Triplet State (Anti)aromaticity of Some Monoheterocyclic Analogues of Benzene, Naphthalene and Anthracene

Marija Baranac-Stojanović,[a*] Milovan Stojanović,[b] Jovana Aleksić[b]

[a] *University of Belgrade - Faculty of Chemistry, Studentski trg 12-16, P.O.Box 158, 11000 Belgrade, Serbia*

[b] *University of Belgrade - Institute of Chemistry, Technology and Metallurgy - Center for Chemistry, Njegoševa 12, P.O.Box 473, 11000 Belgrade, Serbia*

Supplementary Information

Table of Contents

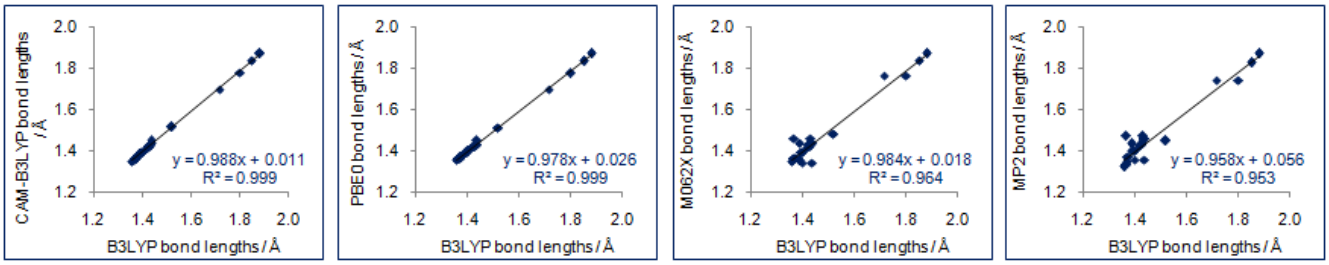

Figure S1. Correlations between B3LYP and CAM-B3LYP, PBE0, M062X and MP2(fc) bond lengths of optimized triplet state structures of monocycles studied.

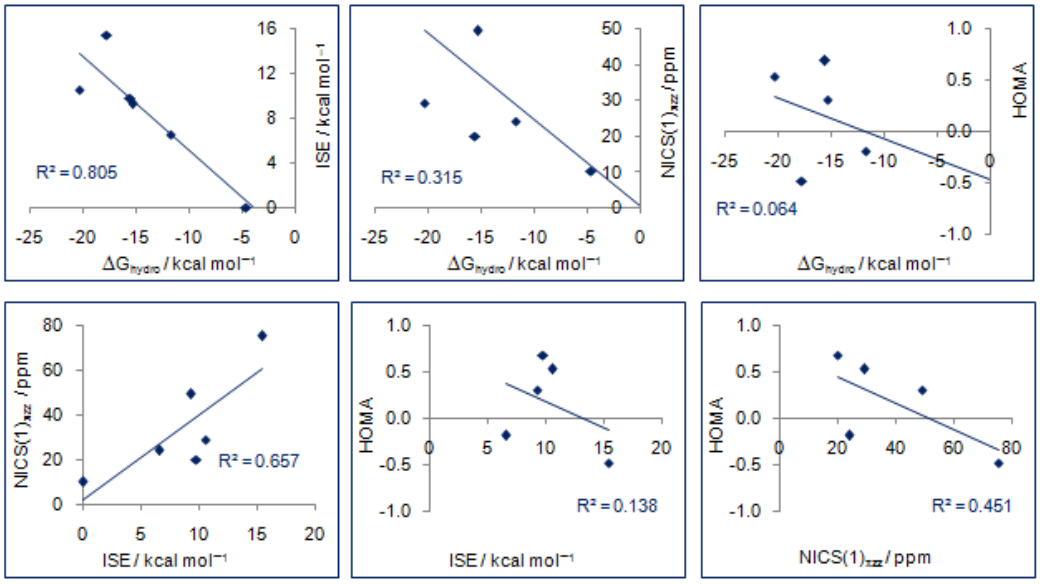

Figure S2. Correlations between different aromaticity indices calculated for monocycles studied.

Table S1. Adiabatic S_0-T_1 energy gaps in eV.

Molecule	B3LYP		CAM-B3LYP		PBE0		M062X		MP2(fc)	
Benzene	D_{2h}	3.8	D_{2h}	3.8	D_{2h}	3.8	C_s	4.0	C_s	5.2
Silabenzene	C_s	2.0	C_s	2.0	C_s	2.0	C_s	2.1	C_s	2.9
Pyridine	C_s	3.6	C_s	3.7	C_s	3.6	C_s	3.8	C_s	4.8
Phosphinine	C_s	2.7	C_1	2.7	C_s	2.7	C_1	2.9	C_s	3.7
Pyrylium ion	C_s	3.3	C_s	3.4	C_s	3.3	C_s	3.5	C_s	3.9
Thiopyrylium ion	C_1	3.2	C_1	3.2	C_1	3.2	C_s	3.5	C_s	3.8

Table S2. Calculated HOMA values for T1 states.

Molecule	B3LYP	CAM-B3LYP	PBE0	M062X	MP2(fc)
Benzene	-0.484	-0.412	-0.342	-0.094	0.491
Silabenzene	/	/	/	/	/
Pyridine	0.689	0.705	0.741	0.729	0.385
Phosphinine	-0.185	-0.106	0.002	-0.123	-0.459
Pyrylium ion	0.313	0.435	0.438	0.418	0.334
Thiopyrylium ion	0.532	0.560	0.598	0.140	0.200

Table S3. Calculated NICS(1)$_{\pi zz}$ values for T1 states in ppm.

Molecule	B3LYP	CAM-B3LYP	PBE0	M062X	MP2(fc)[a]
Benzene	75.4	66.2	70.1	17.7	36.8
Silabenzene	10.2	9.8	9.2	9.7	6.0
Pyridine	20.1	18.5	19.1	19.2	2.8
Phosphinine	24.2	20.3	19.1	18.2	6.9
Pyrylium ion	49.4	47.6	43.4	39.1	6.5
Thiopyrylium ion	29.2	18.3	15.9	38.8	16.7
[a] NICS(1)$_{zz}$ in this case.					

Table S4. Calculated Gibbs energy of hydrogenation for T1 states in kcal/mol.

Molecule	B3LYP	CAM-B3LYP	PBE0	M062X	MP2(fc)
Benzene	-17.8	-21.1	-24.1	-21.8	-32.1
Silabenzene	-4.6	-8.3	-10.9	-9.5	-15.4
Pyridine	-15.6	-19.3	-21.4	-19.3	-24.5
Phosphinine	-11.8	-15.4	-18.1	-15.8	-18.4
Pyrylium ion	-15.3	-18.8	-21.7	-20.1	-24.5
Thiopyrylium ion	-20.4	-24.3	-27.0	-26.4	-44.0

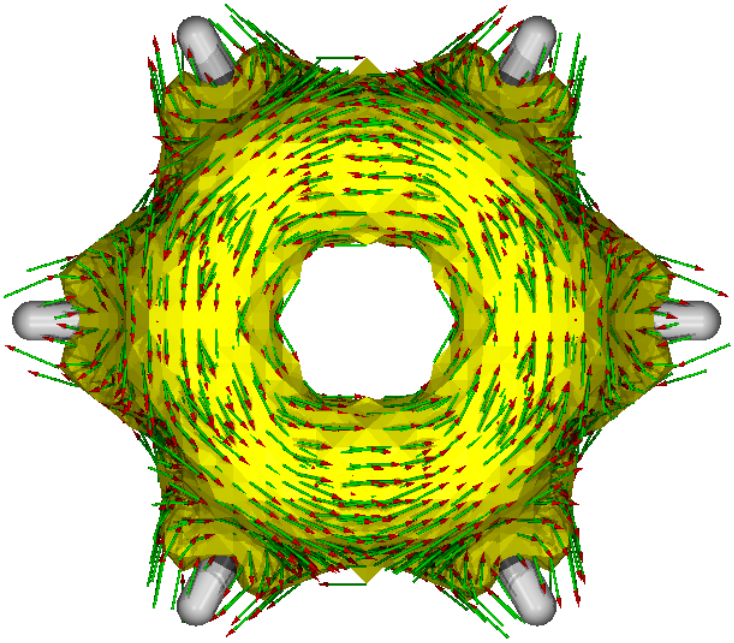

Figure S3. ACID plot of T_1 benzene at an isosurface value of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

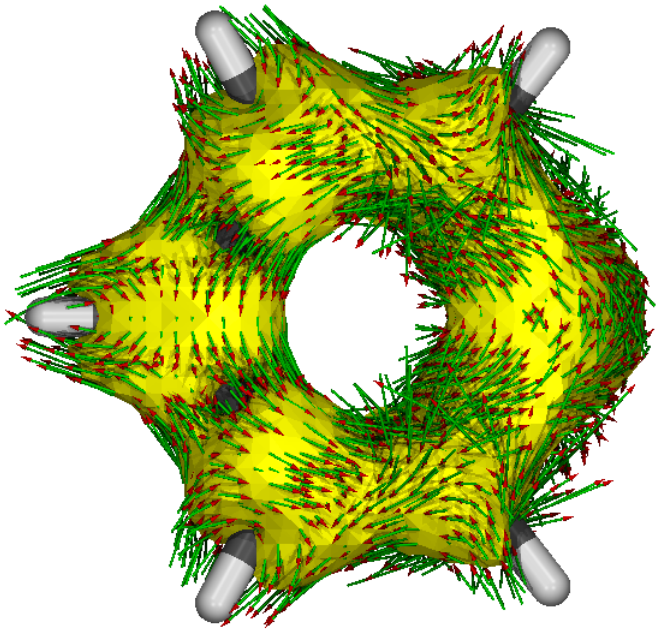

Figure S4. ACID plot of T_1 pyridine at an isosurface value of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

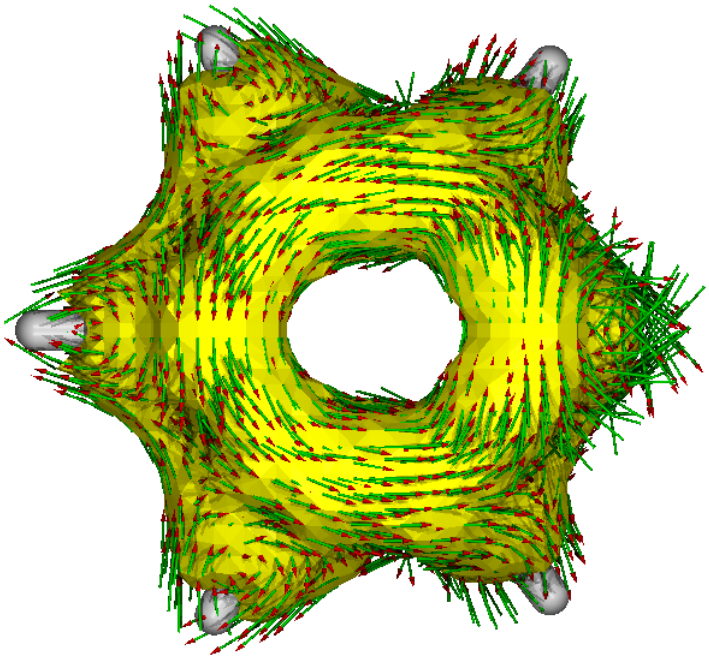

Figure S5. ACID plot of T_1 pyrylium ion at an isosurface value of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

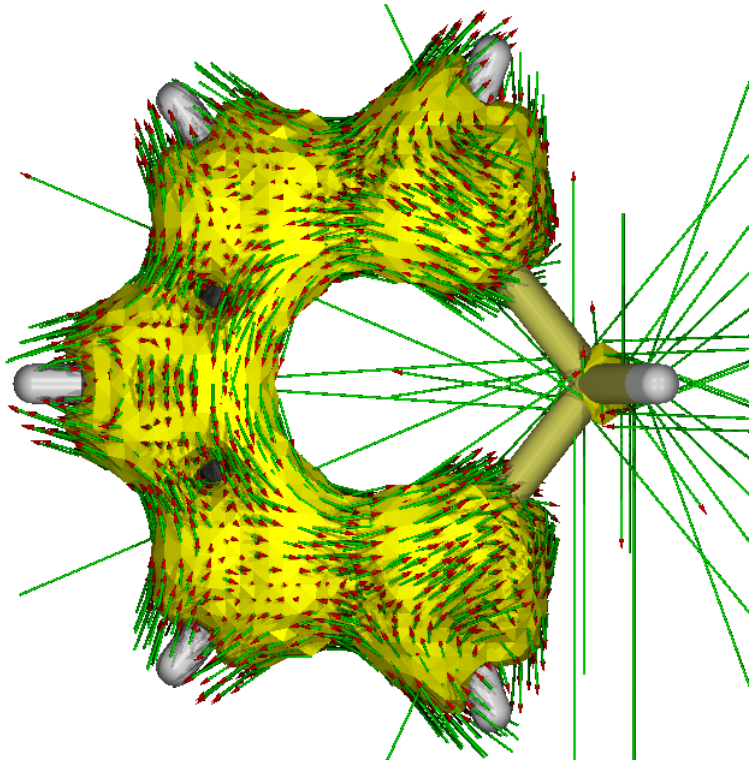

Figure S6. ACID plot of T_1 silabenzene at an isosurface value of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

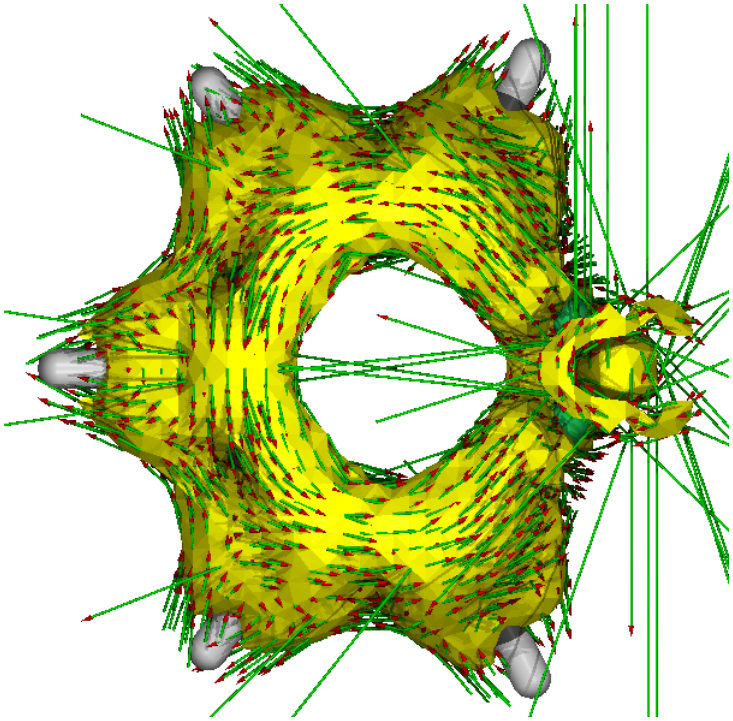

Figure S7. ACID plot of T_1 phosphinine at an isosurface value of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic

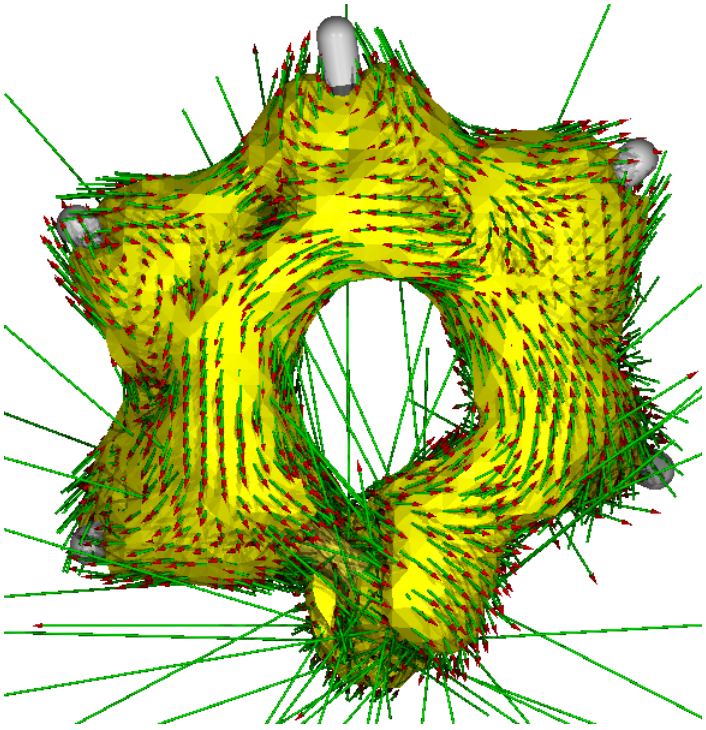

Figure S8. ACID plot of T_1 thiopyrylium ion at an isosurface value of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

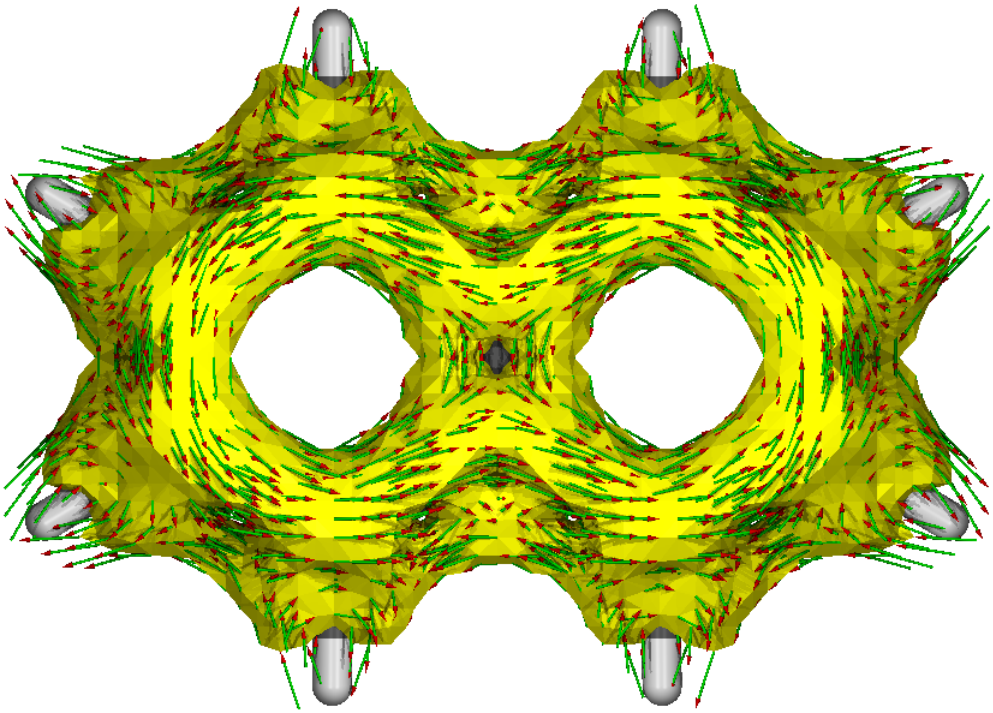

Figure S9. ACID plot of T_1 naphthalene at an isosurface value of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

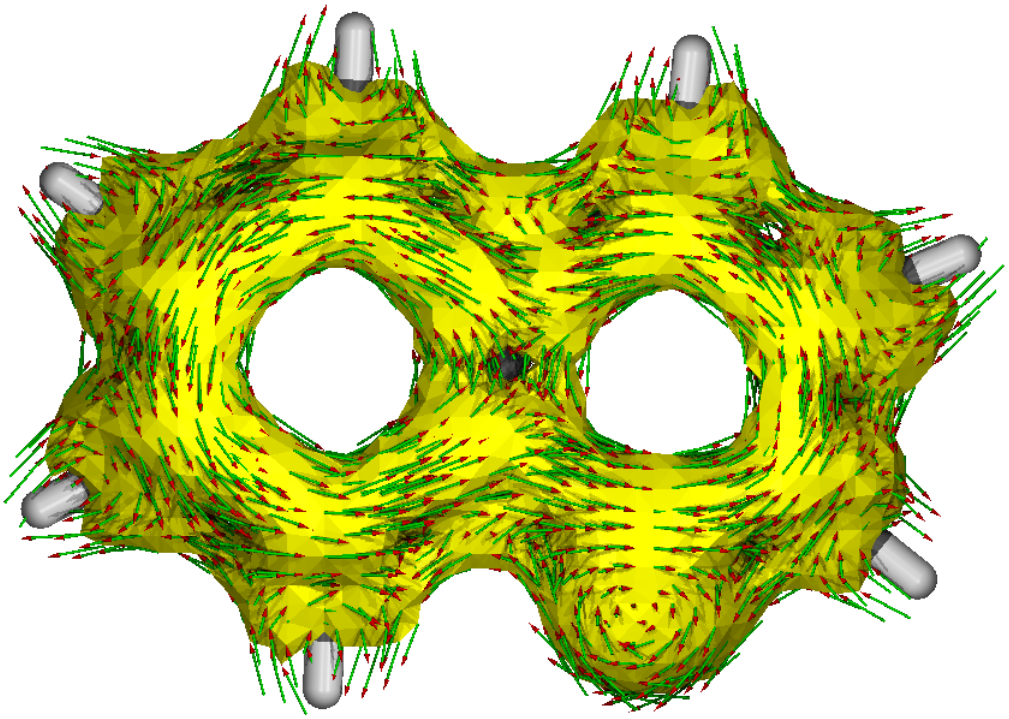

Figure S10. ACID plot of T_1 quinoline at an isosurface value of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

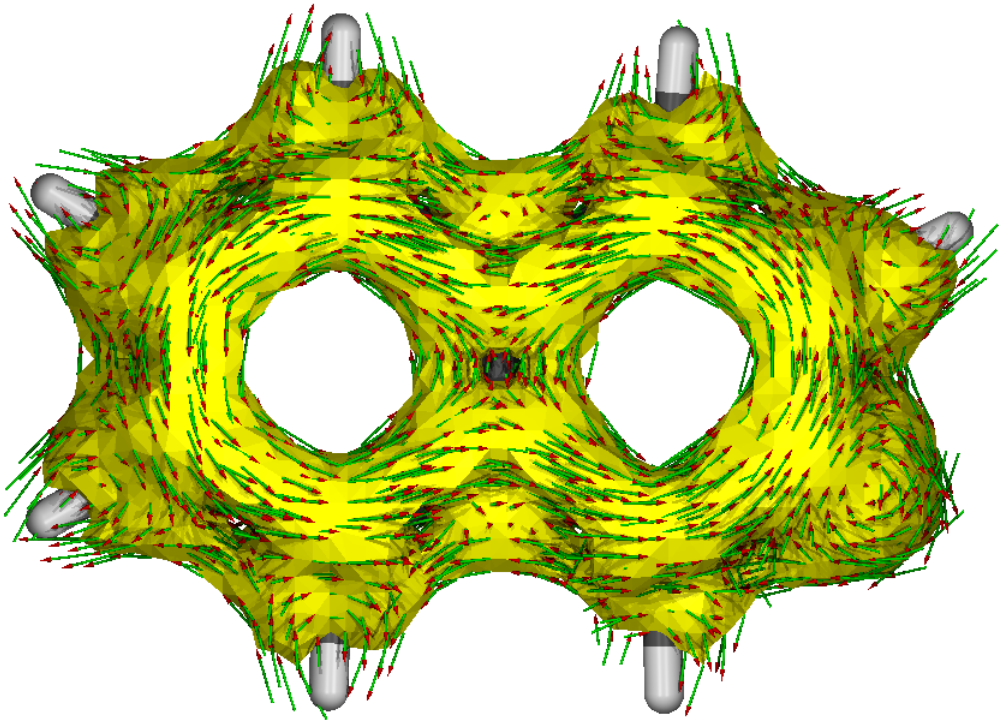

Figure S11. ACID plot of T_1 isoquinoline at an isosurface value of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

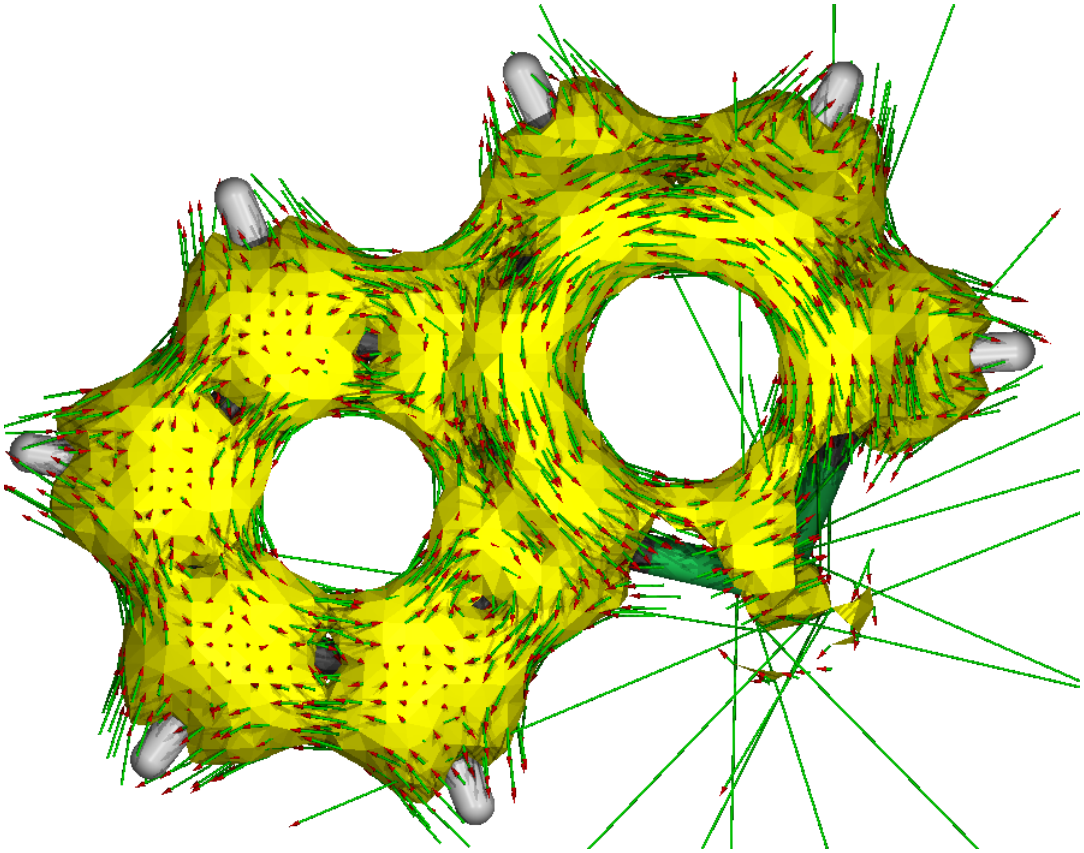

Figure S12. ACID plot of T_1 1-phosphanaphthalene at an isosurface value of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

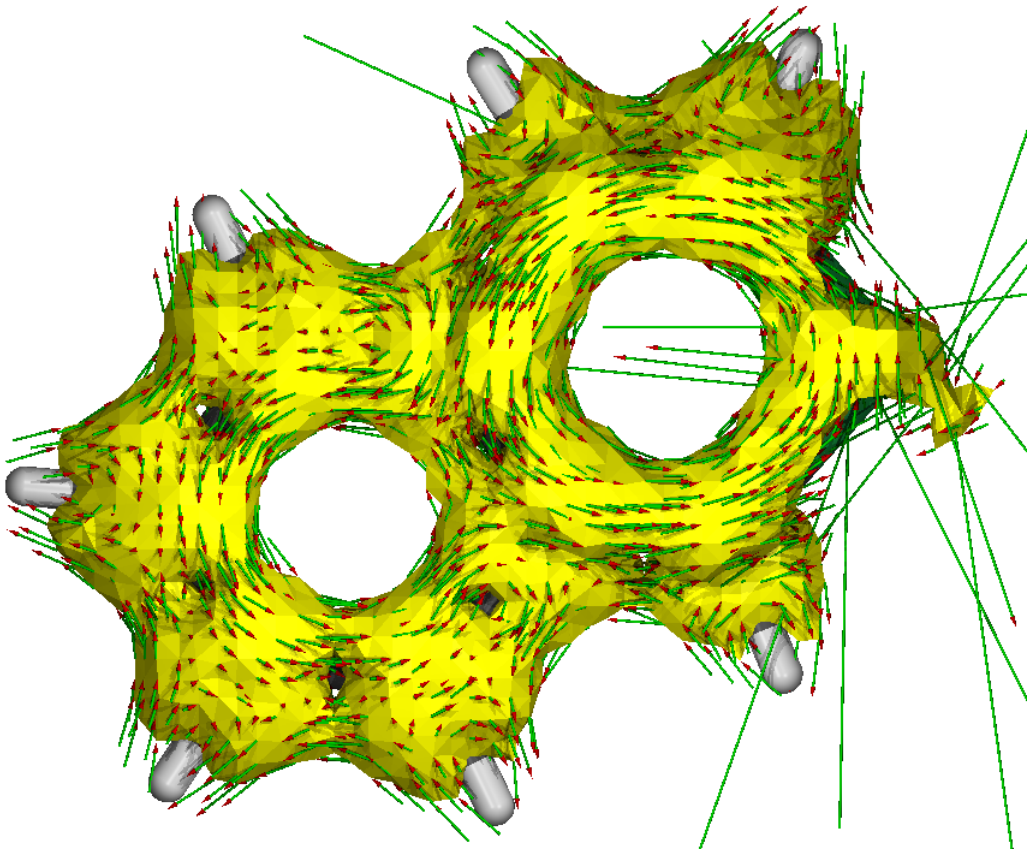

Figure S13. ACID plot of T_1 2-phosphanaphthalene at an isosurface value of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

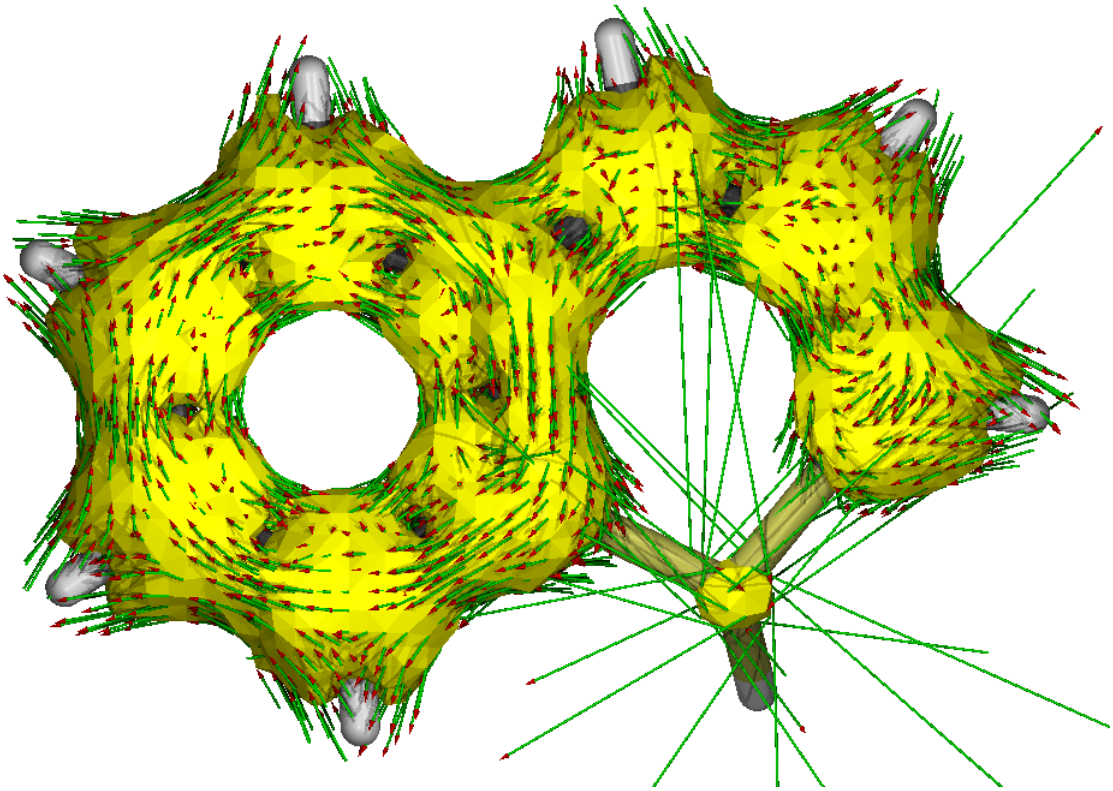

Figure S14. ACID plot of T_1 1-silanaphthalene at an isosurface value of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

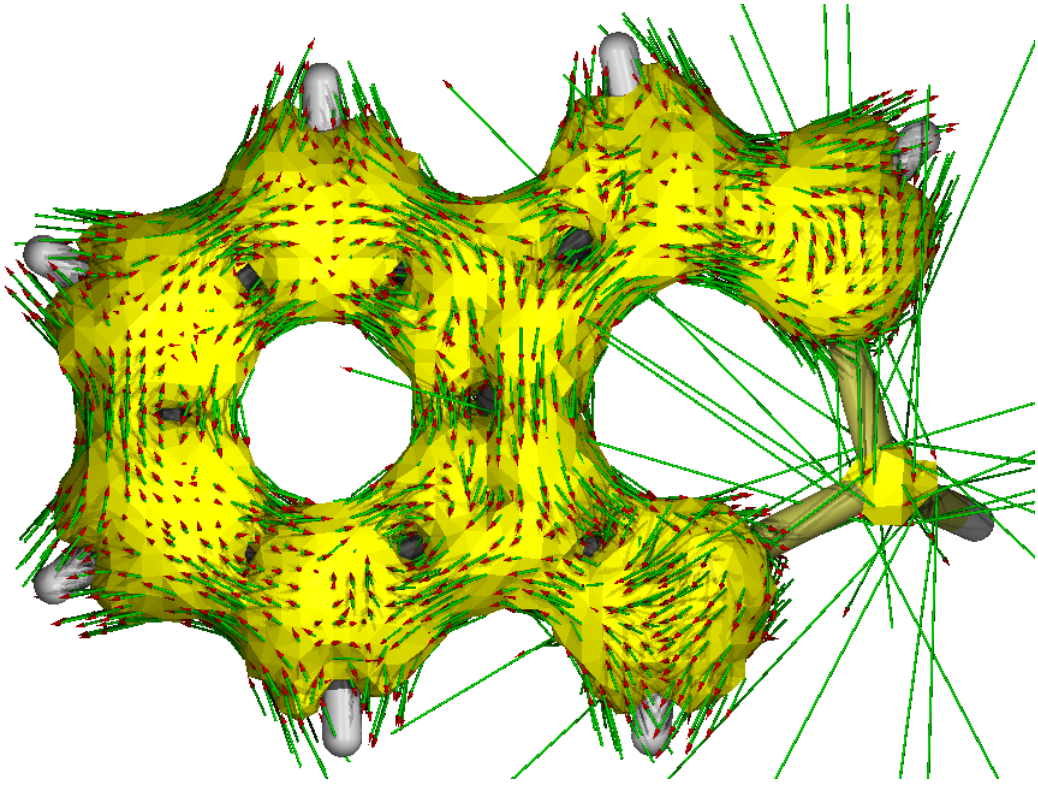

Figure S15. ACID plot of T_1 2-silanaphthalene at an isosurface value of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

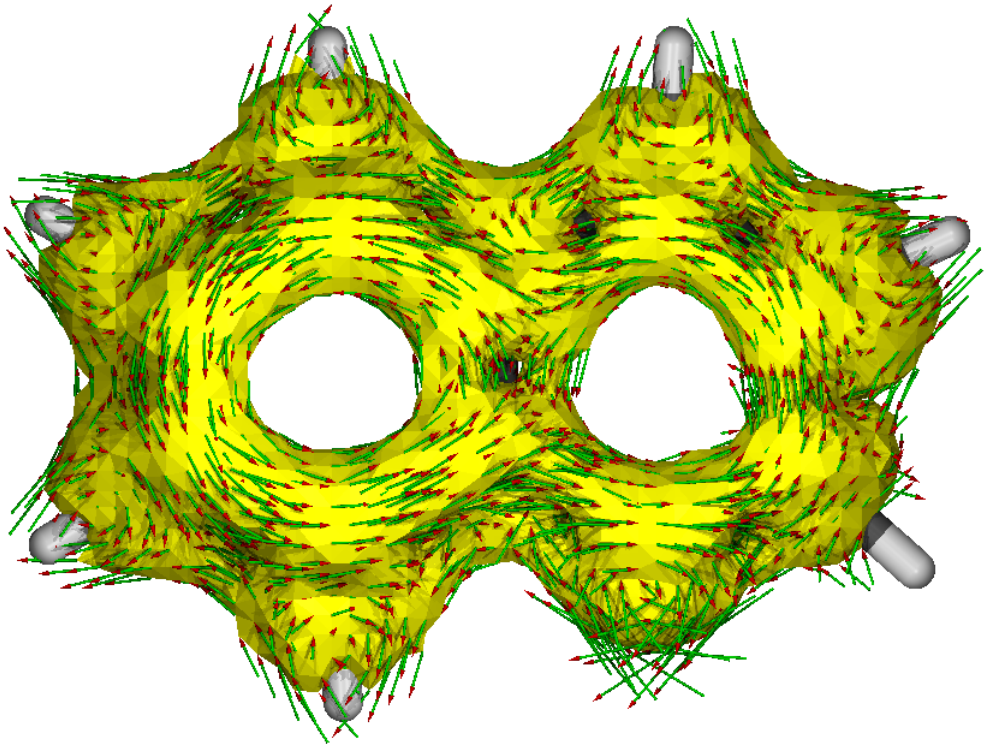

Figure S16. ACID plot of T_1 chromenylium ion at an isosurface value of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

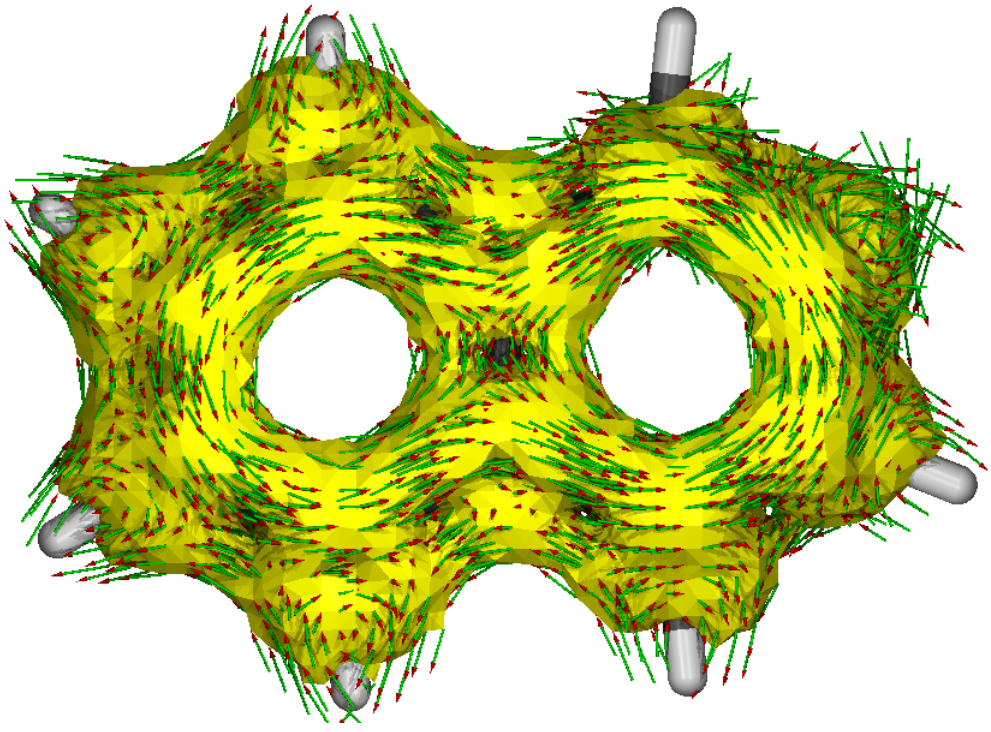

Figure S17. ACID plot of T_1 isochromenylium ion at an isosurface value of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

,

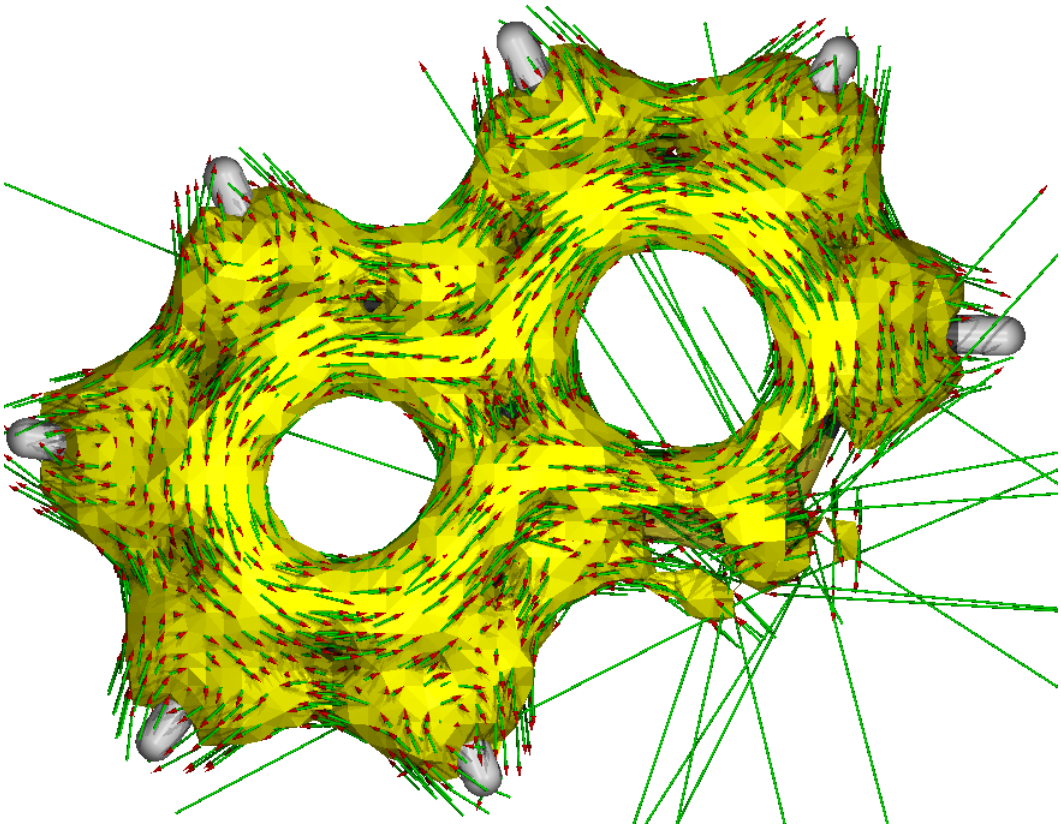

Figure S18. ACID plot of T_1 thiochromenylium ion at an isosurface value of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

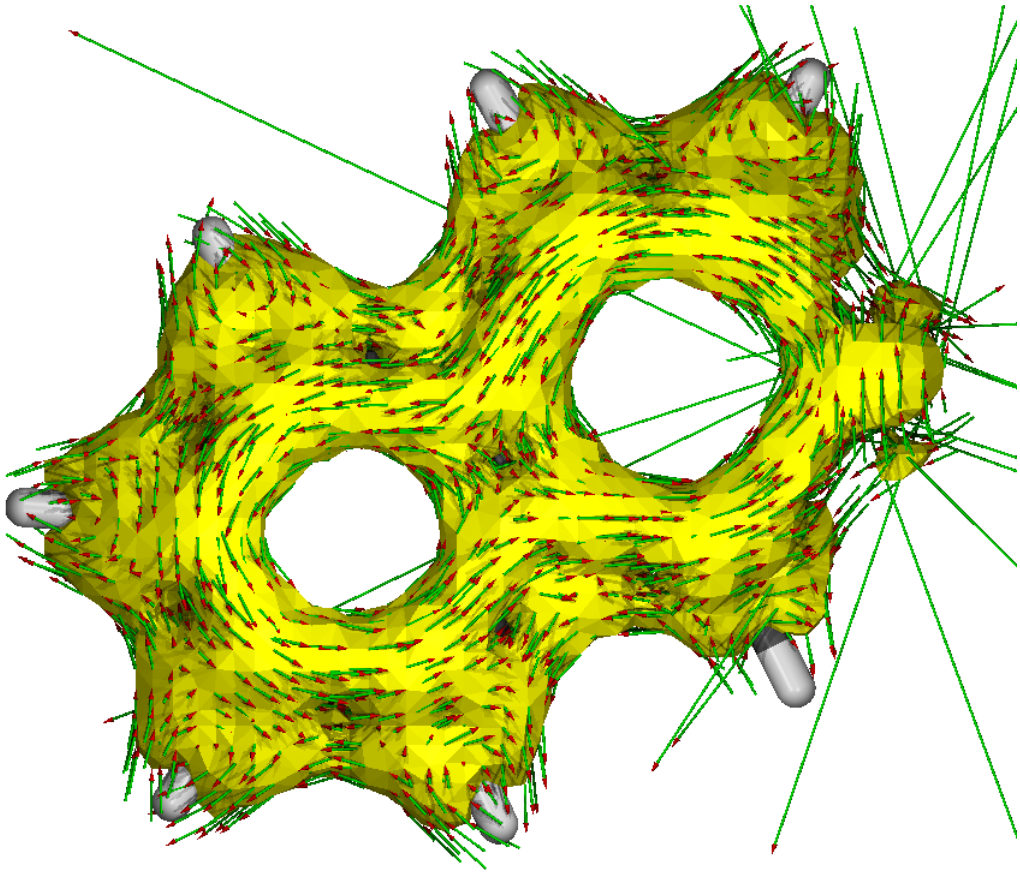

Figure S19. ACID plot of T_1 isothiochromenylium ion at an isosurface value of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

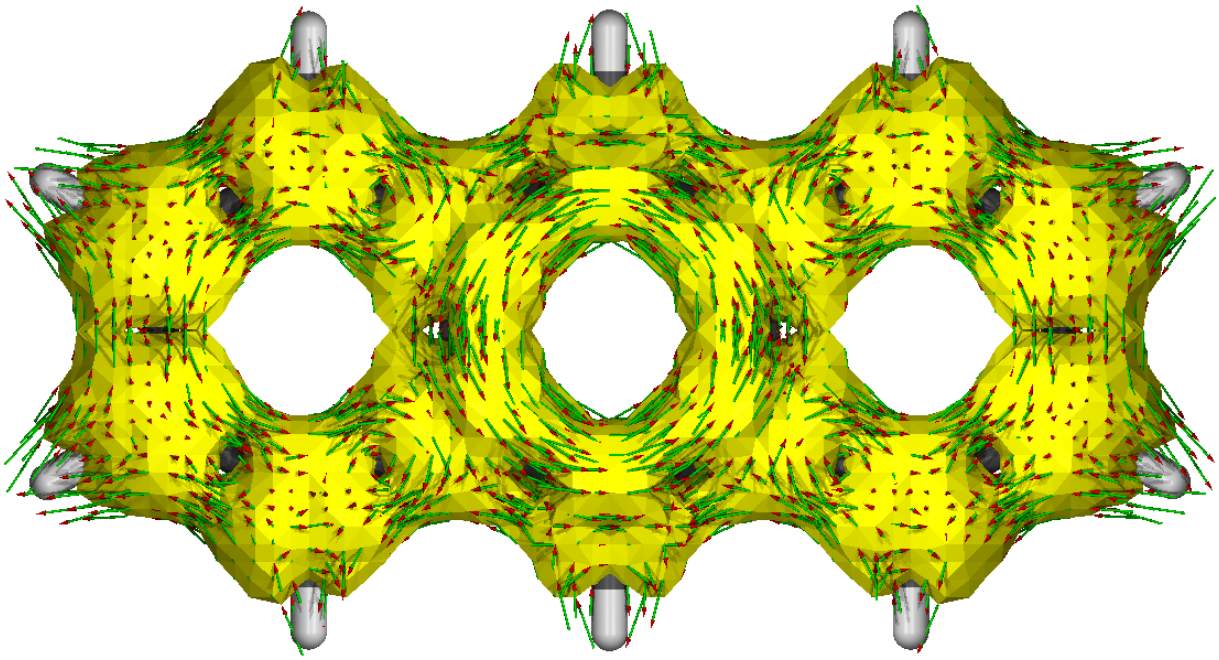

Figure S20. ACID plot of T_1 anthracene at an isosurface value of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

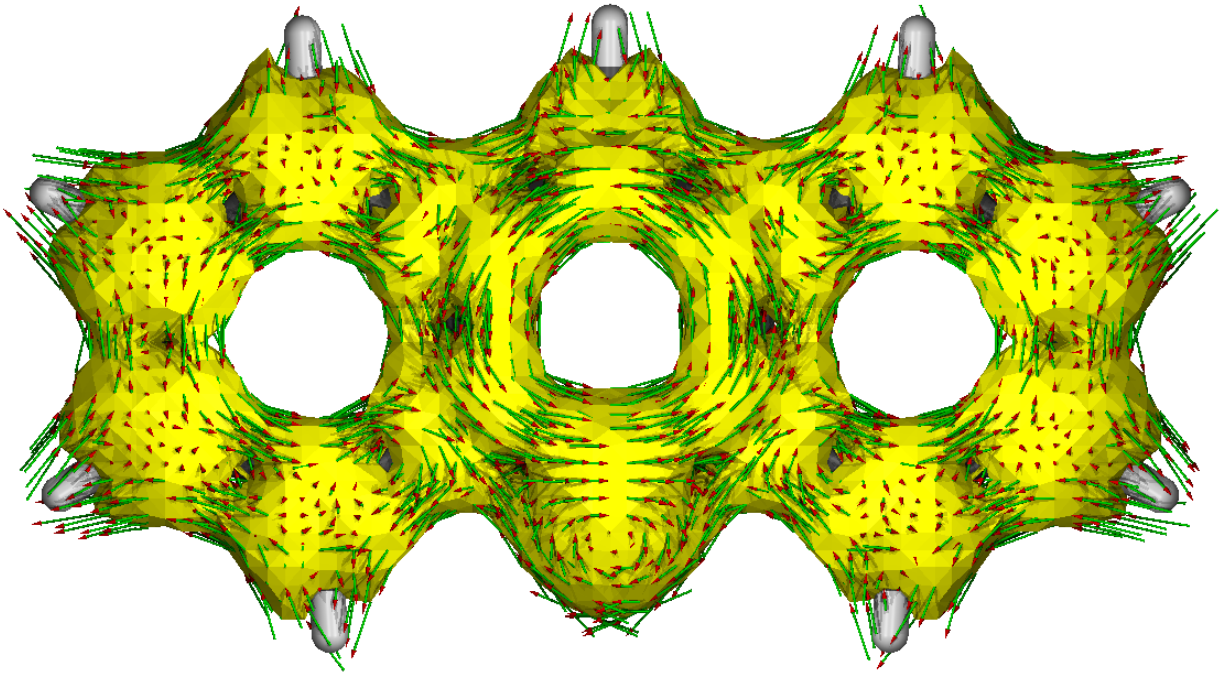

Figure S21. ACID plot of T_1 acridine at an isosurface value of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

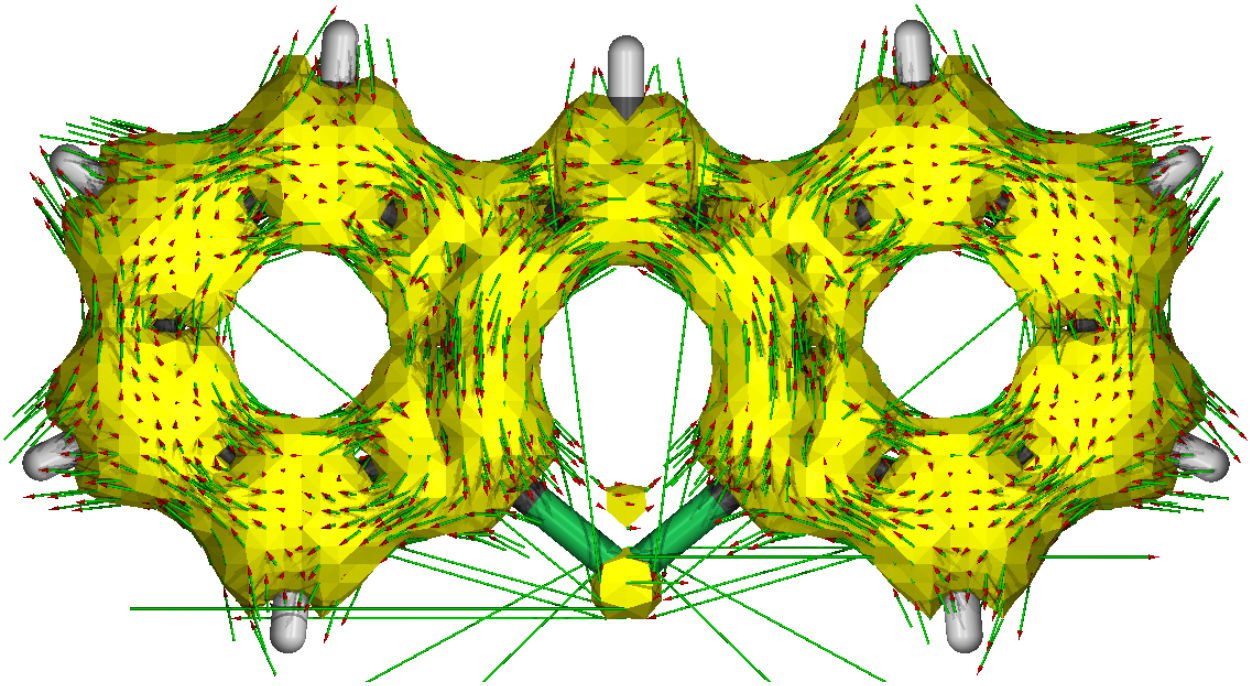

Figure S22. ACID plot of T_1 9-phosphaanthracene at an isosurface value of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

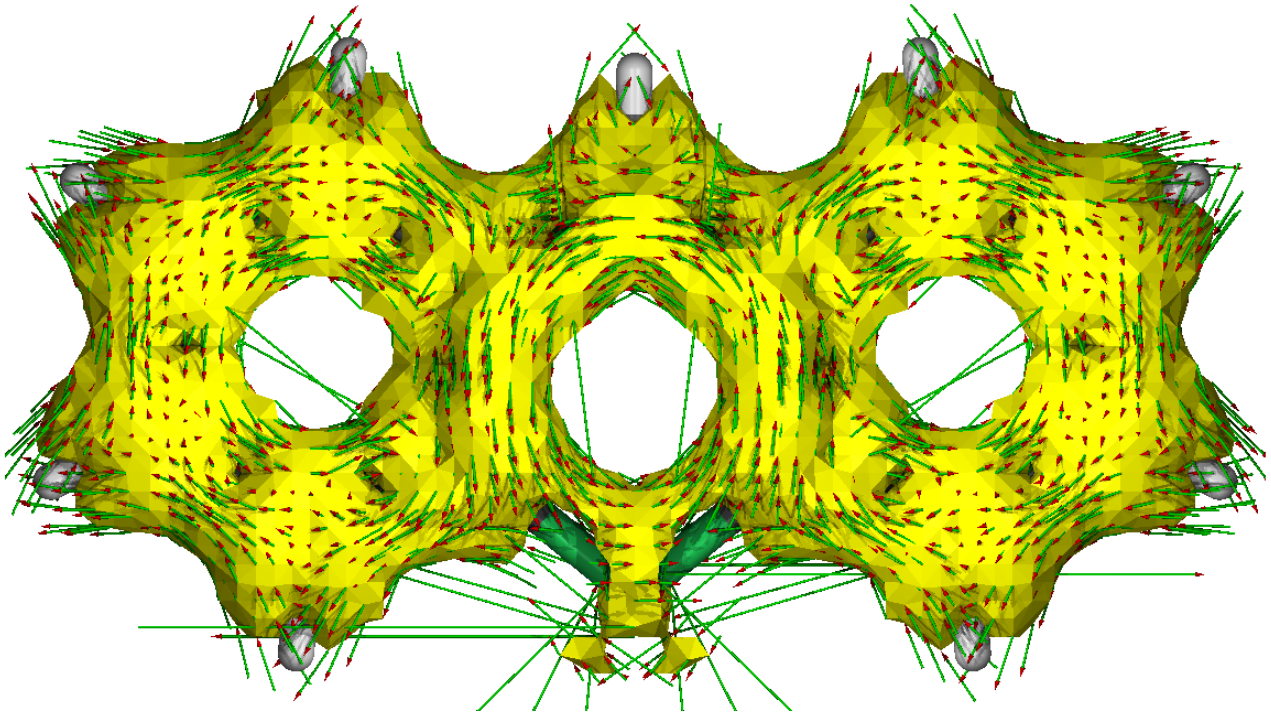

Figure S23. ACID plot of T_1 9-phosphaanthracene at an isosurface value of 0.04 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

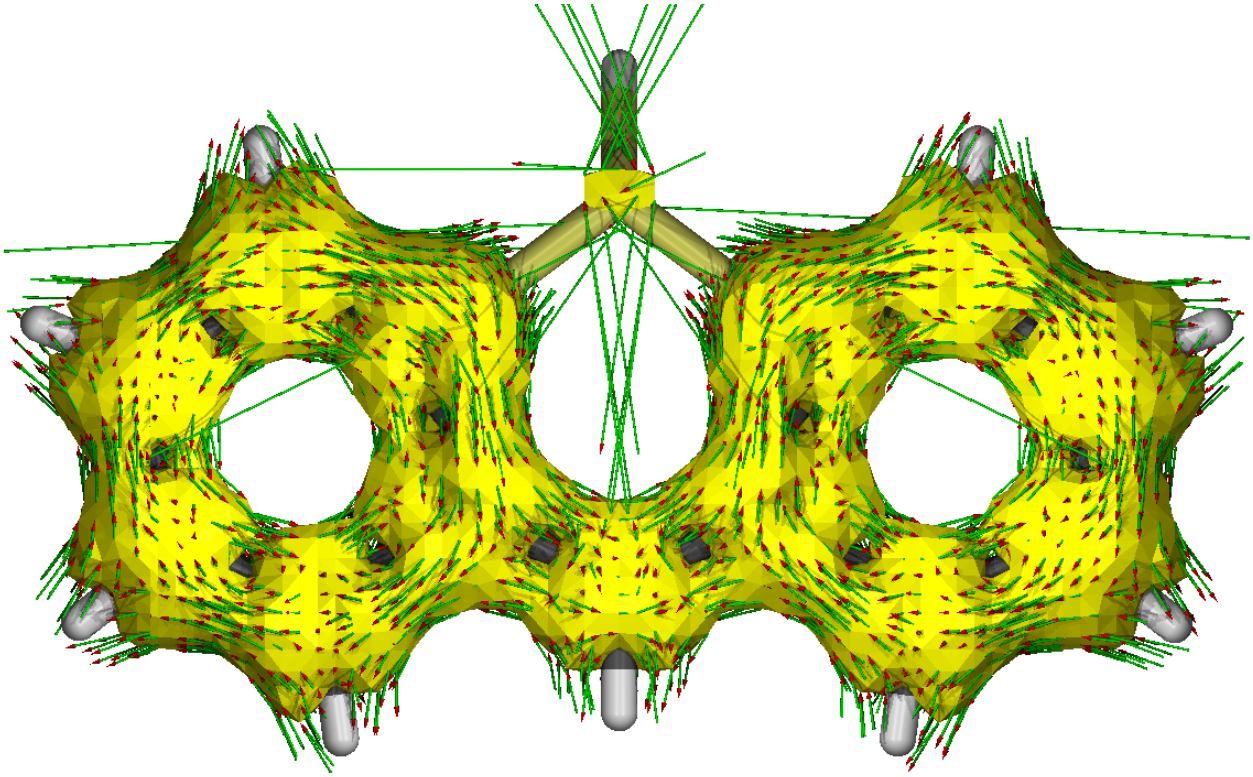

Figure S24. ACID plot of T_1 9-silaanthracene at an isosurface value of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

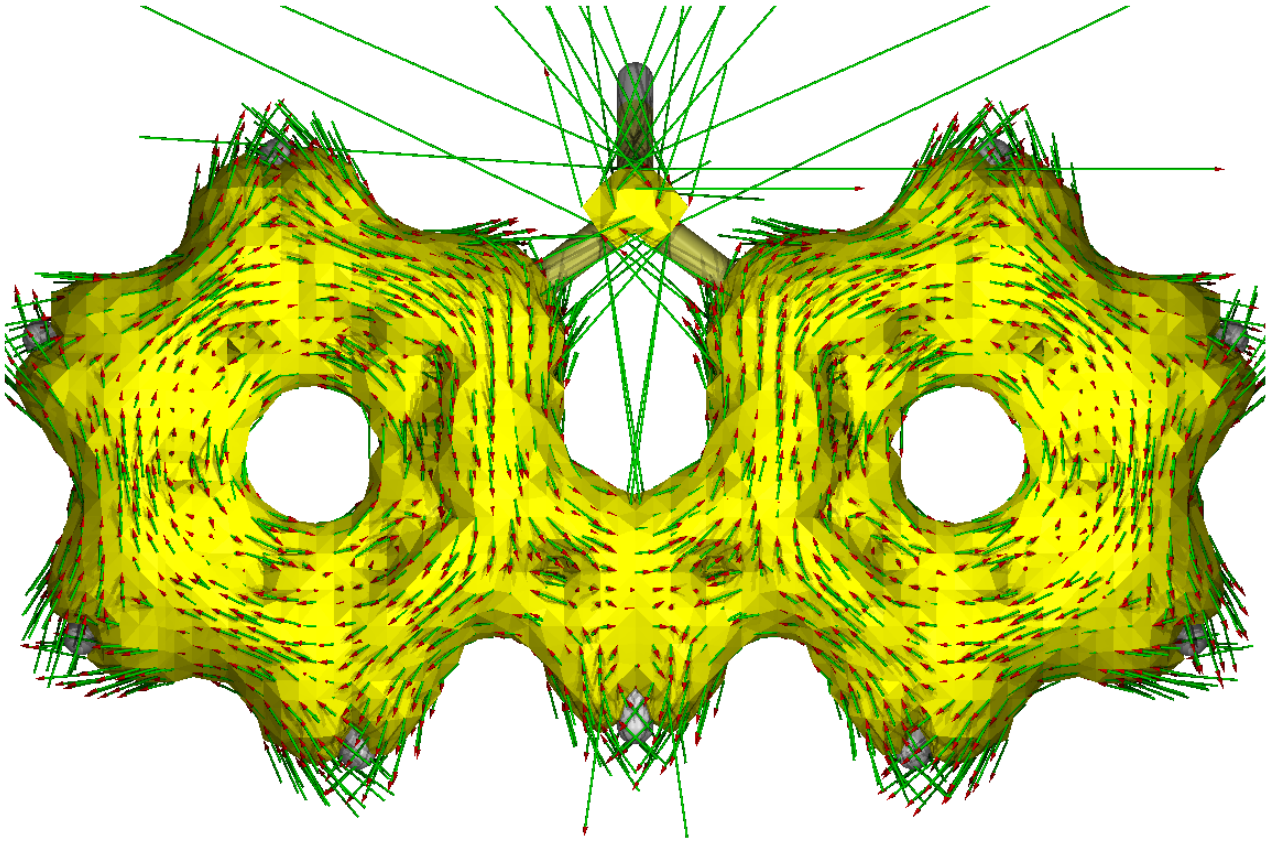

Figure S25. ACID plot of T_1 9-silaanthracene at an isosurface value of 0.03 a.u.. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

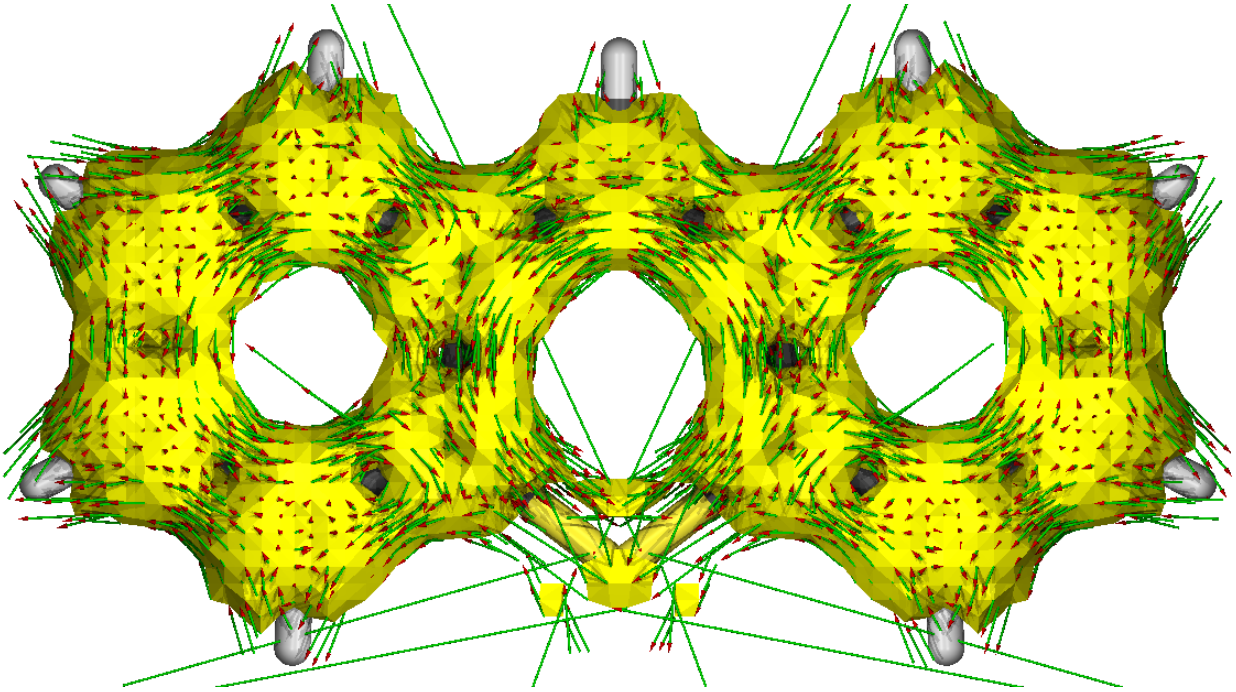

Figure S26. ACID plot of T_1 thioxanthylium ion at an isosurface value of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

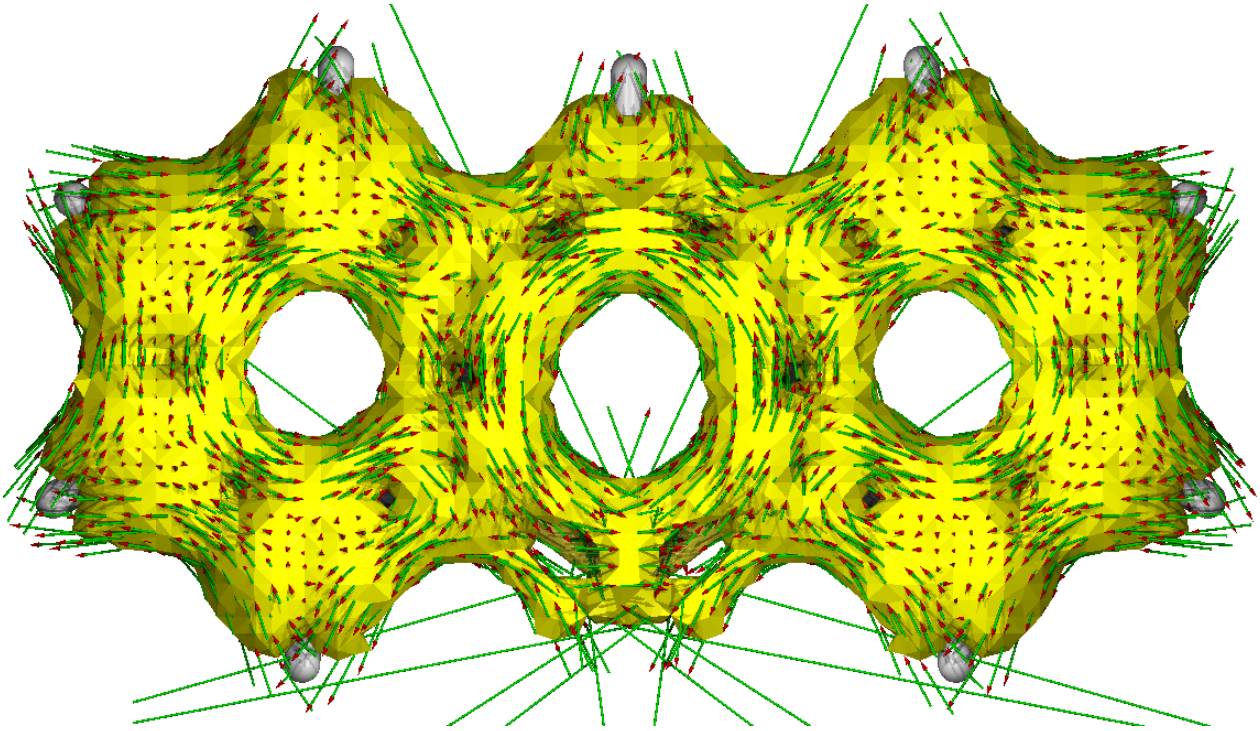

Figure S27. ACID plot of T_1 thioxanthylium ion at an isosurface value of 0.04 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

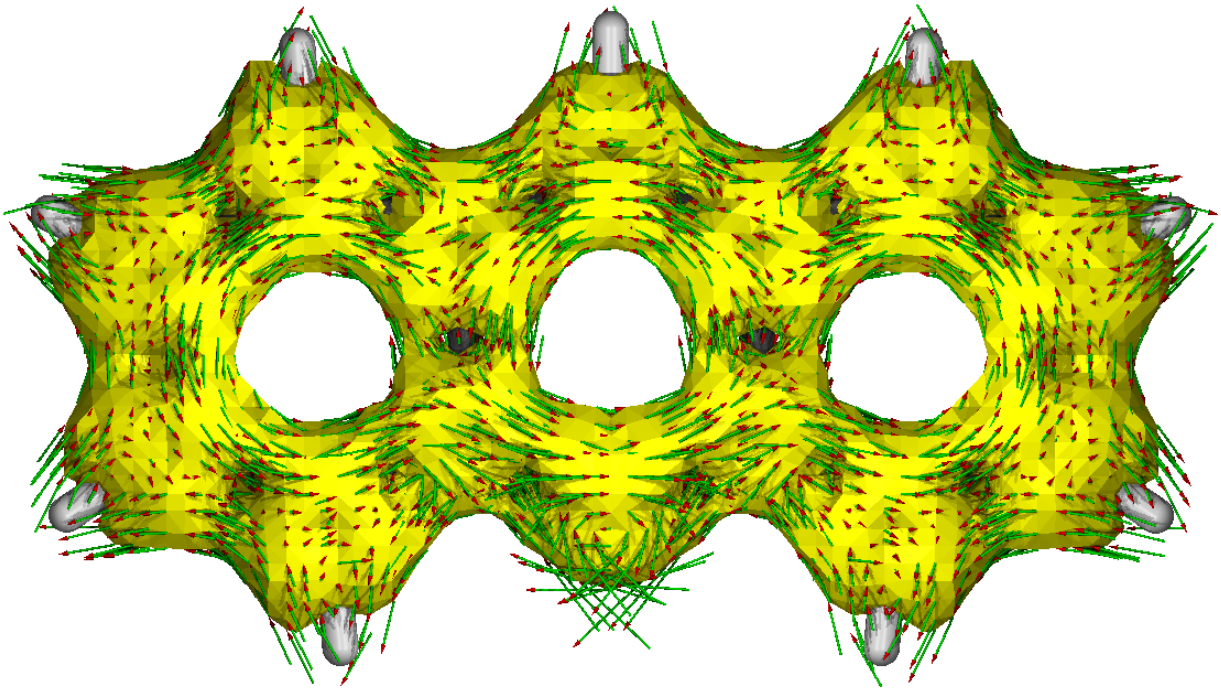

Figure S28. ACID plot of T_1 xanthylium ion at an isosurface value of 0.05 a.u. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

Absolute Energies and x, y, z Coordinates of 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

Pyridine S_0

E = -248.3512166 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.141638	0.721422
2	6	0	0.000000	1.196726	-0.671684
3	6	0	0.000000	0.000000	-1.382952
4	6	0	0.000000	-1.196726	-0.671684
5	6	0	0.000000	-1.141638	0.721422
6	7	0	0.000000	0.000000	1.416462
7	1	0	0.000000	0.000000	-2.467373
8	1	0	0.000000	2.057168	1.306729
9	1	0	0.000000	2.153679	-1.180237
10	1	0	0.000000	-2.153679	-1.180237
11	1	0	0.000000	-2.057168	1.306729

Pyridine T_1

E = -248.2175069 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.076027	-0.728864	1.196978
2	6	0	-0.076027	0.637213	1.227391
3	6	0	0.046814	1.360119	0.000000
4	6	0	-0.076027	0.637213	-1.227391
5	6	0	-0.076027	-0.728864	-1.196978
6	7	0	0.369474	-1.293265	0.000000
7	1	0	0.003602	2.440956	0.000000
8	1	0	-0.275993	-1.379946	2.038164
9	1	0	-0.247084	1.155443	2.164088
10	1	0	-0.247084	1.155443	-2.164088
11	1	0	-0.275993	-1.379946	-2.038164

Pyrylium ion S_0

E = -268.5421271 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.161805	0.681284
2	6	0	0.000000	1.208605	-0.690128
3	6	0	0.000000	0.000000	-1.393802
4	6	0	0.000000	-1.208605	-0.690128
5	6	0	0.000000	-1.161805	0.681284
6	1	0	0.000000	0.000000	-2.478036
7	1	0	0.000000	2.008928	1.354521
8	1	0	0.000000	2.168116	-1.190710
9	1	0	0.000000	-2.168116	-1.190710
10	1	0	0.000000	-2.008928	1.354521
11	8	0	0.000000	0.000000	1.327420

Pyrylium ion T_1

E = -268.4192919 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.050191	-0.701122	1.151469
2	6	0	0.050191	0.714733	1.180547
3	6	0	-0.029747	1.464033	0.000000
4	6	0	0.050191	0.714733	-1.180547
5	6	0	0.050191	-0.701122	-1.151469
6	1	0	-0.059823	2.543165	0.000000
7	1	0	0.241246	-1.340372	2.003149
8	1	0	0.144664	1.188436	2.152674
9	1	0	0.144664	1.188436	-2.152674
10	1	0	0.241246	-1.340372	-2.003149
11	8	0	-0.217263	-1.398353	0.000000

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

Phosphinine S_0

E = -534.9552778 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.335965	0.368049
2	6	0	0.000000	1.224803	-1.018210
3	6	0	0.000000	0.000000	-1.687164
4	6	0	0.000000	-1.224803	-1.018210
5	6	0	0.000000	-1.335965	0.368049
6	1	0	0.000000	0.000000	-2.771736
7	1	0	0.000000	2.332144	0.801292
8	1	0	0.000000	2.133808	-1.613501
9	1	0	0.000000	-2.133808	-1.613501
10	1	0	0.000000	-2.332144	0.801292
11	15	0	0.000000	0.000000	1.488071

Phosphinine T_1

E = -534.8535473 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.191464	-0.373195	1.387954
2	6	0	0.191464	0.977063	1.259780
3	6	0	0.035994	1.650436	0.000000
4	6	0	0.191464	0.977063	-1.259780
5	6	0	0.191464	-0.373195	-1.387954
6	1	0	-0.006099	2.733261	0.000000
7	1	0	0.401897	-0.842450	2.343073
8	1	0	0.384796	1.598242	2.131647
9	1	0	0.384796	1.598242	-2.131647
10	1	0	0.401897	-0.842450	-2.343073
11	15	0	-0.425226	-1.426259	0.000000

Thiopyrylium ion S_0

E = -591.5272925 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-1.331183	0.351397
2	6	0	0.000000	-1.229833	-1.024139
3	6	0	0.000000	0.000000	-1.689611
4	6	0	0.000000	1.229833	-1.024139
5	6	0	0.000000	1.331183	0.351397
6	1	0	0.000000	0.000000	-2.773759
7	1	0	0.000000	-2.289857	0.858378
8	1	0	0.000000	-2.147532	-1.601310
9	1	0	0.000000	2.147532	-1.601310
10	1	0	0.000000	2.289857	0.858378
11	16	0	0.000000	0.000000	1.404387

Thiopyrylium ion T_1

E = -591.4105558 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.506383	1.259931	-0.170624
2	6	0	-0.889124	1.287173	-0.080120
3	6	0	-1.728779	0.149383	0.142160
4	6	0	-1.208202	-1.112018	0.051430
5	6	0	0.182062	-1.343189	-0.224240
6	1	0	-2.783712	0.301904	0.325651
7	1	0	1.066993	2.165353	-0.378515
8	1	0	-1.356176	2.265507	-0.154639
9	1	0	-1.858036	-1.981912	0.109718
10	1	0	0.496235	-2.107389	-0.930697
11	16	0	1.453791	-0.130696	0.169803

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

Quinoline S_0

E = -402.0310543 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.445032	0.551568	0.000000
2	6	0	-1.321000	1.338394	0.000000
3	6	0	-0.044134	0.725023	0.000000
4	6	0	0.000000	-0.704675	0.000000
5	6	0	-2.290556	-0.856485	0.000000
6	1	0	1.133037	2.540232	0.000000
7	1	0	-3.438512	0.984068	0.000000
8	1	0	-1.394227	2.421377	0.000000
9	6	0	1.171993	1.455632	0.000000
10	6	0	1.262163	-1.352348	0.000000
11	1	0	-3.172836	-1.492476	0.000000
12	6	0	2.422682	-0.616406	0.000000
13	6	0	2.379032	0.799027	0.000000
14	1	0	1.272696	-2.435728	0.000000
15	1	0	3.383121	-1.119526	0.000000
16	1	0	3.304838	1.363034	0.000000
17	7	0	-1.128429	-1.471337	0.000000

Quinoline T_1

E = -401.9294179 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.499841	0.462174	0.000000
2	6	0	-1.354313	1.315961	0.000000
3	6	0	-0.076579	0.738934	0.000000
4	6	0	0.000000	-0.706741	0.000000
5	6	0	-2.320358	-0.890945	0.000000
6	1	0	1.082543	2.561518	0.000000
7	1	0	-3.498062	0.883417	0.000000
8	1	0	-1.467948	2.393890	0.000000
9	6	0	1.127650	1.477943	0.000000
10	6	0	1.287935	-1.318245	0.000000
11	1	0	-3.163814	-1.572325	0.000000
12	6	0	2.497378	-0.532987	0.000000
13	6	0	2.421857	0.822558	0.000000
14	1	0	1.326889	-2.400416	0.000000
15	1	0	3.455674	-1.038322	0.000000
16	1	0	3.317886	1.431746	0.000000
17	7	0	-1.079363	-1.495916	0.000000

Isoquinoline S_0

E = -402.0291583 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.420786	0.676921	0.000000
2	6	0	1.241625	1.382538	0.000000
3	6	0	0.000000	0.698479	0.000000
4	6	0	-0.018989	-0.727420	0.000000
5	6	0	1.214655	-1.428624	0.000000
6	6	0	2.404111	-0.739526	0.000000
7	1	0	-1.259556	2.462975	0.000000
8	1	0	3.370209	1.199911	0.000000
9	1	0	1.245619	2.467619	0.000000
10	6	0	-1.250332	1.374127	0.000000
11	6	0	-1.288235	-1.358034	0.000000
12	1	0	1.205362	-2.513392	0.000000
13	1	0	3.343095	-1.281762	0.000000
14	6	0	-2.425154	-0.587843	0.000000
15	1	0	-1.358544	-2.440351	0.000000
16	1	0	-3.407118	-1.050029	0.000000
17	7	0	-2.418551	0.773046	0.000000

Isoquinoline T_1

E = -401.9303076 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.476241	0.620926	0.000000
2	6	0	1.243653	1.368435	0.000000
3	6	0	0.000000	0.713045	0.000000
4	6	0	-0.022362	-0.731664	0.000000
5	6	0	1.198084	-1.436907	0.000000
6	6	0	2.457094	-0.741444	0.000000
7	1	0	-1.259160	2.474365	0.000000
8	1	0	3.416754	1.159535	0.000000
9	1	0	1.276192	2.451970	0.000000
10	6	0	-1.235924	1.390037	0.000000
11	6	0	-1.283051	-1.346933	0.000000
12	1	0	1.182522	-2.521035	0.000000
13	1	0	3.378450	-1.310999	0.000000
14	6	0	-2.476864	-0.532174	0.000000
15	1	0	-1.373273	-2.427200	0.000000
16	1	0	-3.446962	-1.024806	0.000000
17	7	0	-2.473678	0.768321	0.000000

Chromenylium ion S_0

E = -422.2396314 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.395244	-0.721585	0.000000
2	6	0	-1.199472	-1.434188	0.000000
3	6	0	0.030619	-0.754595	0.000000
4	6	0	0.000000	0.667344	0.000000
5	6	0	-2.339312	0.654889	0.000000
6	1	0	1.343958	-2.476013	0.000000
7	1	0	-3.358810	-1.212502	0.000000
8	1	0	-1.211934	-2.519019	0.000000
9	6	0	1.298794	-1.393509	0.000000
10	6	0	1.156997	1.441140	0.000000
11	1	0	-3.196367	1.316142	0.000000
12	6	0	2.371387	0.778966	0.000000
13	6	0	2.443823	-0.634291	0.000000
14	1	0	1.087090	2.521326	0.000000
15	1	0	3.288418	1.356041	0.000000
16	1	0	3.414044	-1.114997	0.000000
17	8	0	-1.196493	1.313000	0.000000

Chromenylium ion T_1

E = -422.1528952 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.448042	-0.619303	0.000000
2	6	0	-1.278281	-1.423210	0.000000
3	6	0	-0.027281	-0.771354	0.000000
4	6	0	0.000000	0.640609	0.000000
5	6	0	-2.358043	0.735131	0.000000
6	1	0	1.277404	-2.500132	0.000000
7	1	0	-3.432498	-1.069692	0.000000
8	1	0	-1.344506	-2.502478	0.000000
9	6	0	1.240900	-1.416643	0.000000
10	6	0	1.211624	1.370958	0.000000
11	1	0	-3.164310	1.450835	0.000000
12	6	0	2.466996	0.692801	0.000000
13	6	0	2.478489	-0.672038	0.000000
14	1	0	1.156961	2.453965	0.000000
15	1	0	3.382954	1.268177	0.000000
16	1	0	3.412208	-1.220877	0.000000
17	8	0	-1.125798	1.362313	0.000000

Isochromenylium ion S_0

E = -422.235895 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.406306	0.805140	0.000000
2	6	0	1.201510	1.459312	0.000000
3	6	0	0.000000	0.695460	0.000000
4	6	0	0.046862	-0.742837	0.000000
5	6	0	1.301380	-1.376499	0.000000
6	6	0	2.451933	-0.611831	0.000000
7	1	0	-1.415137	2.371134	0.000000
8	1	0	3.331942	1.367078	0.000000
9	1	0	1.150801	2.541795	0.000000
10	6	0	-1.247337	1.300591	0.000000
11	6	0	-1.194959	-1.439313	0.000000
12	1	0	1.358116	-2.458232	0.000000
13	1	0	3.417364	-1.104664	0.000000
14	6	0	-2.357369	-0.746816	0.000000
15	1	0	-1.227686	-2.521620	0.000000
16	1	0	-3.358429	-1.150699	0.000000
17	8	0	-2.363365	0.611995	0.000000

Isochromenylium ion T_1

E = -422.1527117 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.499586	0.579041	0.000000
2	6	0	1.294555	1.352774	0.000000
3	6	0	0.029437	0.719690	0.000000
4	6	0	0.000000	-0.717748	0.000000
5	6	0	1.210948	-1.447870	0.000000
6	6	0	2.468151	-0.795759	0.000000
7	1	0	-1.296683	2.491547	0.000000
8	1	0	3.447985	1.103623	0.000000
9	1	0	1.358889	2.434337	0.000000
10	6	0	-1.169018	1.421233	0.000000
11	6	0	-1.271513	-1.342022	0.000000
12	1	0	1.166112	-2.531844	0.000000
13	1	0	3.379990	-1.377338	0.000000
14	6	0	-2.411220	-0.565904	0.000000
15	1	0	-1.378378	-2.419277	0.000000
16	1	0	-3.416890	-0.968652	0.000000
17	8	0	-2.395823	0.755874	0.000000

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

Phosphinoline S_0

E = -688.6328577 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.794343	-1.735138	0.000000
2	6	0	-0.423832	-1.851721	0.000000
3	6	0	0.471905	-0.747596	0.000000
4	6	0	0.000000	0.603411	0.000000
5	6	0	-2.467906	-0.497684	0.000000
6	1	0	2.231818	-2.003298	0.000000
7	1	0	-2.387602	-2.644991	0.000000
8	1	0	0.013580	-2.845204	0.000000
9	6	0	1.875624	-0.978205	0.000000
10	6	0	0.953142	1.655224	0.000000
11	1	0	-3.554041	-0.511897	0.000000
12	6	0	2.305018	1.397807	0.000000
13	6	0	2.770260	0.064532	0.000000
14	1	0	0.597790	2.680903	0.000000
15	1	0	3.015018	2.217083	0.000000
16	1	0	3.836180	-0.133690	0.000000
17	15	0	-1.726130	1.051821	0.000000

Phosphinoline T_1

E = -688.5551304 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.765753	-1.821992	0.000000
2	6	0	-0.335139	-1.871886	0.000000
3	6	0	0.520006	-0.722484	0.000000
4	6	0	0.000000	0.611543	0.000000
5	6	0	-2.496234	-0.680508	0.000000
6	1	0	2.316830	-1.900704	0.000000
7	1	0	-2.286373	-2.776675	0.000000
8	1	0	0.140069	-2.846466	0.000000
9	6	0	1.914698	-0.892715	0.000000
10	6	0	0.888732	1.680023	0.000000
11	1	0	-3.579924	-0.736317	0.000000
12	6	0	2.288826	1.486775	0.000000
13	6	0	2.794512	0.202066	0.000000
14	1	0	0.498215	2.693247	0.000000
15	1	0	2.951471	2.344255	0.000000
16	1	0	3.864955	0.031110	0.000000
17	15	0	-1.784209	1.016441	0.000000

Isophosphinoline S_0

E = -688.6327594 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.206981	1.756742	0.000000
2	6	0	0.838526	1.867847	0.000000
3	6	0	0.000000	0.716151	0.000000
4	6	0	0.620704	-0.575835	0.000000
5	6	0	2.038284	-0.652478	0.000000
6	6	0	2.815965	0.480531	0.000000
7	1	0	-1.794719	1.876992	0.000000
8	1	0	2.825046	2.647494	0.000000
9	1	0	0.369707	2.846068	0.000000
10	6	0	-1.410132	0.860000	0.000000
11	6	0	-0.155400	-1.769104	0.000000
12	1	0	2.502790	-1.633043	0.000000
13	1	0	3.896941	0.399585	0.000000
14	6	0	-1.524480	-1.808814	0.000000
15	1	0	0.395762	-2.706942	0.000000
16	1	0	-2.012313	-2.779153	0.000000
17	15	0	-2.584393	-0.393416	0.000000

Isophosphinoline T_1

E = -688.5466139 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.235467	1.802619	0.000000
2	6	0	0.837907	1.902600	0.000000
3	6	0	0.000000	0.750334	0.000000
4	6	0	0.645528	-0.542434	0.000000
5	6	0	2.024622	-0.609042	0.000000
6	6	0	2.838715	0.560211	0.000000
7	1	0	-1.808923	1.883472	0.000000
8	1	0	2.836811	2.704740	0.000000
9	1	0	0.368165	2.880129	0.000000
10	6	0	-1.392868	0.880291	0.000000
11	6	0	-0.139728	-1.772455	0.000000
12	1	0	2.503381	-1.583067	0.000000
13	1	0	3.917623	0.464853	0.000000
14	6	0	-1.508644	-1.849758	0.000000
15	1	0	0.433073	-2.696646	0.000000
16	1	0	-1.957623	-2.839488	0.000000
17	15	0	-2.635900	-0.503213	0.000000

Thiochromenylium ion S_0

E = -745.2197693 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.700105	-1.823091	0.000000
2	6	0	-0.311692	-1.866852	0.000000
3	6	0	0.528920	-0.734144	0.000000
4	6	0	0.000000	0.595809	0.000000
5	6	0	-2.405027	-0.632414	0.000000
6	1	0	2.354360	-1.891303	0.000000
7	1	0	-2.263159	-2.748648	0.000000
8	1	0	0.167016	-2.840595	0.000000
9	6	0	1.942339	-0.888988	0.000000
10	6	0	0.855313	1.708639	0.000000
11	1	0	-3.489580	-0.613892	0.000000
12	6	0	2.222322	1.509691	0.000000
13	6	0	2.768469	0.208363	0.000000
14	1	0	0.447116	2.712605	0.000000
15	1	0	2.883689	2.367941	0.000000
16	1	0	3.843718	0.079694	0.000000
17	16	0	-1.709149	0.904507	0.000000

Thiochromenylium ion T_1

E = -745.1401746 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.720579	-1.831755	0.000000
2	6	0	-0.299557	-1.902460	0.000000
3	6	0	0.525560	-0.750840	0.000000
4	6	0	0.000000	0.569610	0.000000
5	6	0	-2.445346	-0.679264	0.000000
6	1	0	2.377658	-1.854334	0.000000
7	1	0	-2.275985	-2.764094	0.000000
8	1	0	0.170270	-2.877174	0.000000
9	6	0	1.937840	-0.863185	0.000000
10	6	0	0.851749	1.688025	0.000000
11	1	0	-3.526404	-0.648587	0.000000
12	6	0	2.264272	1.538747	0.000000
13	6	0	2.795281	0.274546	0.000000
14	1	0	0.423651	2.685393	0.000000
15	1	0	2.894489	2.418308	0.000000
16	1	0	3.868030	0.124188	0.000000
17	16	0	-1.711689	0.915985	0.000000

Isothiochromenylium ion S_0

E = -745.21877 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.146118	1.850082	0.000000
2	6	0	0.776918	1.917141	0.000000
3	6	0	0.000000	0.720878	0.000000
4	6	0	0.666661	-0.559066	0.000000
5	6	0	2.076107	-0.582366	0.000000
6	6	0	2.797008	0.593506	0.000000
7	1	0	-1.881060	1.781477	0.000000
8	1	0	2.735524	2.758683	0.000000
9	1	0	0.269430	2.874603	0.000000
10	6	0	-1.392048	0.812625	0.000000
11	6	0	-0.074448	-1.774991	0.000000
12	1	0	2.588716	-1.536915	0.000000
13	1	0	3.880104	0.557414	0.000000
14	6	0	-1.432921	-1.853063	0.000000
15	1	0	0.481664	-2.706785	0.000000
16	1	0	-1.964780	-2.796396	0.000000
17	16	0	-2.468123	-0.480035	0.000000

Isothiochromenylium ion T_1

E = -745.1394644 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.252355	1.789604	0.000000
2	6	0	0.833122	1.888928	0.000000
3	6	0	0.000000	0.735692	0.000000
4	6	0	0.653068	-0.544001	0.000000
5	6	0	2.062518	-0.603213	0.000000
6	6	0	2.870796	0.562471	0.000000
7	1	0	-1.872097	1.839603	0.000000
8	1	0	2.837974	2.701379	0.000000
9	1	0	0.373305	2.870332	0.000000
10	6	0	-1.387923	0.872361	0.000000
11	6	0	-0.097900	-1.753613	0.000000
12	1	0	2.538969	-1.578124	0.000000
13	1	0	3.948820	0.473661	0.000000
14	6	0	-1.473334	-1.816292	0.000000
15	1	0	0.441493	-2.695003	0.000000
16	1	0	-1.983480	-2.773270	0.000000
17	16	0	-2.535075	-0.476887	0.000000

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

Acridine S_0

E = -555.7047893 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-3.582838	0.767687
2	6	0	0.000000	-2.383389	1.424361
3	6	0	0.000000	-1.153809	0.695972
4	6	0	0.000000	-1.210179	-0.746749
5	6	0	0.000000	-2.483668	-1.392118
6	6	0	0.000000	-3.636206	-0.656655
7	6	0	0.000000	0.000000	-1.441813
8	6	0	0.000000	1.210179	-0.746749
9	6	0	0.000000	1.153809	0.695972
10	6	0	0.000000	2.383389	1.424361
11	1	0	0.000000	2.323218	2.506026
12	6	0	0.000000	3.582838	0.767687
13	6	0	0.000000	3.636206	-0.656655
14	6	0	0.000000	2.483668	-1.392118
15	1	0	0.000000	-4.508977	1.331662
16	1	0	0.000000	-2.323218	2.506026
17	1	0	0.000000	-2.518335	-2.476779
18	1	0	0.000000	-4.599791	-1.153249
19	1	0	0.000000	0.000000	-2.528274
20	1	0	0.000000	4.508977	1.331662
21	1	0	0.000000	4.599791	-1.153249
22	1	0	0.000000	2.518335	-2.476779
23	7	0	0.000000	0.000000	1.379124

Acridine T_1

E = -555.6340314 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-3.625069	0.757351
2	6	0	0.000000	-2.374098	1.410643
3	6	0	0.000000	-1.176734	0.685429
4	6	0	0.000000	-1.233009	-0.754606
5	6	0	0.000000	-2.483019	-1.377172
6	6	0	0.000000	-3.678608	-0.622168
7	6	0	0.000000	0.000000	-1.466896
8	6	0	0.000000	1.233009	-0.754606
9	6	0	0.000000	1.176734	0.685429
10	6	0	0.000000	2.374098	1.410643
11	1	0	0.000000	2.307839	2.492098
12	6	0	0.000000	3.625069	0.757351
13	6	0	0.000000	3.678608	-0.622168
14	6	0	0.000000	2.483019	-1.377172
15	1	0	0.000000	-4.536744	1.343019
16	1	0	0.000000	-2.307839	2.492098
17	1	0	0.000000	-2.533595	-2.461205
18	1	0	0.000000	-4.633525	-1.134823
19	1	0	0.000000	0.000000	-2.551493
20	1	0	0.000000	4.536744	1.343019
21	1	0	0.000000	4.633525	-1.134823
22	1	0	0.000000	2.533595	-2.461205
23	7	0	0.000000	0.000000	1.382996

Xanthylium ion S_0

E = -575.932669 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	3.559598	0.761806
2	6	0	0.000000	2.345761	1.424123
3	6	0	0.000000	1.179743	0.660122
4	6	0	0.000000	1.217715	-0.764592
5	6	0	0.000000	2.489530	-1.404963
6	6	0	0.000000	3.635556	-0.651950
7	6	0	0.000000	0.000000	-1.452792
8	6	0	0.000000	-1.217715	-0.764592
9	6	0	0.000000	-1.179743	0.660122
10	6	0	0.000000	-2.345761	1.424123
11	1	0	0.000000	-2.279720	2.504449
12	6	0	0.000000	-3.559598	0.761806
13	6	0	0.000000	-3.635556	-0.651950
14	6	0	0.000000	-2.489530	-1.404963
15	1	0	0.000000	4.475975	1.340273
16	1	0	0.000000	2.279720	2.504449
17	1	0	0.000000	2.530482	-2.487842
18	1	0	0.000000	4.605537	-1.132672
19	1	0	0.000000	0.000000	-2.538773
20	1	0	0.000000	-4.475975	1.340273
21	1	0	0.000000	-4.605537	-1.132672
22	1	0	0.000000	-2.530482	-2.487842
23	8	0	0.000000	0.000000	1.314068

Xanthylium ion T_1

E = -575.8611094 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-3.593739	0.797069
2	6	0	0.000000	-2.336162	1.413973
3	6	0	0.000000	-1.184921	0.620465
4	6	0	0.000000	-1.224538	-0.799052
5	6	0	0.000000	-2.498888	-1.382539
6	6	0	0.000000	-3.670187	-0.587950
7	6	0	0.000000	0.000000	-1.521920
8	6	0	0.000000	1.224538	-0.799052
9	6	0	0.000000	1.184921	0.620465
10	6	0	0.000000	2.336162	1.413973
11	1	0	0.000000	2.230010	2.492159
12	6	0	0.000000	3.593739	0.797069
13	6	0	0.000000	3.670187	-0.587950
14	6	0	0.000000	2.498888	-1.382539
15	1	0	0.000000	-4.491096	1.401512
16	1	0	0.000000	-2.230010	2.492159
17	1	0	0.000000	-2.586311	-2.462770
18	1	0	0.000000	-4.636208	-1.078190
19	1	0	0.000000	0.000000	-2.604041
20	1	0	0.000000	4.491096	1.401512
21	1	0	0.000000	4.636208	-1.078190
22	1	0	0.000000	2.586311	-2.462770
23	8	0	0.000000	0.000000	1.285817

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

9-Phosphaanthracene S_0

E = -842.3040281 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	3.798226	0.426040
2	6	0	0.000000	2.675932	1.211513
3	6	0	0.000000	1.366531	0.642807
4	6	0	0.000000	1.246358	-0.792683
5	6	0	0.000000	2.444975	-1.576555
6	6	0	0.000000	3.679773	-0.989942
7	6	0	0.000000	0.000000	-1.431828
8	6	0	0.000000	-1.246358	-0.792683
9	6	0	0.000000	-1.366531	0.642807
10	6	0	0.000000	-2.675932	1.211513
11	1	0	0.000000	-2.771190	2.292674
12	6	0	0.000000	-3.798226	0.426040
13	6	0	0.000000	-3.679773	-0.989942
14	6	0	0.000000	-2.444975	-1.576555
15	1	0	0.000000	4.781646	0.882267
16	1	0	0.000000	2.771190	2.292674
17	1	0	0.000000	2.351819	-2.657672
18	1	0	0.000000	4.574125	-1.602733
19	1	0	0.000000	0.000000	-2.518181
20	1	0	0.000000	-4.781646	0.882267
21	1	0	0.000000	-4.574125	-1.602733
22	1	0	0.000000	-2.351819	-2.657672
23	15	0	0.000000	0.000000	1.748395

9-Phosphaanthracene T_1

E = -842.2540693 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	3.844104	0.396454
2	6	0	0.000000	2.686301	1.194273
3	6	0	0.000000	1.411061	0.634448
4	6	0	0.000000	1.275619	-0.788798
5	6	0	0.000000	2.448023	-1.568133
6	6	0	0.000000	3.718434	-0.984492
7	6	0	0.000000	0.000000	-1.433521
8	6	0	0.000000	-1.275619	-0.788798
9	6	0	0.000000	-1.411061	0.634448
10	6	0	0.000000	-2.686301	1.194273
11	1	0	0.000000	-2.789712	2.275166
12	6	0	0.000000	-3.844104	0.396454
13	6	0	0.000000	-3.718434	-0.984492
14	6	0	0.000000	-2.448023	-1.568133
15	1	0	0.000000	4.822300	0.862781
16	1	0	0.000000	2.789712	2.275166
17	1	0	0.000000	2.355566	-2.649422
18	1	0	0.000000	4.599883	-1.615652
19	1	0	0.000000	0.000000	-2.518952
20	1	0	0.000000	-4.822300	0.862781
21	1	0	0.000000	-4.599883	-1.615652
22	1	0	0.000000	-2.355566	-2.649422
23	15	0	0.000000	0.000000	1.784619

Thioxanthylium ion S_0

E = -898.9075673 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	3.772531	0.422308
2	6	0	0.000000	2.643270	1.217456
3	6	0	0.000000	1.373180	0.618314
4	6	0	0.000000	1.250083	-0.807364
5	6	0	0.000000	2.444913	-1.587871
6	6	0	0.000000	3.676810	-0.987297
7	6	0	0.000000	0.000000	-1.440161
8	6	0	0.000000	-1.250083	-0.807364
9	6	0	0.000000	-1.373180	0.618314
10	6	0	0.000000	-2.643270	1.217456
11	1	0	0.000000	-2.735132	2.297210
12	6	0	0.000000	-3.772531	0.422308
13	6	0	0.000000	-3.676810	-0.987297
14	6	0	0.000000	-2.444913	-1.587871
15	1	0	0.000000	4.749528	0.891120
16	1	0	0.000000	2.735132	2.297210
17	1	0	0.000000	2.355779	-2.668045
18	1	0	0.000000	4.578484	-1.586592
19	1	0	0.000000	0.000000	-2.526248
20	1	0	0.000000	-4.749528	0.891120
21	1	0	0.000000	-4.578484	-1.586592
22	1	0	0.000000	-2.355779	-2.668045
23	16	0	0.000000	0.000000	1.674579

Thioxanthylium ion T_1

E = -898.8460121 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	3.810175	0.453918
2	6	0	0.000000	2.636568	1.215550
3	6	0	0.000000	1.384886	0.583952
4	6	0	0.000000	1.260918	-0.835395
5	6	0	0.000000	2.461487	-1.565460
6	6	0	0.000000	3.716288	-0.930665
7	6	0	0.000000	0.000000	-1.497451
8	6	0	0.000000	-1.260918	-0.835395
9	6	0	0.000000	-1.384886	0.583952
10	6	0	0.000000	-2.636568	1.215550
11	1	0	0.000000	-2.695557	2.298601
12	6	0	0.000000	-3.810175	0.453918
13	6	0	0.000000	-3.716288	-0.930665
14	6	0	0.000000	-2.461487	-1.565460
15	1	0	0.000000	4.773350	0.947082
16	1	0	0.000000	2.695557	2.298601
17	1	0	0.000000	2.413771	-2.648332
18	1	0	0.000000	4.614234	-1.536846
19	1	0	0.000000	0.000000	-2.580500
20	1	0	0.000000	-4.773350	0.947082
21	1	0	0.000000	-4.614234	-1.536846
22	1	0	0.000000	-2.413771	-2.648332
23	16	0	0.000000	0.000000	1.648838