
30	1	0	4.731207	0.836745	1.518327

8-Silabenz[*a*]anthracene S_0

E = -944.7035741 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.159862	-3.832905	0.000000
2	6	0	-2.113293	-2.455061	0.000000
3	6	0	-0.937071	-1.636032	0.000000
4	6	0	0.401500	-2.179028	0.000000
5	6	0	-1.045155	-4.715531	0.000000
6	6	0	-1.079517	-0.232595	0.000000
7	6	0	1.488319	-1.294565	0.000000
8	6	0	1.326601	0.090643	0.000000
9	6	0	0.000000	0.645131	0.000000
10	6	0	-0.153880	2.102109	0.000000
11	6	0	1.009284	2.920951	0.000000
12	6	0	2.315261	2.313618	0.000000
13	6	0	2.465309	0.967944	0.000000
14	1	0	-2.090277	0.156432	0.000000
15	1	0	-3.149508	-4.283830	0.000000
16	1	0	-3.060367	-1.925134	0.000000
17	1	0	1.843276	-4.671620	0.000000
18	1	0	-1.234610	-5.782334	0.000000
19	1	0	2.500676	-1.689415	0.000000
20	1	0	3.183113	2.964668	0.000000
21	1	0	3.455367	0.523916	0.000000
22	6	0	0.873474	4.324831	0.000000
23	1	0	1.771137	4.934488	0.000000
24	6	0	-1.411210	2.739947	0.000000

25	1	0	-2.317914	2.148939	0.000000
26	6	0	-0.372029	4.921594	0.000000
27	1	0	-0.461084	6.001981	0.000000
28	6	0	-1.522482	4.119033	0.000000
29	1	0	-2.504239	4.578915	0.000000
30	14	0	0.539495	-3.982679	0.000000

8-Silabenz[*a*]anthracene T_1

E = -944.6520372 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.065869	-1.760166	0.011112
2	6	0	-2.647155	-1.847290	-0.009637
3	6	0	-1.712238	-0.762642	-0.020766
4	6	0	-2.122661	0.620780	-0.022002
5	6	0	-4.810339	-0.610514	-0.011283
6	6	0	-0.340889	-1.056322	-0.005883
7	6	0	-1.145485	1.591031	-0.021428
8	6	0	0.245547	1.294195	-0.014537
9	6	0	0.660334	-0.065697	-0.007560
10	6	0	2.082357	-0.371411	0.000899
11	6	0	3.020604	0.703649	0.000246
12	6	0	2.551309	2.054567	-0.009815
13	6	0	1.217434	2.336512	-0.017615
14	1	0	-0.057933	-2.101621	0.021481
15	1	0	-4.589147	-2.714700	0.039602
16	1	0	-2.221114	-2.845560	-0.008369
17	1	0	-5.892276	-0.699336	-0.001295
18	1	0	-1.427960	2.640996	-0.029975
19	1	0	3.282494	2.855917	-0.010259
20	1	0	0.874065	3.365730	-0.024462
21	6	0	4.406470	0.419480	0.008858
22	1	0	5.106691	1.248353	0.008283
23	6	0	2.587906	-1.691608	0.008972
24	1	0	1.905601	-2.531714	0.007756
25	6	0	4.866128	-0.878897	0.017703
26	1	0	5.930802	-1.082596	0.024309

27	6	0	3.945003	-1.942627	0.017629
28	1	0	4.302463	-2.966110	0.024055
29	14	0	-3.951289	1.049373	-0.049657
30	1	0	-4.326365	1.941160	1.094726

11-Silabenz[*a*]anthracene S_0

E = -944.7036776 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.758538	-4.703252	0.000000
2	6	0	-0.500726	-1.792573	0.000000
3	6	0	0.907694	-2.114725	0.000000
4	6	0	1.408381	-3.457569	0.000000
5	6	0	0.660661	-4.615492	0.000000
6	6	0	-0.904091	-0.447304	0.000000
7	6	0	1.812115	-1.036563	0.000000
8	6	0	1.401696	0.293750	0.000000
9	6	0	0.000000	0.613755	0.000000
10	6	0	-0.409865	2.017768	0.000000
11	6	0	0.590118	3.029382	0.000000
12	6	0	1.981885	2.658428	0.000000
13	6	0	2.368020	1.361083	0.000000
14	1	0	-1.967269	-0.236671	0.000000
15	1	0	-1.212473	-5.687062	0.000000
16	1	0	-3.105149	-3.019270	0.000000
17	1	0	2.488683	-3.560629	0.000000
18	1	0	1.215615	-5.550798	0.000000
19	1	0	2.876653	-1.251139	0.000000
20	1	0	2.722302	3.451601	0.000000
21	1	0	3.420848	1.099397	0.000000
22	6	0	0.210603	4.387449	0.000000
23	1	0	0.987320	5.145206	0.000000
24	6	0	-1.760111	2.424990	0.000000
25	1	0	-2.549869	1.684724	0.000000
26	6	0	-1.120536	4.756262	0.000000
27	1	0	-1.398639	5.803969	0.000000
28	6	0	-2.111383	3.763272	0.000000

29	1	0	-3.158776	4.043419	0.000000
30	14	0	-1.641056	-3.196765	0.000000

11-Silabenz[*a*]anthracene T_1

E = -944.6516437 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.727706	-0.780161	-0.023299
2	6	0	-1.779738	-0.521159	-0.019198
3	6	0	-2.112256	0.882166	-0.017457
4	6	0	-3.462795	1.364665	-0.010957
5	6	0	-4.651535	0.588192	0.002130
6	6	0	-0.450778	-0.895116	-0.016552
7	6	0	-1.061161	1.803727	0.002919
8	6	0	0.294292	1.416109	0.005307
9	6	0	0.625446	0.034016	-0.005001
10	6	0	2.018180	-0.363928	-0.006260
11	6	0	3.027135	0.646780	0.007336
12	6	0	2.646336	2.026527	0.021482
13	6	0	1.337964	2.396492	0.021109
14	1	0	-0.218233	-1.954008	-0.025946
15	1	0	-5.711280	-1.239657	-0.020755
16	1	0	-3.050213	-2.750700	1.102607
17	1	0	-3.583418	2.443290	-0.008666
18	1	0	-5.579358	1.157684	0.025333
19	1	0	-1.292382	2.864646	0.031163
20	1	0	3.429339	2.777432	0.033004
21	1	0	1.062604	3.445762	0.032274
22	6	0	4.390372	0.273379	0.007855
23	1	0	5.143287	1.054634	0.018387
24	6	0	2.437883	-1.716267	-0.019297
25	1	0	1.703499	-2.510887	-0.030341
26	6	0	4.764482	-1.052696	-0.005077
27	1	0	5.813465	-1.325896	-0.004912
28	6	0	3.775320	-2.053872	-0.018717
29	1	0	4.065538	-3.098426	-0.029125
30	14	0	-3.157964	-1.796929	-0.048640

1,4-Disilabenz[*a*]anthracene S_0

E = -1196.0651133 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.692047	3.377240	0.000000
2	6	0	3.245526	2.081703	0.000000
3	6	0	1.850006	1.789271	0.000000
4	6	0	0.917223	2.881221	0.000000
5	6	0	1.419016	4.215009	0.000000
6	6	0	2.767818	4.457014	0.000000
7	6	0	1.361425	0.472139	0.000000
8	6	0	-0.453970	2.585898	0.000000
9	6	0	-0.928480	1.276506	0.000000
10	6	0	0.000000	0.172795	0.000000
11	6	0	-0.510205	-1.201587	0.000000
12	6	0	-1.924717	-1.409648	0.000000
13	6	0	-2.806264	-0.267970	0.000000
14	6	0	-2.337596	1.004432	0.000000
15	1	0	2.091340	-0.329040	0.000000
16	1	0	4.755972	3.585760	0.000000
17	1	0	3.951399	1.257515	0.000000
18	1	0	0.711956	5.038062	0.000000
19	1	0	3.138084	5.475987	0.000000
20	1	0	-1.169727	3.402586	0.000000
21	1	0	-3.878584	-0.438714	0.000000
22	1	0	-3.025239	1.843799	0.000000
23	1	0	-4.164213	-3.150215	0.000000
24	1	0	2.038180	-2.572667	0.000000
25	6	0	-1.602899	-4.441419	0.000000
26	1	0	-1.990125	-5.457492	0.000000
27	6	0	-0.210898	-4.254655	0.000000
28	1	0	0.424123	-5.138653	0.000000
29	14	0	-2.694358	-3.048787	0.000000
30	14	0	0.569261	-2.661542	0.000000

1,4-Disilabenz[*a*]anthracene T_1 ap

E = -1196.0263183 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.750015	-1.495708	-0.008608
2	6	0	3.406776	-1.753036	0.011200
3	6	0	2.455689	-0.686694	0.007621
4	6	0	2.940667	0.669531	-0.018001
5	6	0	4.350479	0.894815	-0.038515
6	6	0	5.228437	-0.154289	-0.033848
7	6	0	1.075806	-0.919235	0.028301
8	6	0	2.011165	1.714827	-0.023921
9	6	0	0.634801	1.478325	-0.004377
10	6	0	0.136860	0.121855	0.025279
11	6	0	-1.288407	-0.119201	0.047865
12	6	0	-2.167987	0.966036	0.026387
13	6	0	-1.645995	2.303241	-0.003186
14	6	0	-0.305511	2.550514	-0.021261
15	1	0	0.736002	-1.949888	0.047236
16	1	0	5.460940	-2.314204	-0.005446
17	1	0	3.042108	-2.774736	0.030255
18	1	0	4.713458	1.917116	-0.057995
19	1	0	6.296780	0.029451	-0.049532
20	1	0	2.367626	2.740337	-0.046720
21	1	0	-2.339186	3.139095	-0.010461
22	1	0	0.066536	3.569697	-0.049643
23	1	0	-4.738640	1.857243	-0.611477
24	1	0	-1.439260	-2.722288	1.144535
25	6	0	-4.619882	-0.924312	-0.167319
26	1	0	-5.689424	-1.094470	-0.296616
27	6	0	-3.786397	-1.989080	-0.161102
28	1	0	-4.214198	-2.982769	-0.303095
29	14	0	-4.025666	0.801833	0.158041
30	14	0	-1.925893	-1.898984	-0.000193

1,4-Disilabenz[*a*]anthracene T_1 sp

E = -1196.0291343 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.762539	-1.483491	-0.029803
2	6	0	-3.420912	-1.746087	-0.071691
3	6	0	-2.464140	-0.685459	-0.031451
4	6	0	-2.942141	0.670544	0.054276
5	6	0	-4.350758	0.901807	0.096515
6	6	0	-5.233970	-0.141863	0.055582
7	6	0	-1.085831	-0.925501	-0.071619
8	6	0	-2.007011	1.709380	0.089645
9	6	0	-0.631750	1.466937	0.043838
10	6	0	-0.140697	0.108924	-0.035545
11	6	0	1.285408	-0.129657	-0.085823
12	6	0	2.164470	0.954324	-0.080547
13	6	0	1.650533	2.289564	-0.000863
14	6	0	0.310280	2.536911	0.063558
15	1	0	-0.755040	-1.955491	-0.133764
16	1	0	-5.477691	-2.297703	-0.061176
17	1	0	-3.061724	-2.767883	-0.136179
18	1	0	-4.708240	1.924195	0.161134
19	1	0	-6.301219	0.046070	0.087758
20	1	0	-2.357091	2.735467	0.151579
21	1	0	2.345230	3.123897	0.013554
22	1	0	-0.059469	3.555426	0.125292
23	1	0	4.738929	1.909248	0.415841
24	6	0	4.609065	-0.898428	0.314845
25	1	0	5.647135	-1.028745	0.619597
26	6	0	3.772092	-1.958384	0.327152
27	1	0	4.149557	-2.931066	0.644693
28	14	0	4.026566	0.778202	-0.242064
29	14	0	1.983350	-1.880091	-0.203970
30	1	0	1.188208	-2.904096	0.527725

8,11-Disilabenz[*a*]anthracene S_0

E = -1196.0680954 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.352906	-4.466578	0.000000
2	6	0	0.604785	-1.509203	0.000000
3	6	0	-0.796614	-1.873714	0.000000
4	6	0	-0.021570	-4.822304	0.000000
5	6	0	0.947165	-0.145675	0.000000
6	6	0	-1.743582	-0.839033	0.000000
7	6	0	-1.387566	0.511427	0.000000
8	6	0	0.000000	0.879660	0.000000
9	6	0	0.356558	2.298171	0.000000
10	6	0	-0.681367	3.271495	0.000000
11	6	0	-2.057850	2.850031	0.000000
12	6	0	-2.393901	1.537871	0.000000
13	1	0	2.000207	0.111533	0.000000
14	1	0	2.083867	-5.271906	0.000000
15	1	0	3.319637	-2.388854	0.000000
16	1	0	-2.749008	-3.955502	0.000000
17	1	0	-0.270020	-5.881138	0.000000
18	1	0	-2.802717	-1.083225	0.000000
19	1	0	-2.827510	3.614700	0.000000
20	1	0	-3.435955	1.235708	0.000000
21	6	0	-0.352206	4.643085	0.000000
22	1	0	-1.156435	5.371515	0.000000
23	6	0	1.690773	2.755451	0.000000
24	1	0	2.507500	2.045244	0.000000
25	6	0	0.964057	5.060729	0.000000
26	1	0	1.202767	6.118106	0.000000
27	6	0	1.991747	4.105633	0.000000
28	1	0	3.027809	4.424883	0.000000
29	14	0	-1.312792	-3.625901	0.000000
30	14	0	1.902782	-2.794337	0.000000

8,11-Disilabenz[*a*]anthracene T_1 ap

E = -1196.0379106 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.524244	-1.313040	-0.000137
2	6	0	1.501065	-0.590383	-0.000818
3	6	0	1.856836	0.802328	0.010313
4	6	0	4.858045	-0.000573	-0.025430
5	6	0	0.155699	-0.941764	-0.000978
6	6	0	0.834266	1.739589	0.018790
7	6	0	-0.533528	1.382177	0.022565
8	6	0	-0.892104	0.006841	0.000199
9	6	0	-2.299063	-0.360158	-0.009351
10	6	0	-3.282185	0.672508	0.010418
11	6	0	-2.870478	2.044603	0.035009
12	6	0	-1.554613	2.385108	0.039367
13	1	0	-0.098541	-1.995812	0.011280
14	1	0	5.327700	-2.050965	0.010933
15	1	0	2.487405	-3.122872	-0.707208
16	1	0	5.916164	0.263578	-0.053091
17	1	0	1.072566	2.800546	0.010320
18	1	0	-3.636963	2.812294	0.048910
19	1	0	-1.255495	3.427832	0.055710
20	6	0	-4.653813	0.330919	0.003613
21	1	0	-5.388604	1.129122	0.019320
22	6	0	-2.747661	-1.700658	-0.038248
23	1	0	-2.031106	-2.511364	-0.057809
24	6	0	-5.058313	-0.986226	-0.022652
25	1	0	-6.113396	-1.234874	-0.027605
26	6	0	-4.093176	-2.008977	-0.044393
27	1	0	-4.406558	-3.046579	-0.066930
28	14	0	3.627248	1.390110	-0.155209
29	14	0	2.781349	-1.946882	0.158069
30	1	0	3.935153	2.550125	0.726548

8,11-Disilabenz[*a*]anthracene T_1 sp

E = -1196.0414712 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.446108	-1.304525	0.414176
2	6	0	-1.501021	-0.589456	-0.144421
3	6	0	-1.857998	0.800147	-0.127133
4	6	0	-4.781727	0.007606	0.429950
5	6	0	-0.158774	-0.944996	-0.097688
6	6	0	-0.842382	1.741148	-0.062232
7	6	0	0.525155	1.382085	-0.022479
8	6	0	0.885833	0.006608	-0.041339
9	6	0	2.292848	-0.358633	-0.000839
10	6	0	3.273866	0.674597	0.056960
11	6	0	2.860161	2.046165	0.075195
12	6	0	1.544526	2.385221	0.037422
13	1	0	0.094981	-1.998902	-0.099070
14	1	0	-5.163849	-2.040084	0.777755
15	1	0	-2.373944	-3.206424	0.328298
16	1	0	-5.762239	0.299895	0.806063
17	1	0	-1.083701	2.800804	-0.035197
18	1	0	3.624794	2.814501	0.120564
19	1	0	1.243932	3.427575	0.051927
20	6	0	4.645216	0.334157	0.096297
21	1	0	5.378220	1.132989	0.139897
22	6	0	2.743660	-1.698666	-0.017096
23	1	0	2.028942	-2.509985	-0.061486
24	6	0	5.051797	-0.982539	0.079542
25	1	0	6.106685	-1.230218	0.109970
26	6	0	4.088892	-2.005936	0.022266
27	1	0	4.403701	-3.043276	0.008561
28	14	0	-3.649573	1.336260	-0.220923
29	14	0	-2.819630	-1.913089	-0.260476
30	1	0	-3.872348	2.670851	0.400806