The Silacyclobutene Ring: An Indicator of Triplet State Baird-Aromaticity

Rabia Ayub,[1,2] Kjell Jorner,[1,2] and Henrik Ottosson[1,2]*

[1] Department of Chemistry - BMC, Uppsala University, Box 576, 751 23 Uppsala, Sweden.

[2] Department of Chemistry - Ångström Laboratory, Uppsala University, Box 523, 751 20 Uppsala, Sweden.

E-mail: henrik.ottosson@kemi.uu.se

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1. NICS scans

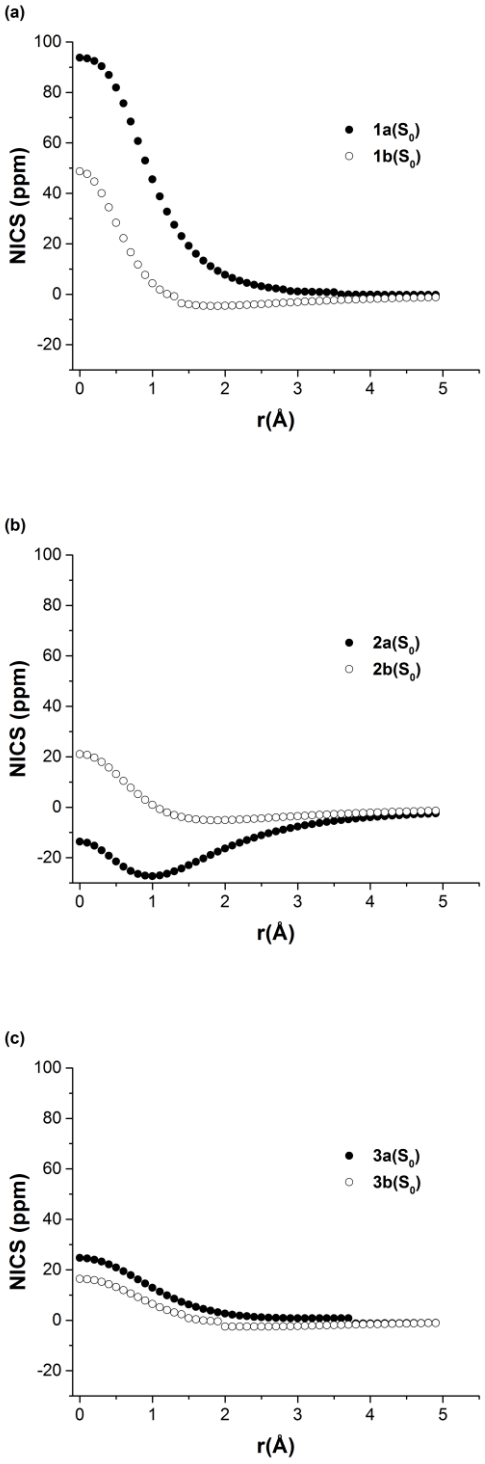


Figure S1: NICS scans at the GIAO-(U)B3LYP/6-311+G(d,p)//(U)B3LYP/6-311G(d,p) level. Only the out-of-plane component of the NICS scans is displayed here.

In the case of **1a(S_0)**, the contribution from the out-of-plane component is positive throughout and approaches zero at long distances revealing that this compound in the S_0 state is antiaromatic. Isomer **1b(S_0)**, on the other hand, displays non-aromatic character.

When going to benzoSCB an opposite behavior is observed (Figure S1). The out-of-plane component in **2a(S_0)** shows a large negative value (-27.3 ppm; 1 Å) and a relatively deep minimum characteristic of aromatic compounds. In **2b(S_0)**, the out-of-plane component is 21.1 ppm at 0 Å, indicating that this isomer is non-aromatic.

The NICS scans show that the isomers **3a(S_0)** and **3b(S_0)** are non-aromatic. Because of the non-planarity, **3b(S_0)** showed some discontinuity.

2. ACID plots

A : Aromatic, AA: antiaromatic, and NA: non-aromatic.

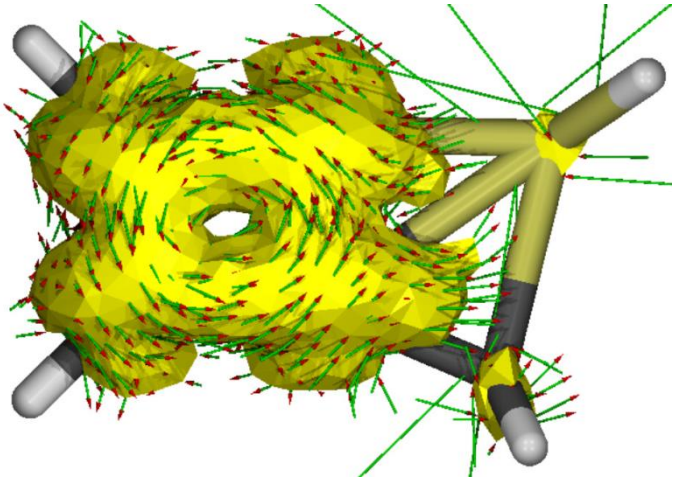


Figure S2: ACID plot of **1a(S_0)** (anti-clockwise ring-currents: AA).

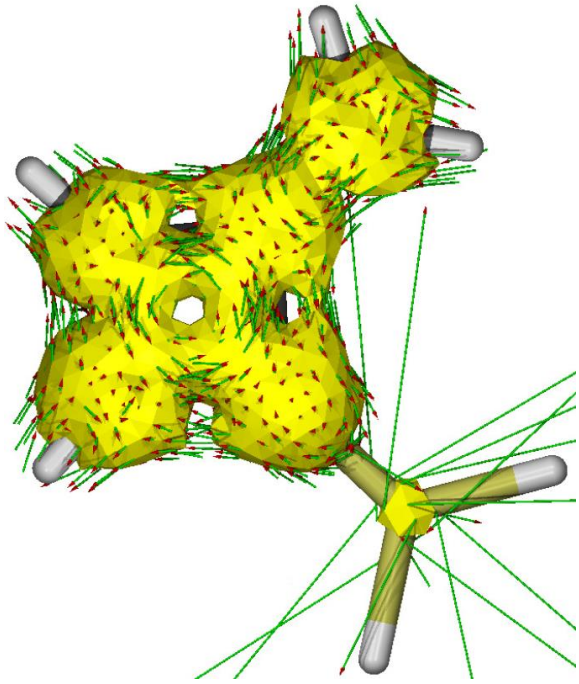


Figure S3: ACID plot of **1b(S_0)** (very weak anti-clockwise ring-currents: weakly AA).

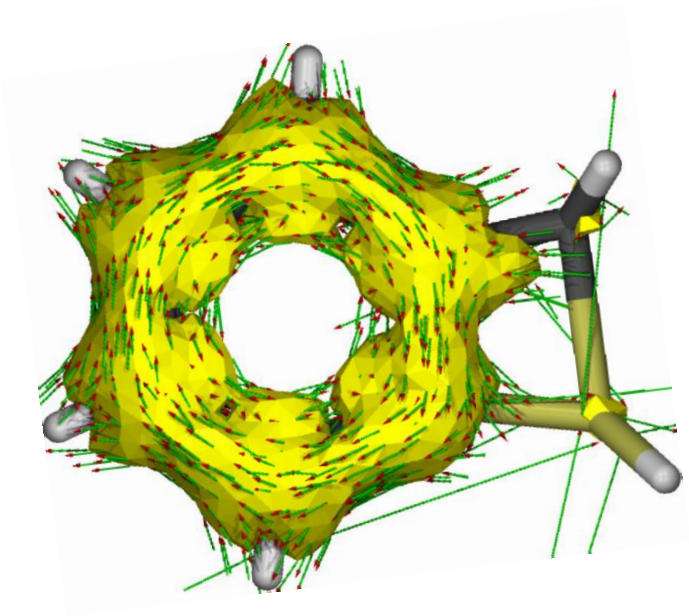


Figure S4: ACID plot of **2a(S_0)** (clockwise ring-currents: A).

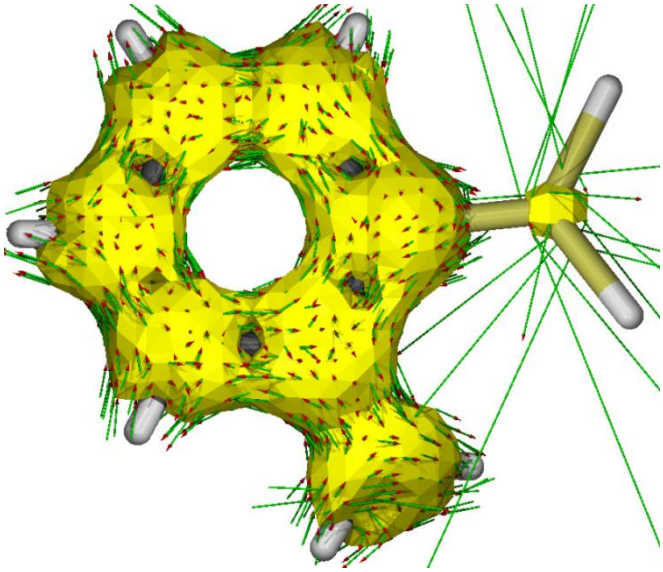


Figure S5: ACID plot of **2b(S_0)** (NA).

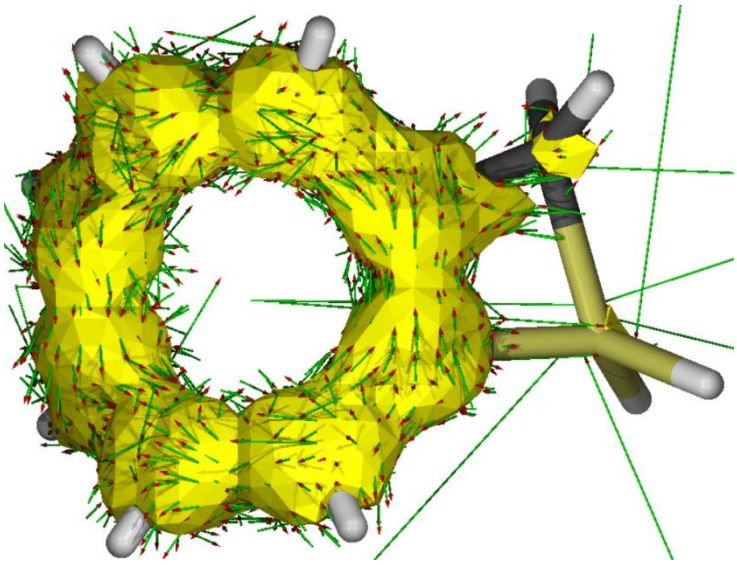


Figure S6: ACID plot of **3a(S_0)** (NA).

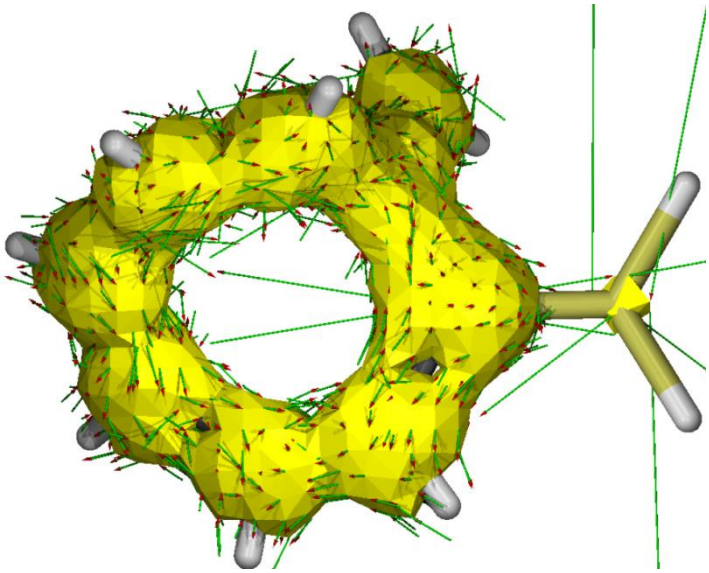


Figure S7: ACID plot of **3b(S_0)** (NA).

3. Geometries and spin densities

The benzene ring in **2a(S_0)** has equalized CC bond lengths which indicate that it is aromatic, and the compound is planar and C_s symmetric (Figure S9). Moreover, bonds *a* (Si-C) and *c* (C-C), both correspond to single bonds (1.872 and 1.529 Å, respectively). In **2a(T_1)**, on the other hand, two of the C-C bonds of the benzene ring change to that of C-C single bonds (1.504 Å), and the ring can be seen as two separate radical segments (Figure S10). Earlier, Zilberg and Haas showed that benzene in the T_1 state can be viewed as having two unpaired electrons in the *para*-positions and two double bonds parallel to the C_2-axis identified as quinoid (**^{3}Q**, either in C_{2v} or D_{2h}) or antiquinoid (**^{3}AQ)** [1]. Our **2a(T_1)** isomer is geometrically most similar to the **^{3}AQ** isomer as it has two long CC bonds and two allylic segments.

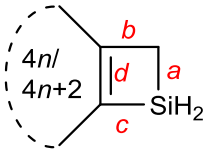


Figure S8: Description about naming of different bonds in the SCB ring.

Upon ring-opening of **2** in T_1, aromaticity is regained as indicated by the fact that the C-C bond lengths in the benzene ring in **2b(T_1)** become more equal (1.394 - 1.422 Å), and the molecule is planar. Bond *c* is intermediate in length (1.407 Å) between a double and a single bond, and bond *a* corresponds to a single bond (1.878 Å). It is a triplet biradical with one electron on the silicon atom and another delocalized in a benzyl radical fragment. The reverse behavior with regard to aromaticity is observed for **2b(S_0)**, with isolated single and double bonds in the six-membered (former benzene) ring. Now, bonds *c* and *a* correspond to exocyclic double bonds with lengths of 1.357 and 1.758 Å, respectively.

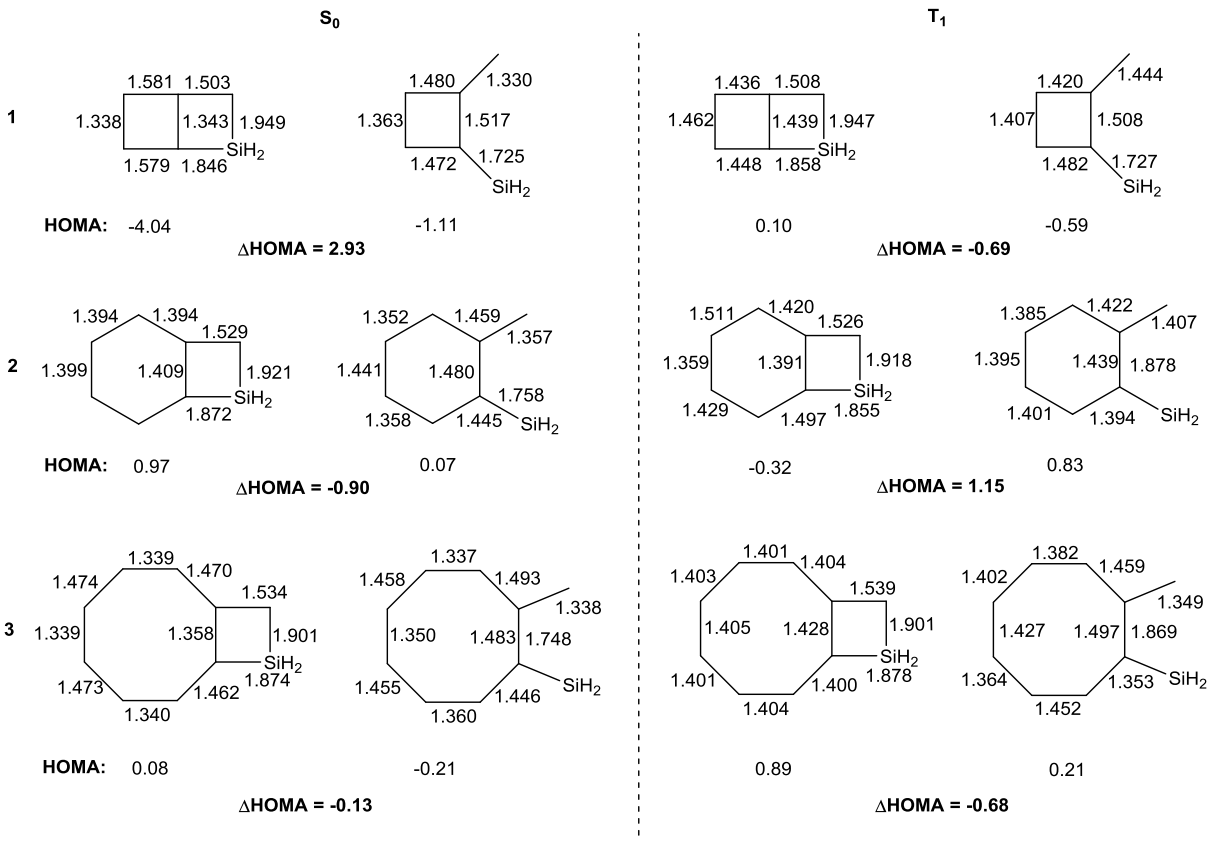


Figure S9: Bond lengths (Å) at the (U)B3LYP/6-311G(d,p) levels in the S_0 and the T_1 states of compounds **1**, **2** and **3**. HOMA values at (U)B3LYP/6-311G(d,p) level is given at the bottom of each compound.

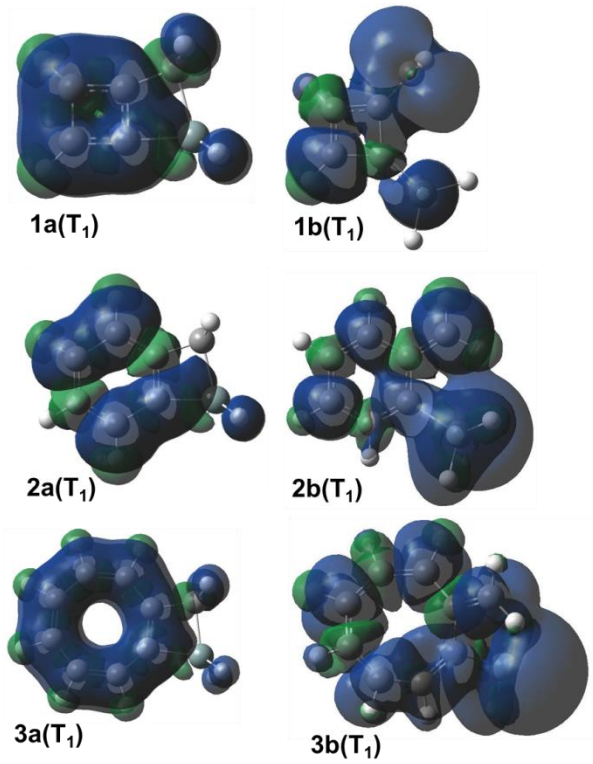


Figure S10: T_1 state spin density maps of **1a(T_1)**, **1b(T_1)**, **2a(T_1)**, **2b(T_1)**, **3a(T_1)**, and **3b(T_1)** at the (U)B3LYP/6-311G(d,p) level (isosurface value: 0.004).

Compounds **1** and **3** show the opposite behavior to that of **2**. In the S_0 state, the isomers **1a(S_0)** and **1b(S_0)** have rectangular four-membered (former CBD) all-C rings with CC bonds in the range 1.338 - 1.581 Å. When going from **1a(S_0)** to **1b(S_0)**, bonds *a* and *c* shorten from 1.846 to 1.725 Å, and from 1.503 to 1.330 Å, respectively, evident of exocyclic Si=C and C=C double bonds. This indicates that antiaromaticity of the rectangular CBD ring is relieved upon ring-opening and a π-conjugated hexatriene path is developed through the whole isomer by formation of Si=C and C=C double bonds. However, when going to the T_1 state, **1a(T_1)** has a nearly square CBD ring with C-C bond lengths of 1.436 - 1.462 Å indicative of aromatic character. Also, the spin density shows that the triplet biradical is evenly distributed over the complete CBD ring (Figure S10). In the SCB ring, the bonds *c* and *a* are 1.508 and 1.858 Å,

corresponding to single bonds. In **1b(T_1)**, on the other hand, the C-C bond lengths of the four-membered (former CBD) ring range from 1.407 to 1.482 Å, and this isomer has no symmetry and is slightly skewed. The exocyclic bonds *c* and *a* also shorten to 1.387 and 1.727 Å, displaying values closer to double bonds. The geometry changes in compound **1** when going from the ring-closed to the ring-opened isomer support our hypothesis that **1a** is T_1-aromatic.

With regard to **3a(S_0)** and **3b(S_0)**, both are non-planar and the C-C bond lengths in COT core range from 1.340 to 1.493 Å. Consequently, both isomers are non-aromatic with isolated single and double bonds. In **3a(T_1)**, on the other hand, the CC bond lengths of the COT ring are 1.401 - 1.405 Å, suggesting aromatic character. Moreover, the geometry is planar and the triplet biradical is distributed uniformly over the cyclooctatetraene ring (Figure S9). In **3b(T_1)**, the C-C bonds in the eight-membered (former COT) ring instead range from 1.353 to 1.549 Å, and the geometry is now skewed. The lengths of the exocyclic bonds *c* and *a* are 1.349 and 1.869 Å, respectively, indicative of exocyclic double bond character in the first but not in the latter of these bonds. The deviation from planarity and the bond length alternation show that the T_1 aromaticity, which exists in the ring-closed isomer, is reduced in the ring-opened isomer. Thus, the T_1-state ring-opening has significant impact on the complete geometry of the molecule.

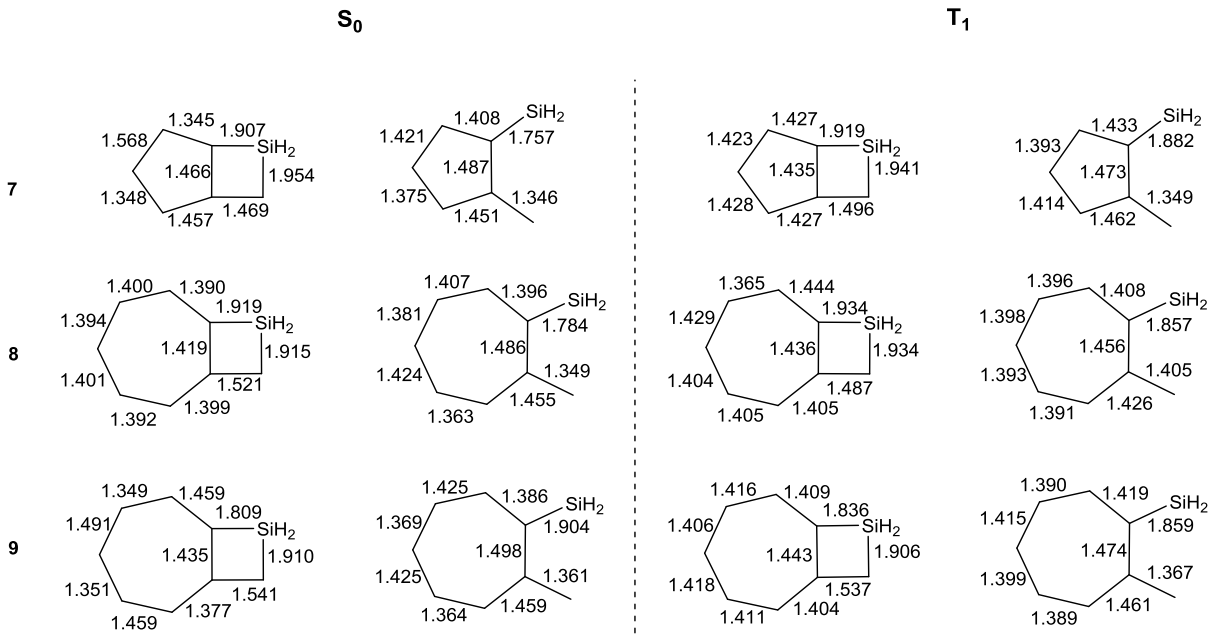


Figure S11: Bond lengths (Å) at the (U)B3LYP/6-311G(d,p) level in the S_0 and the T_1 states of compounds **7**, **8**, and **9**.

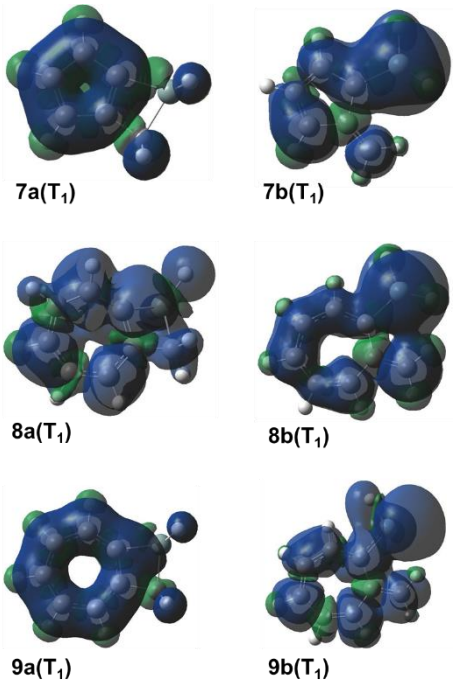


Figure S12: T_1 spin density maps of **7a(T_1)**, **7b(T_1)**, **8a(T_1)**, **8b(T_1)**, **9a(T_1)**, and **9b(T_1)** at the (U)B3LYP/6-311G(d,p) level (isosurface value: 0.004).

4. All carbon analogues of **2** and **3**

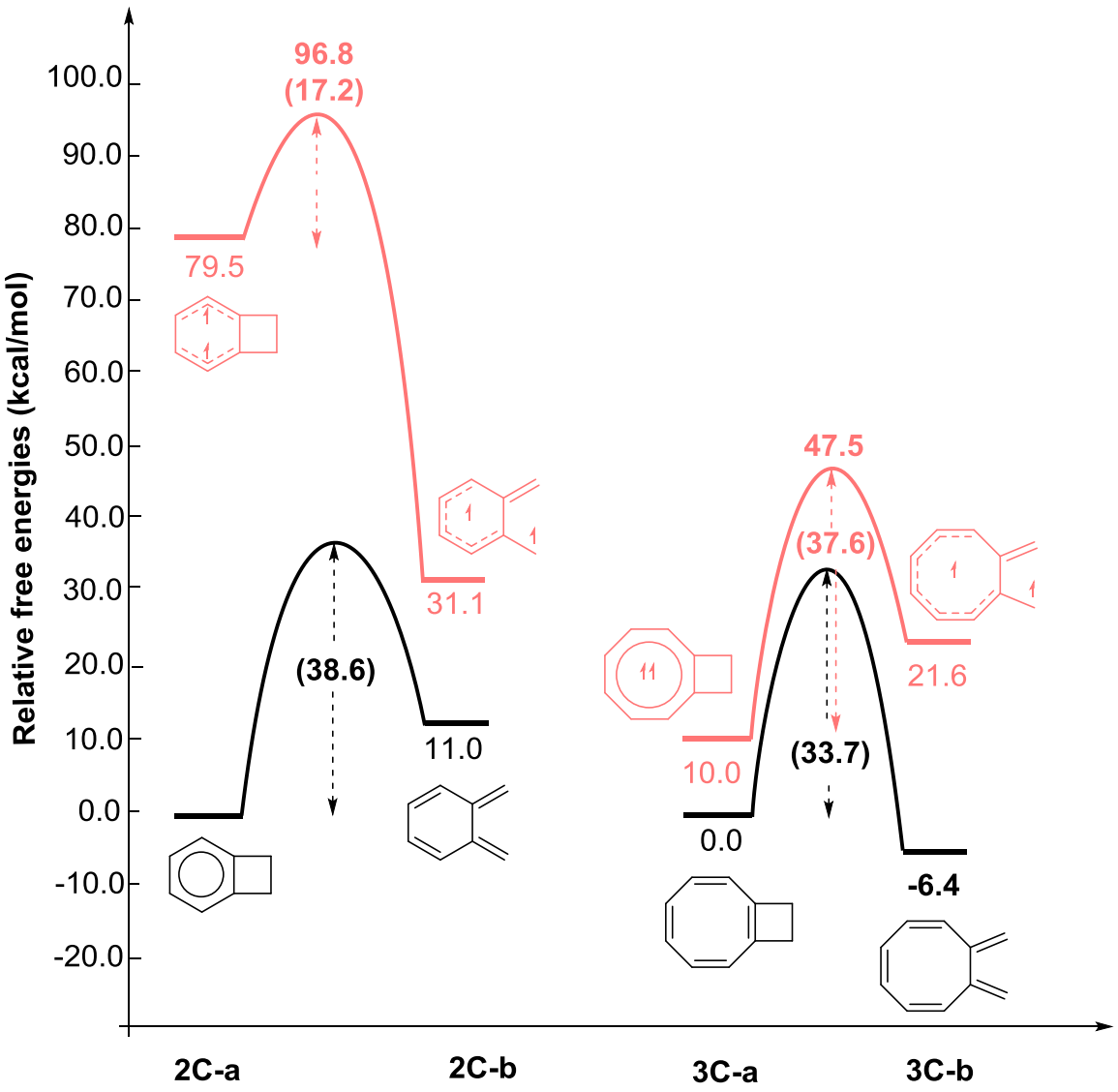
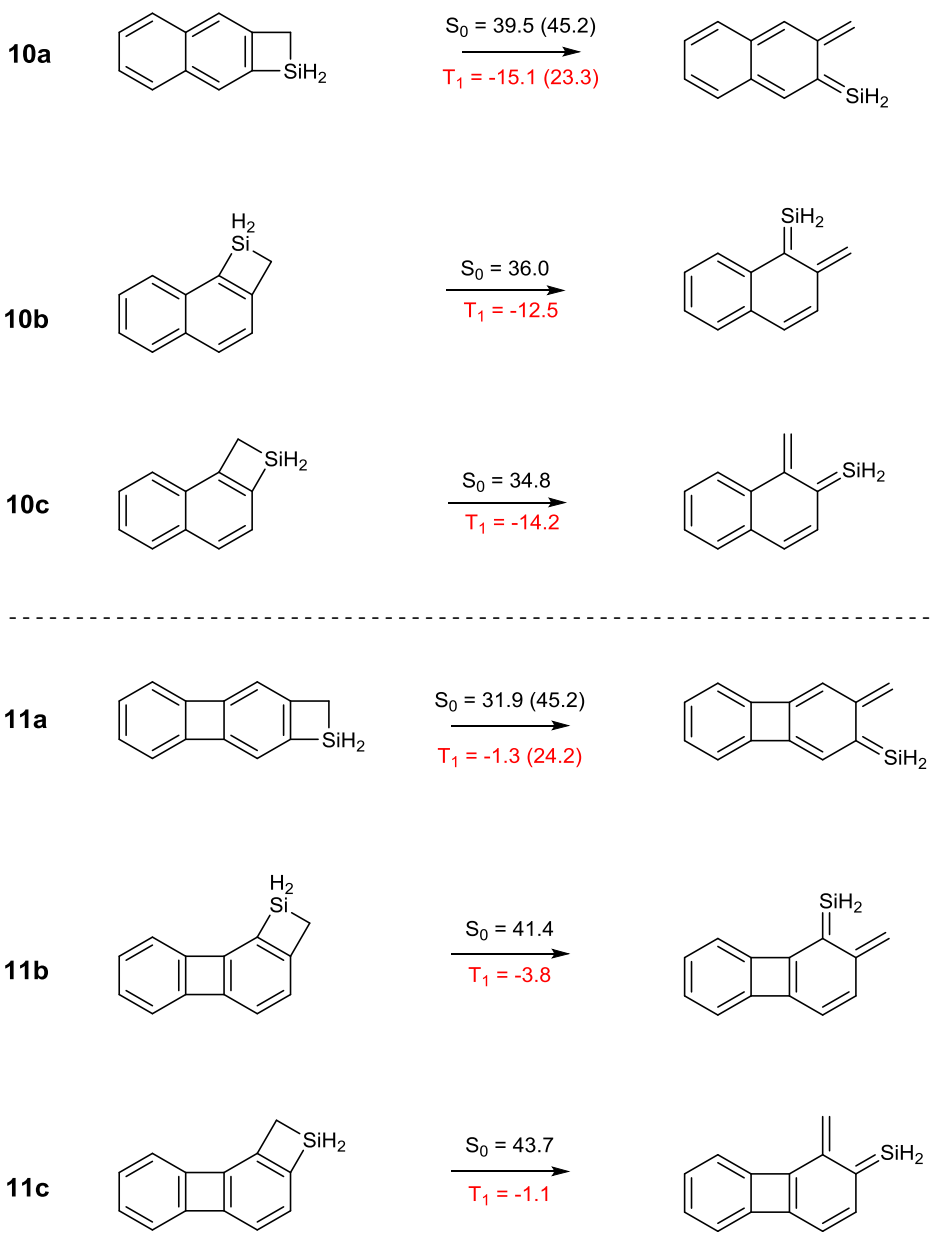


Figure S13: PES for cyclobutene ring-opening of all carbon analogues of **2** and **3** (**2C** and **3C**) at (U)B3LYP/6-311G(d,p) level.

5. Polycyclic structural units fused to SCB ring



Scheme S1: Reaction and activation free energies (kcal/mol) at the (U)B3LYP/6-311G(d,p) level. Activation energies are given in the bracket.

Ottosson and co-workers labelled some compounds as aromatic chameleons because these compounds are influenced by aromaticity in different electronic states [2-5]. The biphenylene is one such example (Figure S14) [6]. It adapts to Hückel's rule in the S_0 state and to Baird's

rule in the T_1 state. Thus, will the SCB ring be able to detect the T_1 aromatcity of the biphenyleno-segments, or will it open?

Figure S14: Aromatic Chameleon personality of biphenylenoSCB (**10a**) in the S_0 and T_1 states.

The biphenylenoSCBs in their T_1 ring-closed structures are 1.1 - 3.8 kcal/mol higher in energy than the ring-opened structure (Scheme S1), considerable smaller than for benzoSCB for which the ring-opening released 36.0 kcal/mol at B3LYP/6-311G(d,p) level.

For naphtho-SCB, reaction energies are exergonic and endergonic in the S_0 and the T_1 states, respectively. However, the activation energy in the T_1 is 14.3 kcal/mol higher than the benzo-SCB.

6. Structures of transition states at the (U)B3LYP/6-311G(d,p) level

(a) Bond lengths (Å)

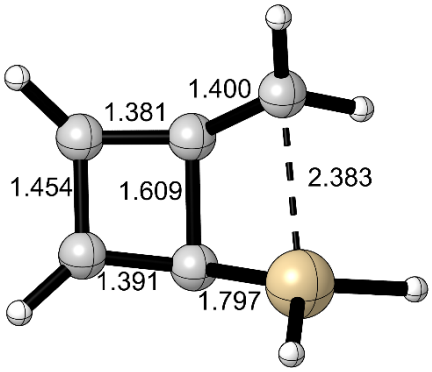


Figure S15: Disrotatory (**1-S$_0$**)

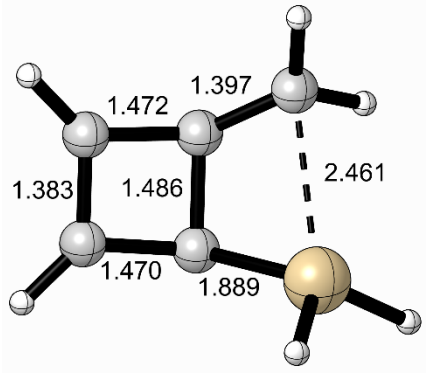


Figure S16: Disrotatory (**1-T$_1$**)

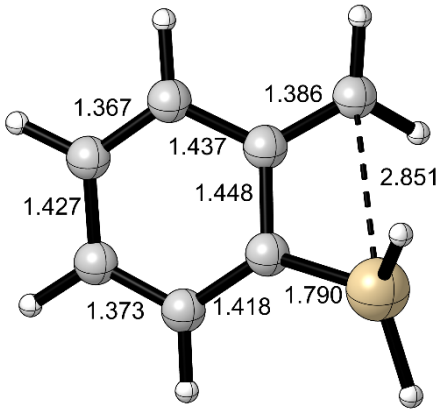


Figure S17: Conrotatory (**2-S$_0$**)

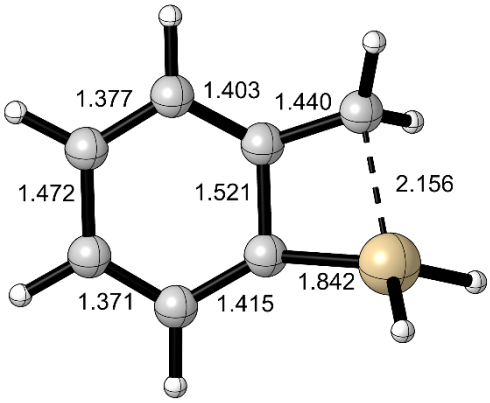


Figure S18: Disrotatory (**2-T$_1$**)

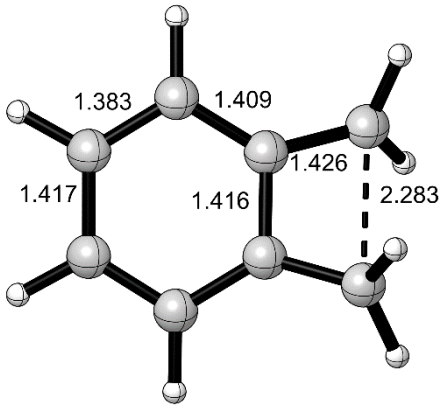


Figure S19: Conrotatory (**2C-S$_0$**)

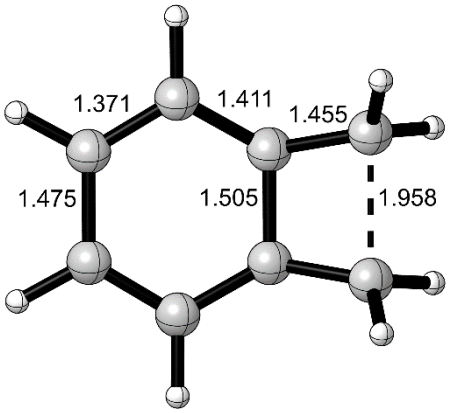


Figure S20: Disrotatory (**2C-T$_1$**)

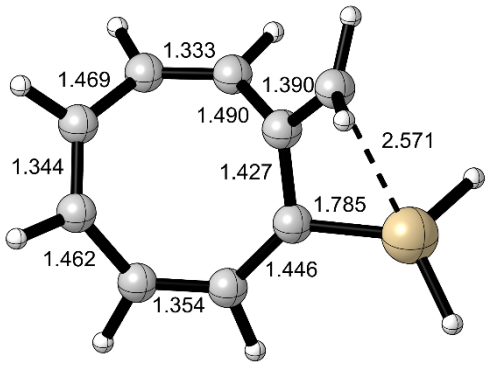


Figure S21: Conrotatory (**3-S$_0$**)

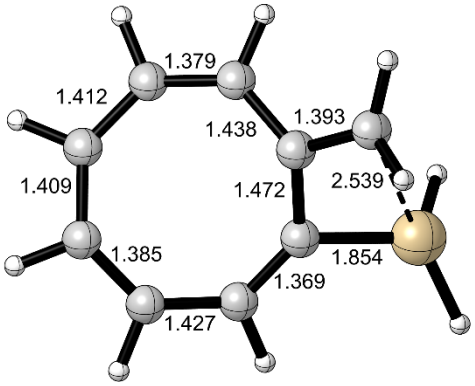


Figure S22: Conrotatory (**3-T$_1$**)

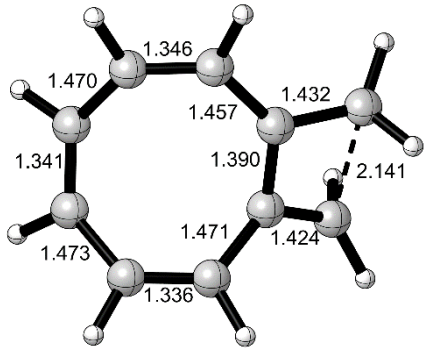


Figure S23: Conrotatory (**3C-S$_0$**)

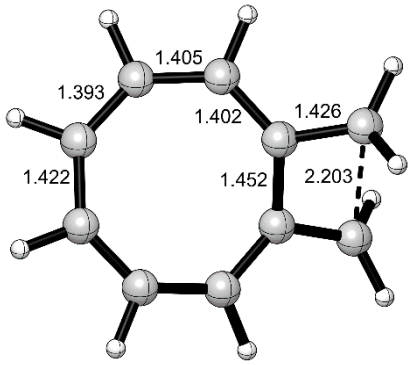


Figure S24: Conrotatory (**3C-T$_1$**)

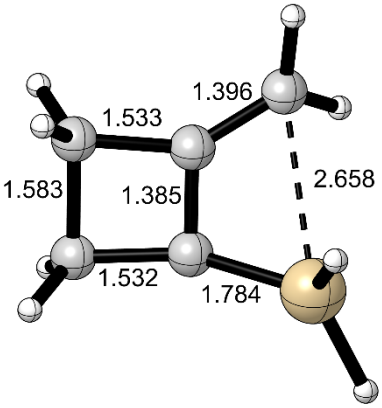


Figure S25: Conrotatory (**4-S$_0$**)

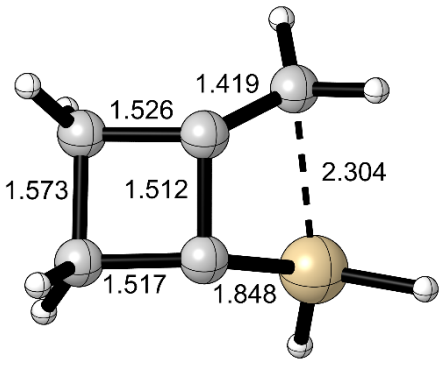


Figure S26: Disrotatory (**4-T$_1$**)

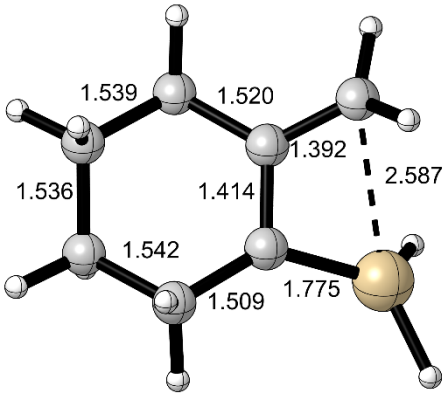


Figure S27: Conrotatory (**5-S$_0$**)

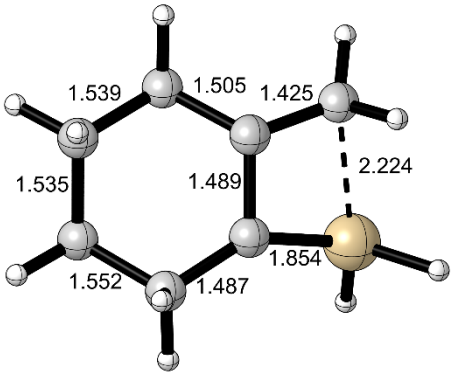


Figure S28: Disrotatory (**5-T$_1$**)

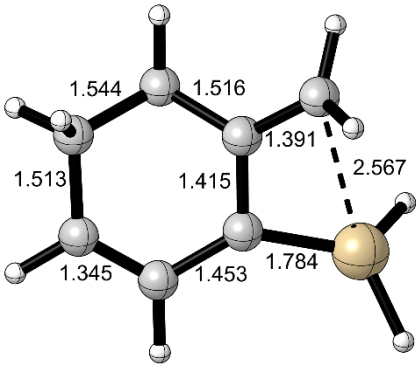


Figure S29: Conrotatory (**6-S$_0$**)

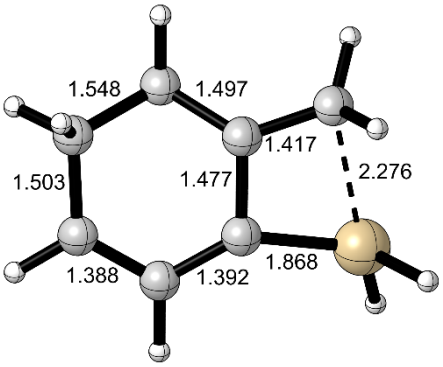


Figure S30: Disrotatory (**6-T$_1$**)

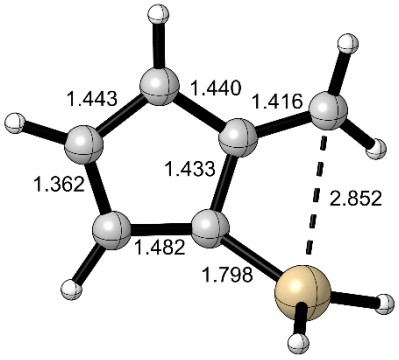


Figure S31: Disrotatory (**7-T$_1$**)

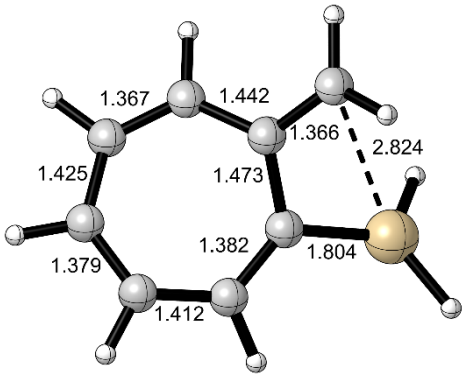


Figure S32: Conrotatory (**8-S$_0$**)

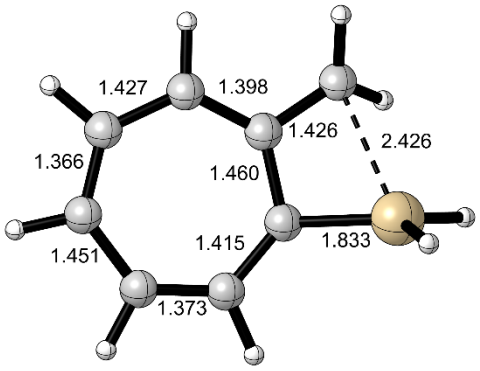


Figure S33: Disrotatory (**8-T$_1$**)

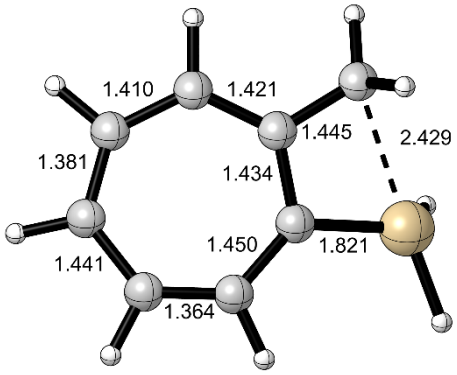


Figure S34: Conrotatory (**9-S$_0$**)

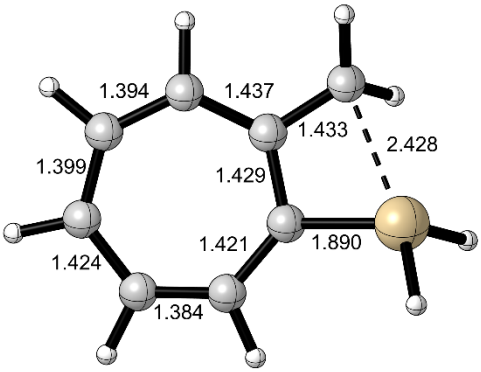


Figure S35: Disrotatory (**9-T$_1$**)

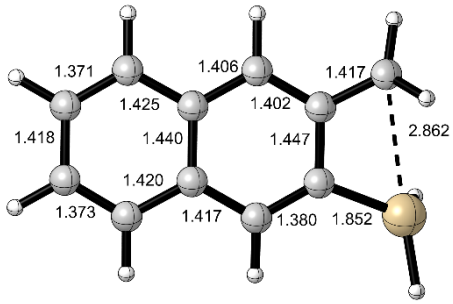


Figure S36: Conrotatory (**10a-S$_0$**)

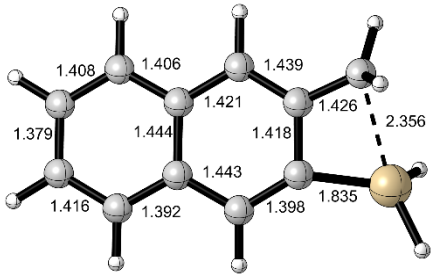


Figure S37: Conrotatory (**10a-T$_1$**)

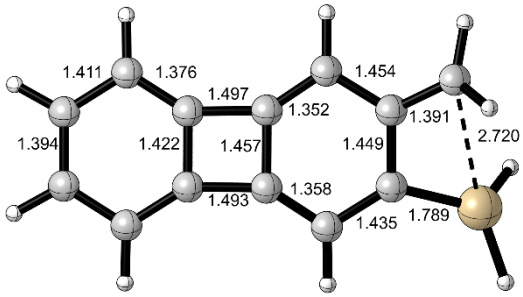


Figure S38: Conrotatory (**11a-S$_0$**)

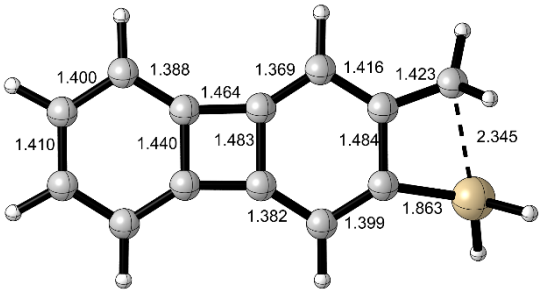


Figure S39: Disrotatory (**11a-T$_1$**)

(b) Dihedral angles (º)

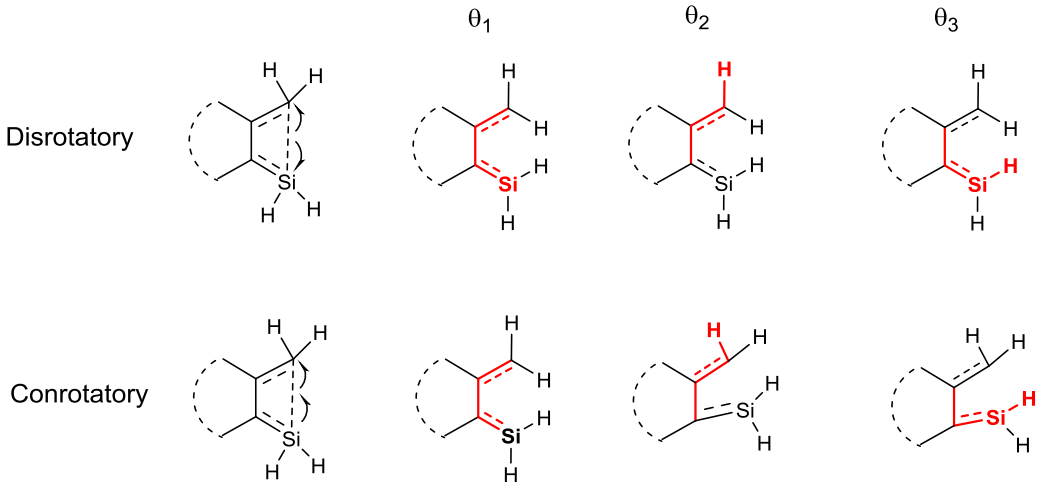


Table S1: Dihedral angles of transition states in S_0 and the T_1 states.

Compound numbers	S_0			T_1		
	θ_1	θ_2	θ_3	θ_1	θ_2	θ_3
1-TS	14.7	-149.7	-93.2	16.5	-146.9	-111.3
2-TS	32.0	-162.9	48.8	13.1	-149.5	-100.4
2C-TS	23.6	-147.8	55.9	0.0	-129.9	-88.5
3-TS	-34.3	157.1	-52.0	-38.5	161.7	-69.9
3C-TS	-21.8	146.7	-61.8	-30.0	149.7	-55.0
4-TS	28.8	-154.1	57.6	-10.1	136.8	96.9
5-TS	-32.4	157.8	-51.9	-18.2	149.4	102.1
6-TS	-30.9	157.9	-56.1	-14.7	151.4	100.7
7-TS				23.4	-161.4	-68.9
8-TS	-40.1	165.3	-42.2	20.3	-156.4	-91.8
9-TS	-16.3	155.3	-70.2	16.9	-157.2	-101.7
10a-TS	-25.0	159.0	-70.3	-21.5	151.9	-74.1
11a-TS	-31.3	160.7	-52.0	-15.0	154.7	95.6

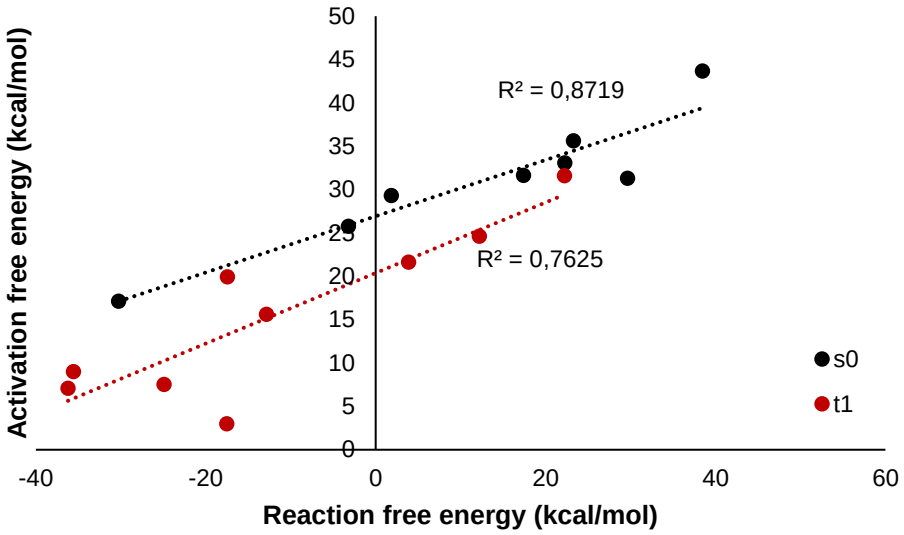


Figure S40: Correlation between reaction and activation free energies for **1 - 9** in the S_0 and the T_1 states at the (U)B3LYP/6-311G(d,p) level.

7. Spin densities for transition states (ISOsurface value: 0.0004).

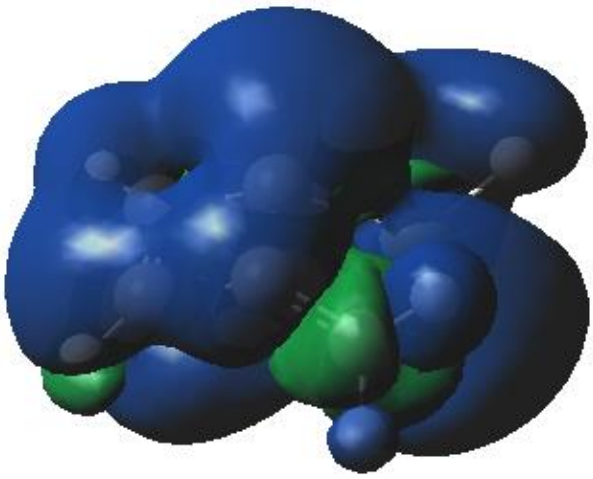


Figure S41: Spin density of **1-T_1**.

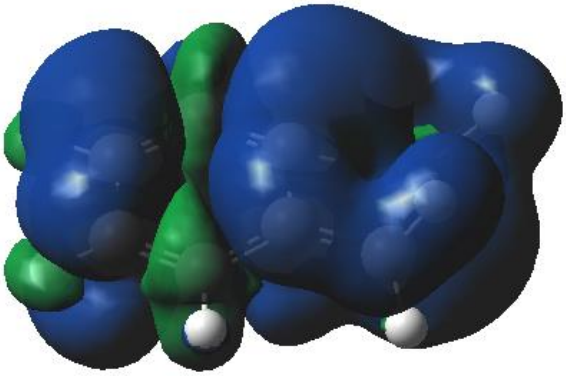


Figure S42: Spin density of **2-T_1**.

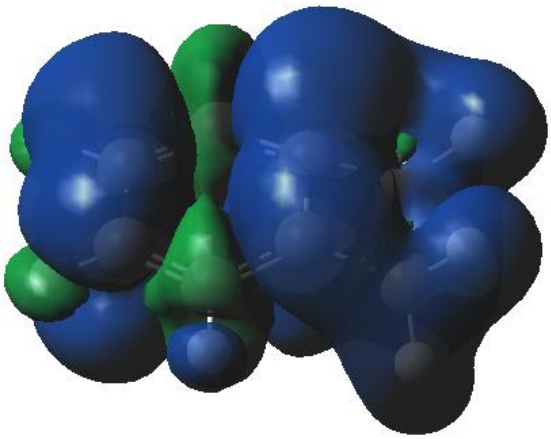


Figure S43: Spin density of **2C-T_1**.

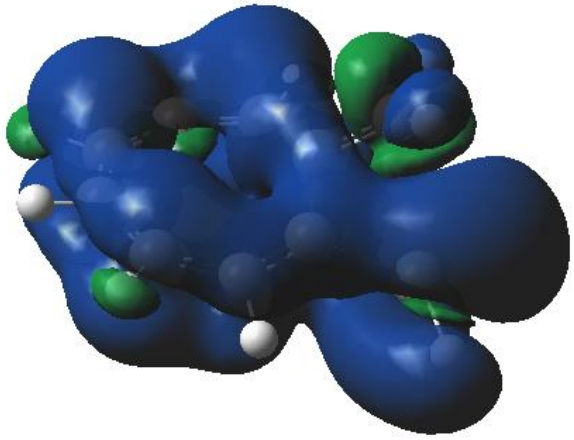


Figure S44: Spin density of **3-T_1**.

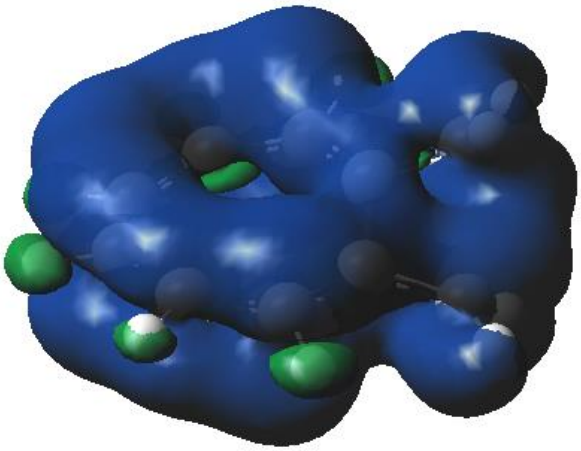


Figure S45: Spin density of **3C-T_1**.

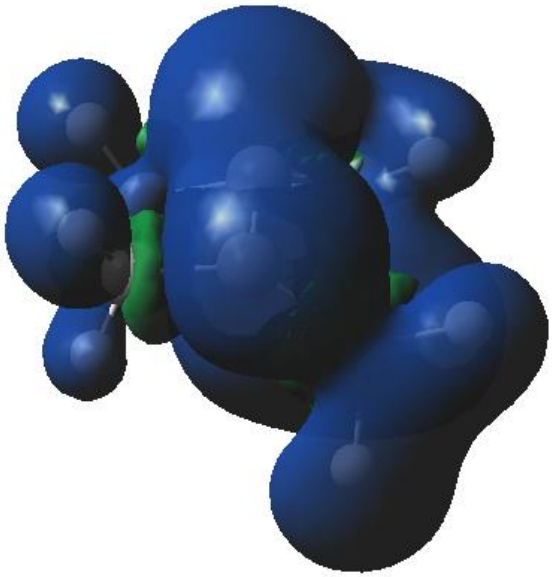


Figure S46: Spin density of **4-T_1**.

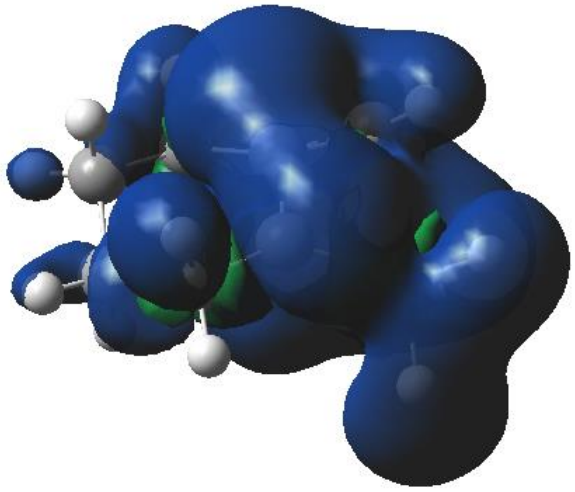


Figure S47: Spin density of **5-T$_1$**.

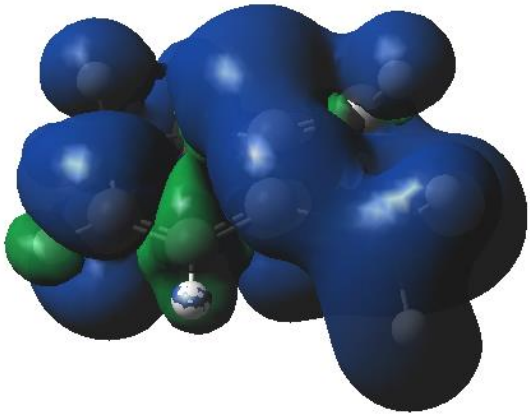


Figure S48: Spin density of **6-T$_1$**.

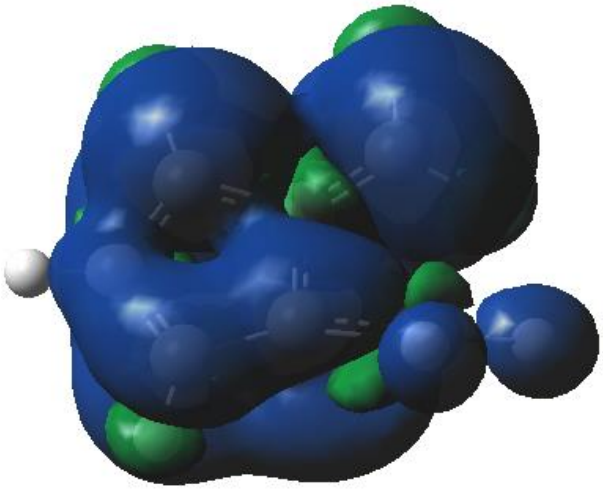


Figure S49: Spin density of **7-T$_1$**.

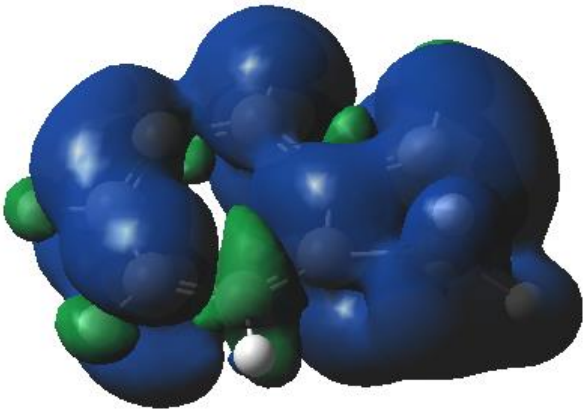


Figure S50: Spin density of **8-T_1**.

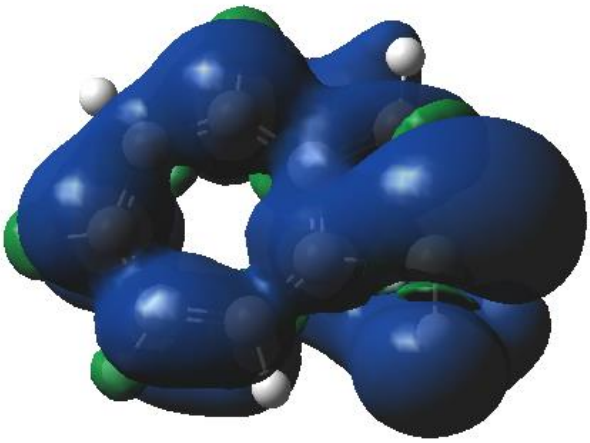


Figure S51: Spin density of **9-T_1**.

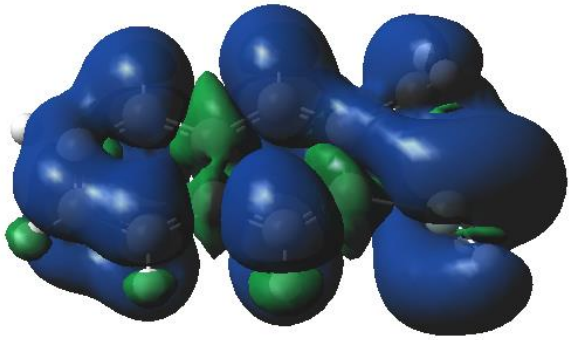


Figure S52: Spin density of **10a-T_1**.

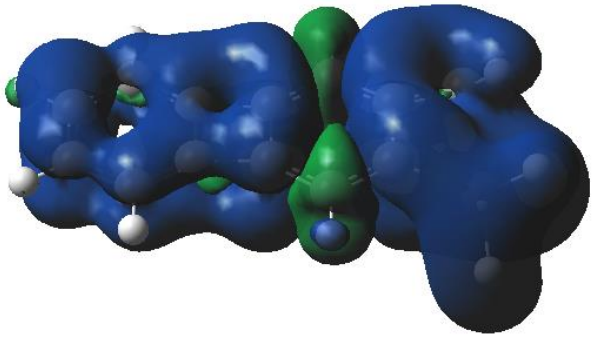


Figure S53: Spin density of **11a-T_1**.

8. ACID plots of transition states

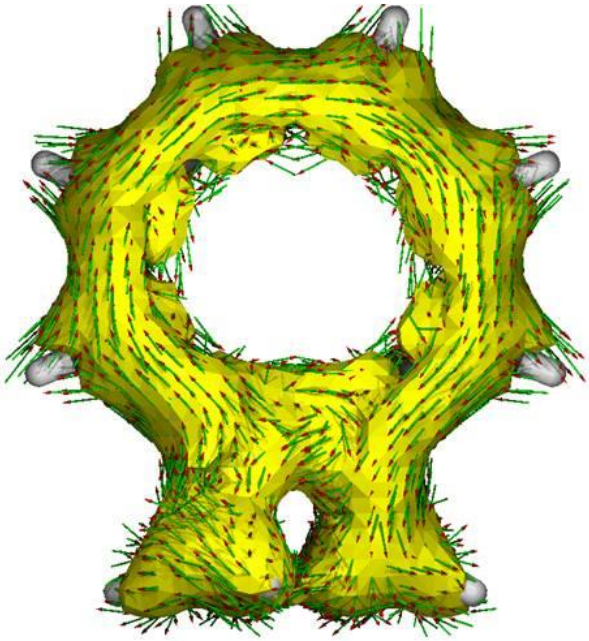


Figure S54: ACID plot of **3-TS(T_1)**.

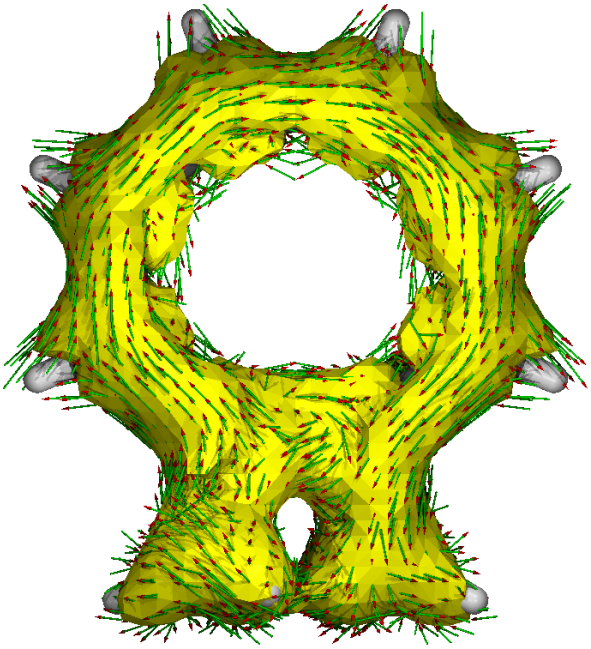


Figure S55: ACID plot of **3C-TS(T_1)**.

* Conjugation to silicon atom is not visible in the ACID isosurface, but the ring current still follows the 10-atom path.

9. Cartesian coordinates and absolute energies at the (U)B3LYP/6-311G(d,p) level

1a(S_0)
Absolute energy: -483.52355713 a.u
Point group: C_s

C	2.016750	0.418470	0.000000
C	0.668682	-0.403707	0.000000
C	0.000000	0.761117	0.000000
C	1.352819	1.580121	0.000000
H	3.062329	0.143446	0.000000
H	1.640745	2.622703	0.000000
C	-1.492189	0.579211	0.000000
H	-2.010917	0.953971	0.888130
H	-2.010917	0.953971	-0.888130
Si	-0.948722	-1.292684	0.000000
H	-1.337753	-2.093894	-1.195799
H	-1.337753	-2.093894	1.195799

1b(S_0)
Absolute energy: -483.57226676 a.u
Point group: C_1

C	-0.45836000	-1.55318300	-0.000094
C	0.29019000	-0.28530800	-0.000107
C	-1.06173300	0.40326000	0.000065
C	-1.67676800	-0.94310500	0.000072
H	-0.13779700	-2.58651900	-0.000225
H	-2.69959300	-1.29561500	0.000575
C	-1.48932400	1.66275400	-0.000080
H	-2.54835500	1.89395600	-0.000011
H	-0.79694700	2.49632800	-0.000176
Si	1.94235200	0.20914400	0.0000060
H	3.04071500	-0.77464700	0.0001670
H	2.32502100	1.63197300	0.0004430

1a(T_1)
Absolute energy: -483.50430731 a.u
Point group: C_1

C	1.788852	-0.897795	0.000540
C	0.347555	-0.761389	-0.010176
C	0.499944	0.670268	-0.007405
C	1.931020	0.556810	0.004624
H	2.480939	-1.727059	0.004052
H	2.771635	1.239019	0.015497
C	-0.851629	1.339444	-0.000621
H	-1.067001	1.945347	0.885601
H	-1.076051	1.944919	-0.884923
Si	-1.491665	-0.499015	0.002855
H	-2.269520	-0.930789	-1.191973
H	-2.251144	-0.929257	1.210006

1b(T_1)
Absolute energy: -483.53195640 a.u
Point group: C_1

C	-0.44171500	-1.53810600	-0.000023
C	0.24177200	-0.28209200	-0.000069
C	-1.10450300	0.39818400	-0.000011
C	-1.71035400	-0.95893700	0.000059
H	-0.09069900	-2.56190300	-0.000038
H	-2.72403700	-1.33591100	0.000112
C	-1.53865400	1.65618900	-0.000021
H	-0.84445600	2.48861700	-0.000082
H	-2.59769300	1.88656300	0.000032
Si	2.00547800	0.29686100	0.0000060
H	2.75035600	-0.14223300	1.2150020
H	2.75056200	-0.14260900	-1.21472300

1-TS(T_1)
Absolute energy: -483.472125370 a.u
Point group: C_1

C	-1.45551	-1.10405	-0.04947
C	-0.17321	-0.62272	-0.58205
C	-0.64744	0.75459	-0.28607
C	-1.88410	0.17337	0.26133
H	-1.85843	-2.09226	0.12981
H	-2.74087	0.57554	0.78855
C	0.34182	1.68738	0.03394
H	1.09617	1.90025	-0.71787
H	0.17608	2.50004	0.73651
Si	1.55159	-0.45097	0.16874
H	1.84805	-1.43418	1.25514
H	2.66737	-0.46711	-0.82058

1-TS(S_0)
Absolute energy: -483.496307115 a.u
Point group: C_1

C	-1.33428	-1.12481	0.01104
C	-0.13149	-0.74095	-0.57240
C	-0.68886	0.73462	-0.25375
C	-1.89766	0.20760	0.15600
H	-1.65052	-2.07194	0.44205
H	-2.76155	0.59920	0.67478
C	0.32092	1.64684	0.07370
H	0.14977	2.48207	0.74938
H	1.06644	1.84206	-0.69402
Si	1.49122	-0.42813	0.13318
H	2.12258	-1.23641	1.22670
H	2.58445	0.03908	-0.75096

2a(S_0)
Absolute energy: -561.056846229 a.u
Point group: C_s

C	1.67288	0.96166	-0.01160
C	0.23325	1.01118	0.00874
C	-0.48963	-0.25620	0.02837
C	0.27200	-1.45159	0.01522
C	1.65195	-1.45010	0.00999
C	2.35751	-0.22230	-0.00778
H	2.21113	1.90342	-0.03054
H	-0.24820	-2.40451	0.02619
H	2.19607	-2.38745	0.02435
H	3.44174	-0.22443	-0.02006
Si	-2.30598	-0.45019	-0.08837
C	-0.39055	2.24624	0.01627
H	-1.46679	2.35445	0.03621
H	0.19573	3.15672	0.00051
H	-3.14389	0.65171	0.44539
H	-2.74645	-1.78062	0.39986

2b(S_0)
Absolute energy: -561.05555649 a.u
Point group: C_1

C	-1.62532700	0.96881400	0.25712800
C	-0.19710400	1.02423800	-0.03893700
C	0.51130000	-0.27374500	-0.10985600
C	-0.29403700	-1.46378500	-0.25820400
C	-1.64548300	-1.43034400	-0.12557600
C	-2.31382200	-0.19312200	0.19130800
H	-2.13506100	1.90506200	0.45837600
H	0.20433200	-2.41368100	-0.42692900
H	-2.22585500	-2.34132200	-0.21506200
H	-3.38480700	-0.20182000	0.36222700
Si	2.23540400	-0.45528100	0.18429500
C	0.39489000	2.21486600	-0.30848300
H	1.41103400	2.28264600	-0.67675100
H	-0.14902000	3.14444600	-0.18926000
H	3.11528900	0.66829200	0.55017500
H	2.88592700	-1.75122100	-0.08720000

2a(T_1)
Absolute energy: -560.98787057 a.u
Point group: C_s

C	0.60915100	-1.69639600	0.00000000
C	-0.35754800	-0.65606800	0.00000000
C	0.00000000	0.67439900	0.00000000
C	1.44573000	1.06234300	0.00000000
C	2.42001900	0.01662500	0.00000000
C	2.06641200	-1.29611800	0.00000000
H	0.33112100	-2.74251800	0.00000000
H	1.74536800	2.10153300	0.00000000
H	3.47138500	0.28602400	0.00000000
H	2.81729200	-2.07619600	0.00000000
Si	-1.78107200	1.19430000	0.00000000
C	-1.88197500	-0.72115900	0.00000000
H	-2.30472300	-1.20124100	0.88729200
H	-2.30472300	-1.20124100	-0.88729200
H	-2.31572200	1.90584300	1.19767300
H	-2.31572200	1.90584300	-1.19767300

2b(T_1)
Absolute energy: -561.04989202 a.u
Point group: C_1

C	-1.63243700	1.01025000	0.00900400
C	-0.21112700	0.99033000	-0.00970300
C	0.44839600	-0.28952300	-0.00847500
C	-0.33014000	-1.44568400	-0.00136100
C	-1.72993100	-1.39634400	0.01317900
C	-2.37490900	-0.15892300	0.01851900
H	-2.13638600	1.97107100	0.01502300
H	0.15504800	-2.41670600	-0.00526200
H	-2.30450200	-2.31531700	0.01780100
H	-3.45815200	-0.11025600	0.02884700
Si	2.31691300	-0.46273700	-0.07184900
C	0.50267100	2.20319700	-0.02578900
H	1.58401900	2.23568900	-0.01409100
H	-0.02184400	3.15035100	-0.04420100
H	3.02928300	0.37977500	0.92989900
H	2.68061000	-1.89610800	0.105619000

2-TS(S_0)
Absolute energy: -561.050364710 a.u
Point group: C_1

C	-1.40076	1.17681	0.29456
C	-0.03485	0.92970	-0.07802
C	0.39162	-0.45222	-0.15723
C	-0.58307	-1.47148	-0.30756
C	-1.90946	-1.17086	-0.11627
C	-2.30466	0.15210	0.24230
H	-1.72078	2.19187	0.50409
H	-0.27404	-2.49819	-0.47564
H	-2.65788	-1.95340	-0.16593
H	-3.35102	0.34825	0.45025
Si	2.14080	-0.54674	0.21109
C	0.86669	1.92249	-0.42713
H	1.63187	1.72542	-1.16422
H	0.71689	2.95757	-0.13810
H	2.62540	0.14909	1.41467
H	2.90521	-1.78542	-0.08417

2-TS(T_1)
Absolute energy: -560.976537949 a.u
Point group: C_1

C	-1.24072	1.35283	0.11478
C	0.03173	0.86892	-0.22572
C	0.27066	-0.63097	-0.30106
C	-0.84673	-1.49209	-0.19456
C	-2.09646	-0.96302	0.00104
C	-2.30664	0.48347	0.17902
H	-1.38800	2.41823	0.26531
H	-0.71703	-2.56868	-0.24162
H	-2.95804	-1.61846	0.06577
H	-3.31233	0.84745	0.34574
Si	2.03750	-0.53465	0.21139
C	1.33394	1.47606	-0.12309
H	1.93289	1.46248	-1.03979
H	1.45511	2.41227	0.41801
H	2.47570	-1.42752	1.33982
H	3.11193	-0.61187	-0.81516

Carbon-2(S_0) closed
Absolute energy: -309.705753315 a.u
Point group: C_{2v}

C	0.00000	1.43609	-0.71865
C	0.00000	0.69667	0.45229
C	-0.00000	-0.69667	0.45229
C	-0.00000	-1.43609	-0.71865
C	-0.00000	-0.69957	-1.91199
C	0.00000	0.69957	-1.91199
H	0.00000	2.52070	-0.73487
H	-0.00000	-2.52070	-0.73487
H	-0.00000	-1.22415	-2.86141
H	0.00000	1.22415	-2.86141
C	0.00000	0.79129	1.97195
H	-0.88857	1.24594	2.41732
H	0.88857	1.24594	2.41732
C	-0.00000	-0.79129	1.97195
H	-0.88857	-1.24594	2.41732
H	0.88857	-1.24594	2.41732

Carbon-2(S_0) open
Absolute energy: -309.684961487 a.u
Point group: C_2

C	0.17998	1.40298	0.67365
C	0.00950	0.74725	-0.62064
C	-0.00950	-0.74725	-0.62064
C	-0.17998	-1.40298	0.67365
C	-0.11176	-0.71677	1.83227
C	0.11176	0.71677	1.83227
H	0.31220	2.47973	0.67505
H	-0.31220	-2.47973	0.67505
H	-0.20450	-1.23339	2.78104
H	0.20450	1.23339	2.78104
C	-0.17998	1.48978	-1.73114
H	-0.40584	1.04823	-2.69335
H	-0.13022	2.57154	-1.68759
C	0.17998	-1.48978	-1.73114
H	0.13022	-2.57154	-1.68759
H	0.40584	-1.04823	-2.69335

Carbon-2(S_0) TS
Absolute energy: -309.640087232 a.u
Point group: C_2

C	0.68686	-1.42256	0.16629
C	-0.51381	-0.70774	-0.01409
C	-0.51381	0.70774	0.01408
C	0.68687	1.42256	-0.16630
C	1.86472	0.70082	-0.10515
C	1.86471	-0.70082	0.10516
H	0.69598	-2.50328	0.26124
H	0.69598	2.50327	-0.26128
H	2.81533	1.21748	-0.17941
H	2.81533	-1.21749	0.17943
C	-1.85411	-1.10108	-0.30189
H	-2.29896	-2.01785	0.08482
H	-2.31438	-0.71090	-1.19698
C	-1.85410	1.10108	0.30189
H	-2.31436	0.71091	1.19699
H	-2.29895	2.01786	-0.08481

Carbon-2(T_1) closed
Absolute energy: -309.566906503 a.u
Point group: C_1

C	-0.61125	1.50566	0.00022
C	0.50106	0.71129	-0.02766
C	0.45814	-0.68552	-0.03090
C	-0.83411	-1.45282	-0.00690
C	-1.97111	-0.66896	0.01451
C	-1.93117	0.73645	0.00479
H	-0.60862	2.58625	0.04280
H	-0.87002	-2.53356	-0.02339
H	-2.94502	-1.14888	0.02468

H	-2.85727	1.29740	-0.00620
C	2.02557	0.72845	0.00125
H	2.47236	1.17630	0.89258
H	2.50633	1.14997	-0.88516
H	2.35331	-1.31800	0.93147
H	2.41738	-1.35129	-0.83822
C	1.95145	-0.85093	0.02160

Carbon-2(T_1) open

Absolute energy: -309.648651907 a.u

Point group: C_{2v}

C	-0.00000	1.38626	0.65677
C	0.00000	0.72666	-0.58107
C	-0.00000	-0.72666	-0.58107
C	-0.00000	-1.38626	0.65677
C	-0.00000	-0.69175	1.87771
C	0.00000	0.69175	1.87771
H	-0.00000	2.47124	0.66298
H	-0.00000	-2.47124	0.66298
H	-0.00000	-1.24352	2.81060
H	0.00000	1.24352	2.81060
C	0.00000	1.48199	-1.78247
H	0.00000	1.02622	-2.76075
H	0.00000	2.56372	-1.73840
H	-0.00000	-1.02622	-2.76075
H	-0.00000	-2.56372	-1.73840
C	-0.00000	-1.48199	-1.78247

Carbon-2(T_1) TS

Absolute energy: -309.541023375 a.u

Point group: C_s

C	-0.70324	1.44146	-0.02065
C	0.50166	0.75265	-0.27607
C	0.50166	-0.75265	-0.27606
C	-0.70324	-1.44146	-0.02065
C	-1.87746	-0.73773	0.05824
C	-1.87746	0.73773	0.05824
H	-0.69943	2.52265	0.08370
H	-0.69943	-2.52265	0.08370
H	-2.82333	-1.25487	0.16621
H	-2.82333	1.25487	0.16621
C	1.87782	0.97919	0.13873
H	2.07572	1.66319	0.96919
H	2.65428	1.03728	-0.62060
H	2.07572	-1.66318	0.96919
H	2.65428	-1.03728	-0.62060
C	1.87782	-0.97919	0.13873

3a(S_0)

Absolute energy: -638.48905419 a.u

Point group: C_1

C	-0.31463300	-1.58214200	-0.71055500
C	-1.59455900	-1.66422900	-0.32104700
C	-0.52993100	1.61598900	-0.64259300
C	-2.28907900	-0.81230700	0.65885200
C	-1.80514000	1.50470100	-0.24879700
C	-2.37694200	0.52366500	0.69042300
C	0.67392800	-0.60220900	-0.26306000
C	0.58746500	0.75293300	-0.23162100
Si	2.45625100	-0.53135500	0.31095800
H	-0.25917600	2.46043700	-1.27432500
H	-2.50163700	2.27192100	-0.58410600
H	-3.00670600	0.95950500	1.46488300
H	-2.85518800	-1.35961500	1.41155000
H	-2.18259700	-2.49971100	-0.69729200
H	0.05426900	-2.35030700	-1.38790700
C	1.93808600	1.30311800	0.24255000
H	2.43971800	1.93358100	-0.49824800
H	1.88225000	1.85650000	1.18380800
H	3.50387300	-0.96331500	-0.65651600
H	2.80250000	-1.10713600	1.63983700

3b(S_0)

Absolute energy: -638.45137381 a.u

Point group: C_1

C	0.31398900	-1.54490000	-0.10780900
C	-0.98242700	-1.86758700	0.14908500
C	-0.68479800	1.38777200	-0.82446900
C	-2.16912800	-1.10068000	0.49751900
C	-1.97051800	1.02355300	-0.84829000
C	-2.61996000	0.09904300	0.07276800
C	1.02472600	-0.28830100	-0.02798100
C	0.30490200	0.98514600	0.21827700
Si	2.76141200	-0.24644700	-0.22474500
H	-0.30949500	2.04688800	-1.60467400
H	-2.61347400	1.46582400	-1.60765900
H	-3.62493600	0.37708300	0.38286900
H	-2.86283600	-1.66169500	1.12155100
H	-1.17916900	-2.93815800	0.14059100
H	0.94790900	-2.40282900	-0.32493800
C	0.55792800	1.77473000	1.26869200
H	0.04355400	2.72076200	1.39552600
H	1.25925600	1.47932800	2.04007000
H	3.50784400	1.02316700	-0.24497800
H	3.52329600	-1.47276600	-0.53868600

3-TS(S_0)

Absolute energy: -638.434422232 a.u

Point group: C_1

C	0.03091	1.66020	-0.33596
C	1.34962	1.80167	-0.06541
C	0.56361	-1.50458	-0.72364
C	2.30505	0.89007	0.56307
C	1.87786	-1.31512	-0.60747
C	2.54219	-0.41433	0.34431
C	-0.83816	0.53246	-0.08426
C	-0.48278	-0.83677	0.10070
Si	-2.61896	0.40845	-0.06644
H	0.19287	-2.22295	-1.45270
H	2.54041	-1.91482	-1.22934
H	3.38134	-0.85508	0.88012
H	2.97938	1.38691	1.25964
H	1.76489	2.78824	-0.26354
H	-0.45975	2.54397	-0.73603
C	-1.32622	-1.58677	0.91131
H	-1.37132	-2.66973	0.82832
H	-1.71203	-1.16802	1.82981
H	-3.28126	-0.56017	-0.95833
H	-3.50173	1.59236	0.15625

3a(T_1)

Absolute energy: -638.46325383 a.u

Point group: C_1

C	-0.19090900	-1.68774600	0.00041400
C	-1.59215900	-1.77954800	-0.00005800
C	-0.43312900	1.73371500	-0.00034400
C	-2.64226800	-0.85196300	-0.00029600
C	-1.82984100	1.61872700	0.00005400
C	-2.73812600	0.54995500	0.00014600
C	0.71218700	-0.61769200	0.00038800
C	0.62151400	0.80738600	0.00006400
Si	2.58866100	-0.53667800	-0.00023400
H	-0.08980600	2.76584400	-0.00073300
H	-2.32743700	2.58508500	0.00025100
H	-3.77087200	0.88924900	0.00045700
H	-3.61791900	-1.33084700	-0.00065700
H	-1.94446200	-2.80807900	-0.00028700
H	0.29095900	-2.66305500	0.00067100
C	2.08096800	1.29491100	0.00027700
H	2.34297200	1.88249000	-0.88476600
H	2.34270700	1.88120500	0.88628000
H	3.30067000	-1.04715100	-1.20479500
H	3.30252500	-1.04771000	1.20298700

3b(T_1)

Absolute energy: -638.42438713 a.u

Point group: C_1

C	0.15144600	-1.52715200	0.19949100
C	-1.22315000	-1.72901100	0.62018100
C	-0.57779100	1.69397800	-0.32558500
C	-2.35286000	-1.04398200	0.28205200

C	-1.80464000	1.25730200	-0.78835400
C	-2.57515200	0.11719400	-0.51736800
C	0.87696200	-0.39352300	0.06187900
C	0.45411300	0.99359100	0.43266700
Si	2.63481700	-0.50656800	-0.56198500
H	-0.36422100	2.74459000	-0.50303000
H	-2.34127700	2.00508200	-1.36776800
H	-3.59063900	0.18165900	-0.89910200
H	-3.27712300	-1.51597500	0.60967200
H	-1.38469800	-2.65508000	1.16769800
H	0.66789400	-2.46411300	-0.01265900
C	1.15823600	1.66373400	1.36757900
H	0.92560200	2.69402500	1.61332400
H	1.95455300	1.18882700	1.92861100
H	2.95540300	0.57418800	-1.53228900
H	2.92407500	-1.85404100	-1.13191700

3-TS(T_1)
Absolute energy: -638.410925301 a.u
Point group: C_1

C	-0.07672	-1.65581	0.07174
C	-1.47586	-1.77163	0.32928
C	-0.41827	1.72416	-0.19535
C	-2.52956	-0.88254	0.19853
C	-1.75129	1.51521	-0.48002
C	-2.64685	0.44674	-0.25351
C	0.76888	-0.57951	0.05214
C	0.58939	0.85151	0.34512
Si	2.55721	-0.51763	-0.43366
H	-0.08023	2.75078	-0.31867
H	-2.25206	2.40517	-0.85283
H	-3.68015	0.73227	-0.43331
H	-3.49623	-1.33672	0.40257
H	-1.78458	-2.78444	0.57665
H	0.40186	-2.61648	-0.11442
C	1.69767	1.41227	0.97512
H	1.84123	2.48973	0.98795
H	2.23867	0.86281	1.73278
H	2.75587	0.19660	-1.71946
H	3.31042	-1.81536	-0.44834

Carbon-3(S_0) closed
Absolute energy: -387.074343219 a.u
Point group: C_s

C	0.53814	-0.04319	1.66813
C	0.30780	-1.36344	1.62708
C	0.53814	-0.04319	-1.66813
C	-0.53632	-2.10486	0.66915
C	0.30780	-1.36344	-1.62708
C	-0.53632	-2.10486	-0.66915
C	0.10509	0.93096	0.67497
C	0.10509	0.93096	-0.67497
H	1.09238	0.35372	-2.51689
H	0.68988	-1.96526	-2.44983
H	-1.23535	-2.78929	-1.14957
H	-1.23535	-2.78929	1.14957
H	0.68988	-1.96526	2.44983
H	1.09238	0.35372	2.51689
C	-0.34791	2.37961	-0.78477
H	0.37567	3.06503	-1.23816
H	-1.32342	2.54131	-1.25320
H	0.37567	3.06503	1.23816
H	-1.32342	2.54131	1.25320
C	-0.34791	2.37961	0.78477

Carbon-3(S_0) open
Absolute energy: -387.082734675 a.u
Point group: C_1

C	-0.53123	1.61852	-0.20005
C	0.76257	1.82755	0.13287
C	0.24286	-1.40438	-0.82041
C	1.86260	0.96602	0.55168
C	1.55479	-1.14526	-0.79412
C	2.23496	-0.26600	0.14737
C	-1.36825	0.42127	-0.14794
C	-0.75358	-0.89912	0.16487
H	-0.14889	-2.05047	-1.60353
H	2.19246	-1.65297	-1.51555
H	3.19926	-0.62169	0.50416
H	2.56491	1.47262	1.21085
H	1.05680	2.87600	0.12341
H	-1.08856	2.51401	-0.46542
C	-1.11155	-1.61092	1.23490
H	-0.67458	-2.58254	1.43719
H	-1.83631	-1.23031	1.94534
H	-3.33452	-0.35051	-0.33847
H	-3.14900	1.46946	-0.62923
C	-2.69009	0.51839	-0.38062

Carbon-3(S_0) TS
Absolute energy: -387.017799454 a.u
Point group: C_1

C	-0.09164	1.71262	-0.40825
C	1.22821	1.70606	-0.14344
C	0.09089	-1.61075	-0.60498
C	2.06205	0.71426	0.55032
C	1.41814	-1.53745	-0.46751
C	2.15814	-0.61592	0.41091
C	-1.06335	0.65600	-0.15791
C	-0.89578	-0.71281	0.01560
H	-0.32430	-2.41557	-1.21165
H	2.02603	-2.28958	-0.96637
H	2.92925	-1.10362	1.00657
H	2.76615	1.16978	1.24602
H	1.76753	2.61861	-0.39274
H	-0.49361	2.61846	-0.85504
C	-2.06505	-1.12441	0.71636
H	-2.53991	-2.09205	0.53190
H	-2.26088	-0.71683	1.69834
H	-3.13618	0.31982	-0.71883
H	-2.91307	1.74114	0.40160
C	-2.47844	0.83737	-0.03439

Carbon-3(T_1) closed
Absolute energy: -387.057336686 a.u
Point group: C_{2v}

C	-0.00000	1.74382	0.03865
C	-0.00000	1.72378	-1.36329
C	-0.00000	-1.74382	0.03865
C	-0.00000	0.70274	-2.33068
C	-0.00000	-1.72378	-1.36329
C	-0.00000	-0.70274	-2.33068
C	-0.00000	0.70879	0.96859
C	-0.00000	-0.70879	0.96859
H	0.00000	-2.73989	0.47547
H	0.00000	-2.71687	-1.80476
H	0.00000	-1.10438	-3.34089
H	0.00000	1.10438	-3.34089
H	0.00000	2.71687	-1.80476
H	0.00000	2.73989	0.47547
C	0.00000	-0.78166	2.48809
H	-0.88818	-1.24250	2.93097
H	0.88818	-1.24250	2.93097
H	-0.88818	1.24250	2.93097
H	0.88818	1.24250	2.93097
C	0.00000	0.78166	2.48809

Carbon-3(T_1) open
Absolute energy: -387.033393901 a.u
Point group: C_2

C	0.10297	1.68688	-0.09580
C	-0.46272	1.61081	1.20995
C	-0.10297	-1.68688	-0.09580
C	-0.35987	0.63248	2.15372
C	0.46272	-1.61081	1.20995
C	0.35987	-0.63248	2.15372
C	0.35987	0.66397	-1.04044
C	-0.35987	-0.66397	-1.04044
H	-0.39387	-2.68711	-0.41015
H	0.92502	-2.53449	1.55382
H	0.78457	-0.88003	3.12453

H	-0.78457	0.88003	3.12453
H	-0.92502	2.53449	1.55382
H	0.39387	2.68711	-0.41015
C	-1.19651	-0.90520	-2.09778
H	-1.69762	-1.86126	-2.20319
H	-1.39922	-0.14736	-2.84283
H	1.39922	0.14736	-2.84283
H	1.69762	1.86126	-2.20319
C	1.19651	0.90520	-2.09778

Carbon-3(T_1) TS
Absolute energy: -386.993881083 a.u
Point group: C_2

C	0.02355	1.73403	0.06940
C	0.27472	1.69283	-1.31255
C	-0.02355	-1.73403	0.06940
C	0.17627	0.68858	-2.27323
C	-0.27472	-1.69283	-1.31255
C	-0.17627	-0.68858	-2.27323
C	-0.17627	0.70406	0.99899
C	0.17627	-0.70406	0.99899
H	0.06569	-2.73530	0.48660
H	-0.49600	-2.66869	-1.73734
H	-0.34604	-1.06045	-3.28071
H	0.34604	1.06045	-3.28071
H	0.49600	2.66869	-1.73734
H	-0.06569	2.73530	0.48660
C	0.60214	-0.92212	2.34199
H	0.47731	-1.89088	2.82954
H	1.38552	-0.30124	2.75431
H	-1.38552	0.30124	2.75431
H	-0.47731	1.89088	2.82954
C	-0.60214	0.92212	2.34199

4a(S_0)
Absolute energy: -484.81603311
Point group: C_1

C	1.76872500	-0.94116000	-0.00020100
C	0.25699200	-0.70520300	-0.00201800
C	0.38608700	0.63370300	-0.00102600
C	1.91206200	0.64068800	0.00110500
C	-0.95722400	1.33576500	-0.00055200
H	-1.16900400	1.93797400	0.88734000
H	-1.16958200	1.93765100	-0.88852000
Si	-1.59034100	-0.50269200	0.00047900
H	-2.36279300	-0.93816600	-1.19711100
H	-2.35683600	-0.93572000	1.20278000
H	2.17204100	-1.43426200	-0.88808200
H	2.38941700	1.06048400	0.89137800
H	2.39234000	1.06201600	-0.88684200
H	2.16934800	-1.43504800	0.88850300

4b(S_0)
Absolute energy: -484.80982751
Point group: C_1

C	0.45589100	-1.57420100	-0.00019500
C	-0.30782500	-0.23849600	-0.00009700
C	0.95467200	0.51905300	0.00008300
C	1.78980300	-0.76026300	0.00022000
C	1.28690600	1.81375000	-0.00012800
Si	-1.98972300	0.16040100	0.00007600
H	0.30115100	-2.19383600	-0.88673700
H	2.41069000	-0.89982500	0.88839400
H	2.41117100	-0.89966200	-0.88765200
H	0.30075300	-2.19420500	0.88602300
H	2.32565800	2.12440100	0.00001500
H	0.53678400	2.59712800	-0.00045100
H	-3.02579200	-0.89035100	-0.00026300
H	-2.48097300	1.55167300	0.00030200

4-TS(S_0)
Energy: -484.767452787
Symmetry: C_1

C	-1.46462	-1.17774	-0.18468
C	-0.04995	-0.59713	-0.27067
C	-0.48066	0.69813	-0.03856
C	-1.90289	0.25612	0.32418
C	0.35576	1.80402	-0.20137
H	0.94888	1.86842	-1.10259
H	0.21006	2.73810	0.33354
Si	1.69163	-0.47399	0.09832
H	2.05207	-0.00253	1.44904
H	2.72437	-1.44405	-0.37190
H	-1.60801	-2.00530	0.51282
H	-2.71353	0.74811	-0.21991
H	-2.12582	0.27235	1.39341
H	-1.91669	-1.43967	-1.14433

4a(T_1)
Absolute energy: -484.71999435
Point group: C_1

C	1.65178900	-0.89522600	0.00098600
C	0.29682700	-0.72052400	-0.64064900
C	0.39374300	0.84796800	-0.52694800
C	1.59917500	0.63623000	0.38975600
C	-0.94417700	1.31566400	-0.02965800
H	-0.92988400	1.96808300	0.84582000
H	-1.58410600	1.75060400	-0.80336800
Si	-1.38679000	-0.57504800	0.16536700
H	-2.53075700	-0.97689200	-0.69647600
H	-1.61576900	-1.11579900	1.54028200
H	2.44922000	-1.07442000	-0.72708800
H	1.39914900	0.82243500	1.45188700
H	2.49639800	1.19081100	0.09851400
H	1.74665800	-1.61882200	0.81437000

4b(T_1)
Absolute energy: -484.77549583
Point group: C_1

C	0.49567400	-1.56897400	0.00024800
C	-0.24413000	-0.22820700	0.00021900
C	0.96254600	0.50725100	-0.00005600
C	1.82865600	-0.75090200	-0.00017300
C	1.26455400	1.84261100	0.00006700
Si	-2.04760400	0.22380300	-0.00009400
H	0.32884300	-2.18963400	-0.88619400
H	2.45008800	-0.88394900	0.88876000
H	2.44936400	-0.88418400	-0.88958800
H	0.32912300	-2.18952500	0.88680500
H	2.29102600	2.18922500	-0.00015200
H	0.48015600	2.59124800	0.00028300
H	-2.75355400	-0.28799000	1.21134300
H	-2.75239200	-0.28910800	-1.21176900

4-TS(T_1)
Energy: -484.707290931
Symmetry: C_1

C	1.51760	-1.05573	-0.05697
C	0.16013	-0.64336	-0.59508
C	0.48677	0.82134	-0.41003
C	1.74461	0.44262	0.36561
C	-0.63399	1.58790	0.00220
H	-0.52887	2.33768	0.78415
H	-1.38853	1.83716	-0.74136
Si	-1.51730	-0.53309	0.17348
H	-2.61657	-0.38543	-0.81940
H	-1.95740	-1.57358	1.16875
H	2.21319	-1.36407	-0.84410
H	1.66192	0.61250	1.44579
H	2.67608	0.89164	0.00926
H	1.53164	-1.80921	0.73378

5a(S_0)
Absolute energy: -563.53306580 a.u
Point group: C_1

C	-2.15333800	-0.82703100	-0.33346600
C	-2.26361200	0.55743600	0.32645100
C	-1.08824900	1.47311500	-0.06602000
C	0.21128100	0.71658800	-0.03886500
C	0.31362700	-0.63028100	0.04344200
C	-0.86442600	-1.56010700	0.08773700

H	-3.02947900	-1.43372700	-0.08484900
H	-3.21355700	1.03025600	0.05989600
H	-1.24078500	1.88823300	-1.07236100
H	-0.97620800	-1.96505500	1.10282500
H	-0.69594600	-2.42819100	-0.55907700
H	-2.15379000	-0.70444200	-1.42324500
H	-2.26984700	0.43326900	1.41593200
H	-1.03040500	2.33866700	0.60479000
C	1.61777000	1.31011400	-0.09503900
Si	2.17417300	-0.51528700	0.03887700
H	1.85686500	1.97701100	0.73896700
H	1.84441000	1.83328800	-1.02920000
H	2.91164200	-0.90528400	1.27452500
H	2.92036900	-1.08901400	-1.11792100

5b(S_0)
Absolute energy: -563.49415179 a.u
Point group: C_1

C	-1.59005700	-1.42674800	-0.10936900
C	-2.29261600	-0.06506800	-0.06487000
C	-1.38447200	1.04948100	-0.61235300
C	-0.02793800	1.07007600	0.07495600
C	0.63112500	-0.24715800	0.19252100
C	-0.25984000	-1.38461500	0.66434700
H	-2.23683400	-2.20372300	0.31142100
H	-3.22457400	-0.09708900	-0.63832900
H	-1.22700700	0.87487800	-1.68496100
H	-0.48695700	-1.23043000	1.72918000
H	0.25319200	-2.34796600	0.59171700
H	-1.39162200	-1.70403200	-1.15153900
H	-2.56704100	0.16882100	0.97098500
H	-1.86849200	2.02472100	-0.51268600
C	0.50419500	2.20832200	0.54225700
Si	2.27131700	-0.49037900	-0.30026800
H	3.10537300	0.59172100	-0.85545700
H	2.91689800	-1.81342300	-0.17174200
H	1.44743100	2.21623600	1.07605500
H	-0.00118000	3.15985900	0.41416600

5-TS(S_0)
Absolute energy: -563.474507350 a.u
Point group: C_1

C	1.94767	-1.05827	0.26112
C	2.28203	0.40886	-0.04582
C	1.15267	1.36357	0.38175
C	-0.19036	0.87523	-0.13700
C	-0.44471	-0.51329	-0.22062
C	0.66311	-1.50927	-0.46216
H	2.78327	-1.70242	-0.03071
H	3.21299	0.69651	0.45245
H	1.11012	1.40755	1.47815
H	0.87156	-1.57851	-1.53915
H	0.37938	-2.51302	-0.13622
H	1.81288	-1.18131	1.34232
H	2.45671	0.51941	-1.12302
H	1.35862	2.37780	0.03068
C	-1.24744	1.72770	-0.44314
Si	-2.15515	-0.59467	0.24573
H	-2.60698	0.04871	1.49325
H	-3.01448	-1.77847	-0.05344
H	-1.89444	1.50965	-1.28045
H	-1.27538	2.75220	-0.07885

5a(T_1)
Absolute energy: -563.41939010 a.u
Point group: C_1

C	-2.09174300	-0.75919800	-0.36062800
C	-2.15805300	0.74629600	-0.06081300
C	-0.80269400	1.44186600	-0.29338000
C	0.26438500	0.79870500	0.55115400
C	0.26831000	-0.72579700	0.40017800
C	-1.00114900	-1.48011700	0.49011200
H	-3.06285000	-1.22763300	-0.17100600
H	-2.92752700	1.21211700	-0.68464100
H	-0.54885600	1.36810000	-1.36894000
H	-1.35223400	-1.48958600	1.53481800
H	-0.89768600	-2.52062500	0.17092800
H	-1.86453800	-0.90796300	-1.42262500
H	-2.46091000	0.89703500	0.98218400
H	-0.86019300	2.51458600	-0.07154600
C	1.72163800	1.17822500	0.37721000
Si	1.95824500	-0.58978300	-0.36664400
H	2.27778600	1.23098700	1.31992200
H	1.90849300	2.08585000	-0.19832200
H	3.03981800	-1.39808800	0.26820500
H	2.12909500	-0.70770200	-1.84895400

5b(T_1)
Absolute energy: -563.45732516 a.u
Point group: C_1

C	-1.69389600	-1.37751000	-0.31752000
C	-2.30467000	-0.16220500	0.37961900
C	-1.61058100	1.11528900	-0.09829500
C	-0.08416500	1.04762000	-0.04256300
C	0.56734500	-0.19831100	-0.01119400
C	-0.20629700	-1.50489700	0.03898700
H	-2.21738000	-2.29730300	-0.03928500
H	-3.37896700	-0.09784000	0.18221900
H	-1.90486600	1.31231700	-1.13711800
H	-0.11510500	-1.92035700	1.05478300
H	0.27138700	-2.24648500	-0.61330900
H	-1.80400400	-1.26469500	-1.40260200
H	-2.18757500	-0.26612600	1.46531800
H	-1.95032400	1.97725000	0.48306300
C	0.60027300	2.25223900	-0.04584400
Si	2.43844600	-0.38800600	0.04191800
H	2.85963100	-1.15018500	1.25656000
H	2.92750800	-1.13543500	-1.15627100
H	1.68394400	2.29069500	-0.03858200
H	0.06944800	3.19688200	-0.06077400

5-TS(T_1)
Absolute energy: -563.406179961 a.u
Point group: C_1

C	2.03135	-0.92024	0.30684
C	2.25529	0.56747	0.00332
C	1.00989	1.40794	0.33638
C	-0.20230	0.87557	-0.37997
C	-0.36260	-0.60508	-0.36728
C	0.82269	-1.49625	-0.47719
H	2.92938	-1.49797	0.06725
H	3.11378	0.93834	0.57155
H	0.83943	1.36914	1.42828
H	1.11135	-1.57040	-1.53860
H	0.59692	-2.51327	-0.14493
H	1.84842	-1.04579	1.38044
H	2.50094	0.69168	-1.05821
H	1.16651	2.46292	0.08787
C	-1.49275	1.47487	-0.29271
Si	-2.08136	-0.57872	0.32710
H	-2.17344	1.34839	-1.13439
H	-1.60847	2.44031	0.19557
H	-3.17119	-0.80995	-0.66861
H	-2.38405	-1.53706	1.45809

6a(S_0)
Absolute energy: -562.30126630 a.u
point group: C_1

C	-1.17750300	1.37495100	-0.23324900
C	0.15675600	0.69764900	-0.06627200
C	0.27519800	-0.65505700	-0.04529200
C	-0.89503700	-1.52240200	-0.15371900
C	-2.11899700	-0.99127300	-0.01535500
C	-2.31344200	0.47657500	0.30274200
H	-1.19425500	2.34922500	0.26442600
H	-0.76863100	-2.58427400	-0.33710800
H	-3.00217500	-1.62056400	-0.06610300
H	-2.37059300	0.58184800	1.39687400
H	-1.32479700	1.57621200	-1.30542900
H	-3.27636200	0.82515100	-0.08109100
C	1.54709400	1.31372900	0.00925300
Si	2.12848300	-0.51145000	0.07638500

H	1.82878900	1.89162500	-0.87745400
H	1.71747900	1.93884600	0.89124400
H	2.94889300	-0.99493800	-1.06992800
H	2.79847900	-0.96786400	1.32654200

6b(S_0)
Absolute energy: -562.27198561 a.u
Point group: C_1

C	-1.51346600	0.88883000	-0.62986600
C	-0.13629200	0.99912200	-0.00689400
C	0.60854000	-0.27857300	0.04552700
C	-0.19822100	-1.48660000	0.18412300
C	-1.54292000	-1.47271900	0.22406400
C	-2.34075700	-0.20705400	0.06744600
H	-2.02899400	1.85102400	-0.58682100
H	0.32109500	-2.43698900	0.27349500
H	-2.08378200	-2.40312700	0.36663400
H	-2.67440600	0.14811400	1.05279200
H	-1.40428700	0.61743900	-1.68693300
H	-3.25298900	-0.40587400	-0.50558500
C	0.31904700	2.15421500	0.49665800
Si	2.33726000	-0.38282300	-0.15929400
H	3.02933700	-1.67752000	-0.00400400
H	3.18924000	0.79577000	-0.39648400
H	1.27073500	2.22137500	1.01126100
H	-0.26317200	3.06598300	0.41941300

6-TS(S_0)
Absolute energy: -562.249344987 a.u
Point group: C_1

C	1.24295	1.20293	0.53233
C	-0.10123	0.82041	-0.05393
C	-0.41522	-0.55833	-0.09978
C	0.65021	-1.54539	-0.11901
C	1.93789	-1.15723	-0.11547
C	2.33010	0.30344	-0.09399
H	1.47268	2.25709	0.36402
H	0.39668	-2.60074	-0.12349
H	2.73277	-1.89548	-0.14610
H	2.53901	0.63303	-1.12303
H	1.22330	1.03197	1.61622
H	3.26536	0.43423	0.45834
C	-1.07665	1.70587	-0.50128
Si	-2.18019	-0.51696	0.15331
H	-3.08021	-1.63524	-0.25384
H	-2.71244	0.14881	1.35575
H	-1.63857	1.48566	-1.39795
H	-1.08432	2.74784	-0.18940

6a(T_1)
Absolute energy: -562.21880896 a.u
Point group: C_1

C	-1.21777000	1.38468200	-0.20077500
C	0.11405000	0.73894500	-0.06959100
C	0.28849000	-0.71191900	-0.04051700
C	-0.76840700	-1.56714100	-0.05867300
C	-2.11552000	-1.00745000	-0.08004300
C	-2.35251700	0.42427500	0.27386100
H	-1.25702300	2.33157700	0.35330900
H	-0.64022100	-2.64476400	-0.06241300
H	-2.96275200	-1.65049700	-0.28724700
H	-2.42381100	0.52370200	1.36980200
H	-1.41100400	1.64653000	-1.25279600
H	-3.31814100	0.76058700	-0.11586200
C	1.50100300	1.33727500	0.03408400
Si	2.14583100	-0.47305200	0.04246300
H	1.79600300	1.96506300	-0.81639300
H	1.67426400	1.92602400	0.94487300
H	2.94492100	-0.89099300	-1.14211200
H	2.86014200	-0.93651100	1.26429200

6b(T_1)
Absolute energy: -562.24020480 a.u
Point group: C_1

C	-1.67347000	0.92395600	-0.35580300
C	-0.18358600	1.01267200	-0.05948600
C	0.54826900	-0.23012300	-0.07350900
C	-0.17745500	-1.45849400	-0.12273200
C	-1.52991400	-1.53226100	0.05796700
C	-2.33646600	-0.29207900	0.30552500
H	-2.17414400	1.84830300	-0.05897600
H	0.37550200	-2.38462500	-0.25603100
H	-2.02424300	-2.49795500	0.07225400
H	-2.42552300	-0.12888200	1.39076200
H	-1.79092500	0.82896900	-1.44316200
H	-3.35853100	-0.41259000	-0.06617900
C	0.39728400	2.22198800	0.15205000
Si	2.42783300	-0.32258700	0.01802700
H	2.96024500	-1.15945300	-1.09697900
H	2.90251400	-0.90612700	1.30826900
H	1.46419300	2.31962800	0.32237100
H	-0.18671400	3.13499200	0.15121400

6-TS(T_1)
Absolute energy: -562.194856512 a.u
Point group: C_1

C	1.23348	1.26761	0.41427
C	-0.06403	0.83885	-0.19714
C	-0.35239	-0.60998	-0.22152
C	0.68565	-1.52816	-0.08879
C	2.00751	-1.10417	-0.06364
C	2.37615	0.35283	-0.09032
H	1.45436	2.31649	0.19709
H	0.46769	-2.58742	0.01226
H	2.80836	-1.83421	-0.01070
H	2.63897	0.64294	-1.11816
H	1.17920	1.17528	1.51196
H	3.28023	0.51764	0.50529
C	-1.28214	1.56198	-0.23962
Si	-2.17332	-0.48978	0.17806
H	-1.35754	2.54841	0.21436
H	-1.89668	1.47453	-1.13664
H	-2.66187	-1.45321	1.22723
H	-3.11165	-0.61732	-0.97494

7a(S_0)
Absolute energy: -522.03171287 a.u
Point group: C_s

C	-1.62134400	0.81280300	0.00000000
C	-2.21978600	-0.63693500	0.00000000
H	-3.28388000	-0.83921700	0.00000000
C	-1.21994800	-1.54056900	0.00000000
H	-1.29202300	-2.61719200	0.00000000
C	-0.28192400	0.69464100	0.00000000
C	0.00000000	-0.74349500	0.00000000
C	1.46308100	-0.87576300	0.00000000
H	1.82655000	-1.45333400	0.86581600
H	1.82655000	-1.45333400	-0.86581600
Si	1.58694700	1.07433800	0.00000000
H	2.11173900	1.67782000	-1.23869800
H	2.11173900	1.67782000	1.23869800
H	-2.23840500	1.70262400	0.00000000

7b(S_0)
Absolute energy: -522.09364994 a.u
Point group: C_1

C	0.30404600	-1.47627800	-0.00009300
C	1.71083500	-1.27357600	0.00004100
H	2.45184700	-2.05958300	0.00007500
C	1.95433400	0.07991100	0.00004100
H	2.92506000	0.55737400	0.00001200
C	-0.36838100	-0.23962300	-0.00002400
C	0.69483400	0.79945400	0.00010100
C	0.56654200	2.13931900	-0.00005300
H	-0.39732400	2.63547900	-0.00006000
H	1.44052800	2.78045100	-0.00021100
Si	-2.12032600	-0.10699800	-0.00000500
H	-2.92904500	-1.33399500	0.00020600
H	-2.80802200	1.19235900	0.00019800
H	-0.17173300	-2.44936000	-0.00022600

7a(T_1)
Absolute energy: -522.03622097 a.u
Point group: C_s

C	-1.25013700	1.39241400	0.00000000
C	-2.27819400	0.40805400	0.00000000
H	-3.34078000	0.61395900	0.00000000
C	-1.69540500	-0.89594500	0.00000000
H	-2.23844200	-1.83160000	0.00000000
C	0.00000000	0.70395300	0.00000000
C	-0.28116300	-0.70314100	0.00000000
C	1.03087400	-1.42253400	0.00000000
H	1.18080400	-2.05917400	0.87929500
H	1.18080400	-2.05917400	-0.87929500
Si	1.88062200	0.32216100	0.00000000
H	2.57183800	0.73347700	-1.23810000
H	2.57183800	0.73347700	1.23810000
H	-1.41061200	2.46198300	0.00000000

7b(T_1)
Absolute energy: -522.02778944 a.u
Point group: C_1

C	-0.45840400	-1.49733700	0.05868100
C	-1.81608900	-1.19435100	-0.00719400
H	-2.62112500	-1.91650600	-0.02534600
C	-1.97976300	0.20931200	-0.04272000
H	-2.91682100	0.74431600	-0.11679300
C	0.30753300	-0.28633600	0.03235800
C	-0.65600600	0.82713300	0.00767600
C	-0.39244200	2.15058200	0.03456200
H	0.61805200	2.53837900	0.07788500
H	-1.19446300	2.87943000	0.01958800
Si	2.18295200	-0.18977100	-0.09297200
H	2.82922800	-1.43868700	0.34912600
H	2.73756400	1.08973700	0.38500600
H	-0.04273100	-2.49389800	0.11196000

7-TS(T_1)
Absolute energy: -521.999117941 a.u
Point group: C_1

C	-1.08029	-1.36849	-0.21594
C	-2.13150	-0.56092	0.09804
H	-3.15648	-0.87526	0.23220
C	-1.66907	0.80090	0.21240
H	-2.26251	1.64930	0.52703
C	0.12049	-0.50892	-0.34103
C	-0.26998	0.85229	-0.12353
C	0.62912	1.94584	-0.08658
H	1.52751	1.95667	-0.69252
H	0.34229	2.88569	0.36644
Si	1.84830	-0.62233	0.14276
H	2.24809	-1.45401	1.29211
H	2.93115	0.02286	-0.61242
H	-1.09886	-2.43682	-0.37162

8a(S_0)
Absolute energy: -599.56693304 a.u
Point group: C_1

C	-2.13700400	1.13478500	-0.00013700
C	-0.81637700	1.57614600	0.00000500
C	0.33739800	0.78452100	0.00009700
C	-2.63086700	-0.17578900	0.00005100
C	0.45060100	-0.63052900	0.00011800
C	-1.93582000	-1.38382400	-0.00000600
C	-0.55145400	-1.59421700	-0.00003000
H	-2.89283700	1.91422100	-0.00031100
H	-0.66781300	2.65233300	0.00004800
H	-3.71298500	-0.26118900	0.00021300
H	-2.55115900	-2.27836700	0.00008100
H	-0.23508400	-2.63363000	0.00000300
C	1.76786300	1.30263700	0.00024900
Si	2.36667600	-0.51682800	0.00001800
H	3.00682400	-1.02356100	1.23171300
H	3.00504900	-1.02128700	-1.23357400
H	2.00407700	1.90310500	0.88305400
H	2.00442100	1.90157600	-0.88355800

8b(S_0)
Absolute energy: -599.51748111 a.u
Point group: C_1

C	2.19661100	0.66383800	-0.53676400
C	1.07052500	1.42687000	-0.44376500
C	-0.18581700	1.06949100	0.19720500
C	2.40485600	-0.64633700	-0.01801600
C	-0.68363300	-0.32824400	0.11158300
C	1.48676100	-1.57971200	0.42095500
C	0.08612400	-1.46885600	0.34525800
H	3.06764700	1.13414900	-0.97939000
H	1.13323800	2.44588600	-0.81573000
H	3.44032700	-0.97474400	-0.01519600
H	1.87677200	-2.54583200	0.72000100
H	-0.45028600	-2.41167600	0.44127900
C	-0.92073100	2.01807700	0.81466300
Si	-2.37318800	-0.57398500	-0.40423600
H	-3.12724800	0.50946900	-1.04921200
H	-3.01930500	-1.87943100	-0.18912500
H	-1.79203000	1.76457000	1.40872100
H	-0.63265800	3.06264600	0.79123900

8-TS(S_0)
Absolute energy: -599.515215999 a.u
Point group: C_1

C	-2.12991	0.89444	-0.44356
C	-0.91584	1.51562	-0.34790
C	0.28380	0.95665	0.22415
C	-2.49011	-0.41941	-0.02686
C	0.58850	-0.47884	0.10039
C	-1.69170	-1.48713	0.32558
C	-0.28178	-1.53876	0.26931
H	-2.94890	1.49947	-0.81745
H	-0.86322	2.55745	-0.65170
H	-3.55751	-0.61870	-0.03577
H	-2.19683	-2.41966	0.55056
H	0.15141	-2.53598	0.31600
C	1.25225	1.73734	0.78809
Si	2.31937	-0.59509	-0.39393
H	3.20677	-1.68700	0.04825
H	2.81720	0.33637	-1.41180
H	1.98557	1.30035	1.46045
H	1.24314	2.81942	0.72135

8a(T_1)
Absolute energy: -599.46197595 a.u
Point group: C_1

C	-0.34505900	-0.70011700	0.36157800
C	-0.50568700	0.72180600	0.48363500
C	0.50740900	1.63415500	0.14408300
C	0.80412400	-1.55353900	0.55399800
C	1.79216400	1.28875700	-0.30795000
C	2.04198500	-1.22840400	0.08060000
C	2.44367700	0.04964700	-0.41853400
H	0.25561800	2.68773100	0.19165100
H	0.66071100	-2.49192300	1.08266100
H	2.40306300	2.13682300	-0.60526000
H	2.82543000	-1.97469600	0.16756100
H	3.45550700	0.09968400	-0.80492700
Si	-2.04368300	-0.60766200	-0.55917700
C	-1.96391400	1.01518600	0.49049200
H	-2.98236200	-1.65234800	-0.08674200
H	-1.94313400	-0.43834900	-2.01980400
H	-2.45326900	0.77595400	1.43981900
H	-2.25819700	1.99943900	0.13610300

8b(T_1)
Absolute energy: -599.49015589 a.u
Point group: C_1

C	-2.37663400	0.67711800	0.02345200
C	-1.21574700	1.44337500	0.02499300
C	0.16171300	1.07833400	-0.00153900
C	-2.51260300	-0.70856900	-0.00667900
C	0.68037700	-0.28210700	0.02037500
C	-1.48020900	-1.65122600	-0.02132500

C	-0.09878500	-1.45416500	0.00436600
H	-3.30182600	1.24413900	0.04207300
H	-1.38528600	2.51500000	0.04369600
H	-3.52411200	-1.09895800	-0.01305600
H	-1.79312000	-2.69054200	-0.03821700
H	0.46295900	-2.38419200	0.01768900
C	1.06279000	2.15494600	-0.04456100
Si	2.50573500	-0.61961600	-0.03710300
H	3.46201300	0.38252900	0.45675900
H	2.83989600	-2.04174800	0.14362000
H	2.13505500	2.02807000	-0.06265400
H	0.69872000	3.17409500	-0.06496400

8-TS(T_1)
Absolute energy: -599.456980581 a.u
Point group: C_1

C	0.55112	-0.54420	-0.21363
C	0.30700	0.89344	-0.13647
C	-0.88904	1.56347	0.13474
C	-0.40417	-1.58723	-0.16693
C	-2.20585	1.01321	0.15879
C	-1.77135	-1.48581	-0.09155
C	-2.58740	-0.29281	0.03952
H	-0.81458	2.63735	0.27012
H	-0.01320	-2.59973	-0.21369
H	-3.00296	1.73782	0.28541
H	-2.32431	-2.41818	-0.11244
H	-3.65518	-0.48136	0.07830
Si	2.33377	-0.60103	0.21052
C	1.51816	1.63710	-0.24846
H	3.43334	-0.55381	-0.77106
H	2.73921	-1.12045	1.53354
H	2.24535	1.38715	-1.02089
H	1.60872	2.64260	0.14735

9a(S_0)
Absolute energy: -599.80005030 a.u
Point group: C_1

C	2.14439100	1.13670600	-0.00025100
C	0.76142600	1.60401300	-0.00015100
C	-0.34617900	0.78641900	-0.00003700
C	2.65249800	-0.11554200	-0.00024100
C	-0.49519300	-0.64085300	0.00001500
C	1.91946000	-1.41397600	-0.00012000
C	0.58661100	-1.62098100	-0.00001300
H	2.88719700	1.93815800	-0.00034700
H	0.60497100	2.67971400	-0.00017700
H	3.73774200	-0.20727400	-0.00033800
H	2.55853300	-2.29653800	-0.00014100
H	0.26959700	-2.66608500	0.00004600
C	-1.79786200	1.30593400	0.00012800
Si	-2.30088700	-0.53670800	0.00028500
H	-3.16363900	-0.99671100	-1.16435800
H	-3.16336000	-0.99666900	1.16514800
H	-2.03488800	1.90440900	-0.88742200
H	-2.03464300	1.90458700	0.88762300

9b(S_0)
Absolute energy: -599.80823683 a.u
Point group: C_1

C	2.37773400	0.68672200	-0.07534700
C	1.23926900	1.43713300	-0.05170700
C	-0.17545900	1.09383500	0.04368700
C	2.52943200	-0.72867100	-0.01670000
C	-0.69977900	-0.30918300	0.07768400
C	1.51165000	-1.64245600	0.05258000
C	0.10187000	-1.43919900	0.08853200
H	3.30699400	1.25190600	-0.14145600
H	1.40367500	2.51357800	-0.09741500
H	3.54848200	-1.10877600	-0.02827200
H	1.81385300	-2.68888400	0.09622500
H	-0.45234000	-2.37511900	0.13931500
C	-1.04988700	2.13545900	0.09598400
Si	-2.56081300	-0.60172500	-0.19970400
H	-3.25211700	0.25363500	0.85237400
H	-2.72035600	-1.97338800	0.44463500
H	-2.11613000	1.98965600	0.18162300
H	-0.68965500	3.15970900	0.06054500

9-TS(S_0)
Absolute energy: -599.758169398 a.u
Point group: C_1

C	2.17492	0.98627	0.24891
C	0.91715	1.57618	0.00505
C	-0.32714	0.91958	-0.19134
C	2.58671	-0.33024	0.19234
C	-0.56826	-0.49365	-0.16378
C	1.77108	-1.47130	-0.13727
C	0.42087	-1.54318	-0.31322
H	2.97069	1.70311	0.46430
H	0.89226	2.66230	-0.02864
H	3.63909	-0.52967	0.37795
H	2.31092	-2.41587	-0.21807
H	0.00865	-2.53844	-0.47945
C	-1.57510	1.64089	-0.28780
Si	-2.34277	-0.60514	0.23023
H	-2.81825	-2.05313	0.08387
H	-2.87121	-0.24391	1.58229
H	-2.13614	1.51082	-1.20825
H	-1.59856	2.66951	0.08555

9a(T_1)
Absolute energy: -599.79432411 a.u
Point group: C_1

C	2.12703100	1.17102800	-0.00015800
C	0.78201300	1.59683900	-0.00011400
C	-0.36556300	0.78715200	-0.00006900
C	2.63842500	-0.15167800	-0.00017200
C	-0.46404100	-0.65216900	-0.00004200
C	1.95455500	-1.37975000	-0.00013600
C	0.55960400	-1.62096200	-0.00006500
H	2.87545400	1.96309300	-0.00019100
H	0.61231500	2.67413500	-0.00012100
H	3.72638100	-0.22547000	-0.00021600
H	2.58643000	-2.26847000	-0.00016400
H	0.25296400	-2.66647800	-0.00003500
C	-1.81325700	1.30470700	0.00003800
Si	-2.29652800	-0.53942300	0.00026400
H	-3.11718800	-1.02081800	-1.17474700
H	-3.11663800	-1.02023300	1.17590700
H	-2.09053700	1.89262000	-0.88670900
H	-2.09039800	1.89254900	0.88688500

9b(T_1)
Absolute energy: -599.77329395 a.u
Point group: C_1

C	2.32162900	0.68266500	-0.27122200
C	1.17699300	1.46558100	-0.19521600
C	-0.20022500	1.09663300	0.12380900
C	2.49211600	-0.69381200	-0.08507400
C	-0.68902900	-0.29317700	0.15487200
C	1.49008600	-1.65483000	0.18978100
C	0.11787800	-1.45333200	0.28581800
H	3.23810600	1.23675500	-0.47866500
H	1.32820000	2.53680900	-0.31421700
H	3.51303800	-1.06486500	-0.15725800
H	1.83066400	-2.68064800	0.32043900
H	-0.44740800	-2.36955200	0.45903800
C	-1.06056300	2.12547200	0.39066400
Si	-2.49239300	-0.58186100	-0.19190800
H	-2.89270200	-0.19595900	-1.60102600
H	-2.75122700	-2.06961900	-0.12861900
H	-2.07313900	1.94210500	0.73289200
H	-0.74533700	3.15983800	0.29354400

9-TS(T_1)
Absolute energy: -599.752867609 a.u
Point group: C_1

C	2.22686	0.97178	-0.16611
C	0.96420	1.56062	-0.12554
C	-0.29672	0.91691	0.12049
C	2.61290	-0.36639	-0.03155
C	-0.55931	-0.48742	0.14384
C	1.76618	-1.50219	0.11199
C	0.38477	-1.54937	0.17630
H	3.05269	1.67335	-0.29637
H	0.92958	2.64488	-0.21045
H	3.68168	-0.56543	-0.06899
H	2.27734	-2.46439	0.14443
H	-0.04447	-2.55066	0.21273
C	-1.51379	1.66625	0.22043
Si	-2.40871	-0.54310	-0.24104
H	-2.71097	-1.82057	-1.03554
H	-3.27504	-0.76996	0.99157
H	-1.54749	2.69270	-0.14696
H	-2.15183	1.50245	1.08509

10a(S_0)
Absolute energy: -714.799105129 a.u
Point group: C_s

C	1.34367	3.28398	0.00000
C	0.11500	2.67158	0.00000
C	0.00000	1.25594	0.00000
C	1.20026	0.46494	0.00000
C	2.45297	1.13452	0.00000
C	2.52514	2.50578	0.00000
H	-2.16398	1.22001	0.00000
H	1.41345	4.36589	0.00000
H	-0.79324	3.26555	0.00000
C	-1.26599	0.60930	0.00000
C	1.11282	-0.95434	0.00000
H	3.36015	0.53904	0.00000
H	3.49107	2.99844	0.00000
C	-0.12452	-1.54749	0.00000
C	-1.32169	-0.76210	0.00000
H	2.02672	-1.54099	0.00000
C	-0.57663	-3.00897	0.00000
H	-0.26891	-3.56988	0.88611
Si	-2.36918	-2.31706	0.00000
H	-3.19703	-2.59407	1.20507
H	-3.19703	-2.59407	-1.20507
H	-0.26891	-3.56988	-0.88611

10b(S_0)
Absolute energy: -714.731585963 a.u
Point group: C_1

C	3.28557	-1.06038	0.00075
C	1.99765	-1.55005	-0.00781
C	0.88876	-0.67281	-0.00761
C	1.11897	0.74329	0.00600
C	2.46070	1.21557	0.01479
C	3.51622	0.33532	0.01209
H	-0.59912	-2.21993	-0.01398
H	4.12738	-1.74322	-0.00133
H	1.81884	-2.62032	-0.01612
C	-0.45173	-1.14335	-0.01249
C	0.01290	1.60786	0.00770
H	2.63756	2.28594	0.02419
H	4.53401	0.70885	0.01909
C	-1.32464	1.14401	-0.00364
C	-1.55060	-0.30366	0.00517
H	0.18711	2.67942	0.01106
C	-2.37137	2.06373	-0.02640
H	-3.40934	1.76014	-0.04790
Si	-3.22987	-1.09369	-0.06543
H	-4.27900	-0.41218	0.73744
H	-3.12602	-2.53164	0.29958
H	-2.16784	3.12733	-0.02727

10(S_0)-TS
Absolute energy: -714.722943916 a.u
Point group: C_1

C	3.34652	-0.95020	-0.03025
C	2.09684	-1.50051	-0.17133
C	0.93239	-0.68928	-0.13519
C	1.07792	0.72888	0.06618
C	2.39189	1.26155	0.21269
C	3.49314	0.44678	0.16470
H	-0.47398	-2.31913	-0.25626
H	4.22729	-1.58103	-0.06718
H	1.98133	-2.56983	-0.31511
C	-0.37076	-1.23834	-0.21859
C	-0.06455	1.54865	0.08228
H	2.50575	2.33022	0.36135
H	4.48559	0.86868	0.27702
C	-1.34059	1.00646	-0.12888
C	-1.48856	-0.43252	-0.14812
H	0.05725	2.62383	0.16912
C	-2.49236	1.79503	-0.37031
H	-3.23263	1.47053	-1.08710
Si	-3.23710	-0.89883	0.24769
H	-3.61840	-2.29595	-0.11045
H	-3.56011	-0.63248	1.67113
H	-2.54402	2.82982	-0.04918

10a(T_1)
Absolute energy: -714.704325495 a.u
Point group: C_s

C	1.41400	3.31149	0.00000
C	0.13139	2.67402	0.00000
C	-0.00000	1.27644	0.00000
C	1.21091	0.47322	0.00000
C	2.45057	1.12713	0.00000
C	2.55035	2.55720	0.00000
H	-2.16265	1.24282	0.00000
H	1.46678	4.39407	0.00000
H	-0.76491	3.28466	0.00000
C	-1.26453	0.63533	0.00000
C	1.10899	-0.94308	0.00000
H	3.35695	0.53121	0.00000
H	3.52887	3.02234	0.00000
C	-0.18991	-1.55928	0.00000
C	-1.33982	-0.80276	0.00000
H	2.01032	-1.54648	0.00000
C	-0.59020	-3.02782	0.00000
H	-0.26305	-3.58048	0.88645
Si	-2.38308	-2.34503	0.00000
H	-3.21834	-2.63423	1.20003
H	-3.21834	-2.63423	-1.20003
H	-0.26305	-3.58048	-0.88645

10b(T_1)
Absolute energy: -714.729398138 a.u
Point group: C_1

C	3.29307	-1.05470	0.00411
C	2.00306	-1.54674	-0.00421
C	0.89693	-0.67229	-0.00428
C	1.12267	0.74037	0.00502
C	2.45964	1.21639	0.01311
C	3.51975	0.33774	0.01271
H	-0.59655	-2.22258	-0.01446
H	4.13539	-1.73687	0.00470
H	1.82623	-2.61738	-0.01051
C	-0.45074	-1.14581	-0.01112
C	0.00908	1.60534	0.00309
H	2.63419	2.28716	0.01955
H	4.53616	0.71502	0.01940
C	-1.32008	1.13716	-0.00901
C	-1.54036	-0.30851	-0.00376
H	0.18210	2.67714	0.00867
C	-2.38218	2.04705	-0.02490
H	-3.41595	1.72861	-0.02694
Si	-3.24420	-1.07748	-0.06499
H	-4.22319	-0.45587	0.86841
H	-3.13162	-2.53975	0.19067
H	-2.19301	3.11325	-0.03433

10(T_1)-TS
Absolute energy: -714.665668719 a.u
Point group: C_1

C	3.44491	-0.82159	-0.01101
C	2.18199	-1.45122	-0.13206
C	0.99867	-0.71881	-0.10530
C	1.07795	0.71518	0.04856
C	2.34443	1.31349	0.17497
C	3.52458	0.54694	0.14319
H	-0.34665	-2.43039	-0.13797
H	4.34541	-1.42454	-0.03408
H	2.13230	-2.52955	-0.23970
C	-0.29865	-1.34728	-0.17049
C	-0.11548	1.48595	0.05235
H	2.40406	2.39011	0.29465
H	4.48692	1.03600	0.23764
C	-1.38299	0.84313	-0.17060
C	-1.46281	-0.57258	-0.16988
H	-0.05686	2.56624	0.12784
C	-2.64328	1.48631	-0.35093
H	-3.19128	1.31486	-1.27025
Si	-3.24227	-0.71020	0.25689
H	-4.01022	-1.92735	-0.16281
H	-3.57965	-0.40807	1.66667
H	-2.80813	2.47837	0.06884

11a(S_0)
Absolute energy: -790.955519548 a.u
Point group: C_s

C	4.10789	1.08902	0.00000
C	3.53184	2.35179	0.00000
C	2.12622	2.53456	0.00000
C	1.37378	1.38775	0.00000
C	1.96383	0.09496	0.00000
C	3.32275	-0.09094	0.00000
H	5.18869	1.00273	0.00000
H	4.17582	3.22417	0.00000
H	1.69615	3.52920	0.00000
H	3.79002	-1.06870	0.00000
C	0.59518	-0.53483	0.00000
C	0.00000	0.76616	0.00000
C	-1.35598	0.96561	0.00000
C	-2.12615	-0.22615	0.00000
C	-1.53917	-1.50175	0.00000
C	-0.13279	-1.69681	0.00000
H	-1.81390	1.94824	0.00000
H	0.30991	-2.68659	0.00000
Si	-3.83381	-0.98557	0.00000
C	-2.68076	-2.51744	0.00000
H	-2.70928	-3.15681	0.88662
H	-2.70928	-3.15681	-0.88662
H	-4.68727	-0.78447	-1.20328
H	-4.68727	-0.78447	1.20328

11b(S_0)
Absolute energy: -790.901403178 a.u
Point group: C_1

C	4.15616	0.44021	-0.14137
C	4.02158	-0.93861	0.05843
C	2.76683	-1.55520	0.18881
C	1.66931	-0.71639	0.10780
C	1.80730	0.68632	-0.09219
C	3.04202	1.29233	-0.22248
H	5.15176	0.85939	-0.23491
H	4.91772	-1.54682	0.11318
H	2.68459	-2.62470	0.34279
H	3.16493	2.35787	-0.37709
C	0.33132	0.85957	-0.06129
C	0.19318	-0.59496	0.13661
C	-1.00319	-1.20858	0.19599
C	-2.19539	-0.37810	0.07477
C	-2.05425	1.11129	0.09740
C	-0.71550	1.69268	-0.10774
H	-1.10621	-2.28616	0.27571
H	-0.63034	2.76824	-0.21686
Si	-3.71061	-1.19430	-0.26797
C	-3.09236	1.93755	0.36012
H	-4.07382	1.57068	0.63240
H	-2.96448	3.01310	0.32783
H	-4.97792	-0.49863	-0.55079
H	-3.77968	-2.66136	-0.12983

11(S_0)-TS
Absolute energy: -790.890605330 a.u
Point group: C_1

C	4.15696	0.54072	0.19460
C	4.08799	-0.83464	-0.02087
C	2.85861	-1.50541	-0.18804
C	1.72985	-0.71731	-0.12577
C	1.80119	0.68564	0.09267
C	2.99851	1.34385	0.25839
H	5.12933	1.00483	0.31555
H	5.00940	-1.40505	-0.05997
H	2.82694	-2.57590	-0.35312
H	3.07036	2.41200	0.42651
C	0.30830	0.78648	0.03441
C	0.23967	-0.65042	-0.19521
C	-0.93626	-1.32469	-0.27568
C	-2.11420	-0.51659	-0.13725
C	-2.04409	0.93049	-0.17548
C	-0.77660	1.59131	0.08924
H	-1.00426	-2.40523	-0.34103
H	-0.73158	2.66798	0.20827
Si	-3.78443	-0.90275	0.37386
C	-3.21377	1.60763	-0.50288
H	-3.89644	1.19311	-1.22943
H	-3.34710	2.65805	-0.26170
H	-4.31144	-0.26459	1.59159
H	-4.33995	-2.26919	0.18044

11a(T_1)
Absolute energy: -790.882241353 a.u
Point group: C_s

C	-1.45471	-1.55823	0.00000
C	-0.08644	-1.73675	0.00000
C	0.65497	-0.54249	0.00000
C	0.00000	0.79990	0.00000
C	-1.39135	0.95079	0.00000
C	-2.10085	-0.23824	0.00000
C	1.93364	0.08846	0.00000
C	3.33243	-0.04121	0.00000
C	4.05013	1.13886	0.00000
C	3.42068	2.43911	0.00000
C	2.04548	2.59898	0.00000
C	1.28945	1.42216	0.00000
H	0.36901	-2.72135	0.00000
H	-1.87900	1.91990	0.00000
H	1.59742	3.58622	0.00000
H	4.06143	3.31328	0.00000
H	5.13379	1.10257	0.00000
H	3.83472	-1.00180	0.00000
Si	-3.79025	-1.04630	0.00000
C	-2.60808	-2.55858	0.00000
H	-2.63697	-3.20081	0.88495
H	-2.63697	-3.20081	-0.88495
H	-4.64605	-0.86280	-1.20425
H	-4.64605	-0.86280	1.20425

11b(T_1)
Absolute energy: -790.883392268 a.u
Point group: C_1

C	-4.20185	0.42346	0.00804
C	-4.05294	-0.96002	0.00762
C	-2.78227	-1.57798	0.00445
C	-1.70094	-0.72501	0.00195
C	-1.85523	0.69099	0.00217
C	-3.08710	1.29591	0.00534
H	-5.20100	0.84422	0.01048
H	-4.94080	-1.58248	0.00973
H	-2.68848	-2.65741	0.00402
H	-3.22226	2.37104	0.00578
C	-0.36037	0.85405	-0.00134
C	-0.21843	-0.57380	0.00098
C	1.02117	-1.18075	-0.00420
C	2.15921	-0.34802	-0.01126

C	2.02522	1.09353	-0.01210
C	0.70247	1.69356	-0.00759
H	1.13151	-2.25987	-0.00620
H	0.61242	2.77406	-0.00715
Si	3.85474	-1.16647	-0.06530
H	3.67415	-2.64467	-0.01386
H	4.76321	-0.72496	1.03242
H	4.15003	1.53992	0.01866
H	3.02564	3.00232	-0.03397
C	3.13928	1.92549	-0.01168

11(T_1)-TS
Absolute energy: -790.842488973 a.u
Point group: C_1

C	-1.99268	0.91730	-0.19107
C	-0.76705	1.59849	0.00517
C	0.34936	0.80646	-0.02404
C	0.28264	-0.66964	-0.14903
C	-0.91504	-1.35799	-0.19518
C	-2.06727	-0.56426	-0.22197
C	1.80927	0.70798	0.03215
C	3.02166	1.37230	0.15072
C	4.16422	0.56377	0.14416
C	4.09648	-0.83940	0.02751
C	2.87902	-1.51849	-0.08946
C	1.74004	-0.72522	-0.08596
H	-0.74086	2.67642	0.12217
H	-0.97248	-2.44112	-0.17041
H	2.84672	-2.59803	-0.17722
H	5.02160	-1.40450	0.02961
H	5.14032	1.02788	0.23137
H	3.10002	2.44911	0.24192
Si	-3.84028	-0.78504	0.30541
C	-3.30898	1.45576	-0.13727
H	-3.98918	1.22107	-0.95413
H	-3.48578	2.43874	0.29151
H	-4.04160	-1.91246	1.27835
H	-4.86496	-0.94898	-0.76333

At OLYP/6-311G(d,p) level

1a(S_0)
Absolute energy: -483.43064386 a.u
Point group: C_1

C	-1.88039400	-0.82535800	0.00923500
C	-0.31420200	-0.72589300	-0.13971300
C	-0.43572800	0.62191300	-0.07952000
C	-2.00490100	0.51400900	0.06211000
H	-2.57774800	-1.65791100	0.04566200
H	-2.84138300	1.20286200	0.15212900
C	0.88182300	1.33750100	-0.01717000
H	1.12898000	1.95704400	-0.88987500
H	1.04982300	1.93422100	0.89091100
Si	1.51216500	-0.50681400	0.03590800
H	2.15598700	-0.88815500	1.33978800
H	2.43444300	-0.98570100	-1.05097700

1b(S_0)
Absolute energy: -483.47795423 a.u
Point group: C_1

C	-0.43995100	-1.55641200	0.00000300
C	0.28705100	-0.28020100	0.00001500
C	-1.07101800	0.39450300	-0.00001300
C	-1.67487000	-0.95449600	-0.00001500
H	-0.10332700	-2.58984700	0.00002100
H	-2.69959100	-1.31707000	-0.00004500
C	-1.51900000	1.65717400	-0.00001200
H	-2.58576900	1.87110500	-0.00002500
H	-0.83855900	2.50510600	0.00000300
Si	1.95258200	0.22070700	0.00001100
H	3.05498500	-0.77559100	0.00002200
H	2.34284200	1.65298600	-0.00000100

1-TS(S_0)
Absolute energy: -483.407471396 a.u
Point group: C_1

C	-1.33087	-1.12522	0.01414
C	-0.13018	-0.73665	-0.59171
C	-0.68957	0.73050	-0.25753
C	-1.90519	0.20373	0.15769
H	-1.63526	-2.07480	0.46208
H	-2.77016	0.59537	0.68476
C	0.31823	1.64829	0.07559
H	0.14575	2.48306	0.75860
H	1.07292	1.84471	-0.68882
Si	1.49151	-0.42567	0.13596
H	2.12367	-1.26010	1.22866
H	2.60751	0.04727	-0.73778

1a(T_1)
Absolute energy: -483.41107796 a.u
Point group: C_1

C	-1.78256800	-0.88857500	0.00543400
C	-0.35197000	-0.76680600	-0.20029400
C	-0.49172500	0.68088100	-0.13824500
C	-1.90834900	0.56109400	0.09194100
H	-2.47967700	-1.71794600	0.07632200
H	-2.72790300	1.24234800	0.31555800
C	0.85690000	1.33981000	-0.02017300
H	1.16941100	1.92200700	-0.89911200
H	1.00258300	1.96619300	0.87037300
Si	1.47338400	-0.50598300	0.05925800
H	2.04928300	-0.92078600	1.38290000
H	2.42519100	-0.96647600	-1.00763300

1b(T_1)
Absolute energy: -483.43594466 a.u
Point group: C_1

C	-0.43038300	-1.54332700	0.00023200
C	0.24340000	-0.27702600	-0.00045800
C	-1.10908600	0.39136900	-0.00022000
C	-1.70728000	-0.96690200	0.00030400
H	-0.06977600	-2.56896300	0.00044300
H	-2.72460400	-1.34900200	0.00059400
C	-1.56161300	1.65286000	-0.00047700
H	-0.87792700	2.49857800	-0.00094100
H	-2.62784900	1.86861400	-0.00025100
Si	2.01120400	0.30599900	0.00003600
H	2.76547900	-0.13488200	1.22205300
H	2.76759000	-0.14017800	-1.21869400

1-TS(T_1)
Absolute energy: -483.381424102 a.u
Point group: C_1

C	-1.49598	-1.09878	-0.09028
C	-0.18737	-0.64319	-0.55324
C	-0.61064	0.73851	-0.21295
C	-1.86794	0.20647	0.29533
H	-1.95493	-2.07744	0.01926
H	-2.71150	0.62694	0.84038
C	0.38001	1.71289	-0.06499
H	1.06137	1.87922	-0.89741
H	0.26303	2.57474	0.59564
Si	1.55362	-0.46217	0.15696
H	1.58954	-0.91648	1.58853
H	2.69334	-1.11196	-0.58707

2a(S_0)
Absolute energy: -560.98826752 a.u
Point group: C_s

C	-0.75613100	1.64336800	0.00000000
C	0.28132900	0.70297200	0.00000000
C	0.00000000	-0.68478300	0.00000000
C	-1.31989400	-1.14758600	0.00000000
C	-2.35472300	-0.20546900	0.00000000
C	-2.07385300	1.17103400	0.00000000
H	-0.55174300	2.71346300	0.00000000
H	-1.54936200	-2.21262300	0.00000000
H	-3.39152100	-0.53882700	0.00000000

H	-2.89926000	1.88179600	0.00000000
Si	1.83482700	-1.07380400	0.00000000
C	1.80182700	0.85007200	0.00000000
H	2.20583900	1.34935700	0.88902200
H	2.20583900	1.34935700	-0.88902200
H	2.41065200	-1.74345800	1.21246700
H	2.41065200	-1.74345800	-1.21246700

2b(S_0)
Absolute energy: -560.92068777 a.u
Point group: C_1

C	1.63525400	0.96285000	-0.25775300
C	0.20825100	1.02737000	0.03597800
C	-0.51050900	-0.26681700	0.11708800
C	0.28364900	-1.46258200	0.25712000
C	1.64660400	-1.43994100	0.12664000
C	2.32278600	-0.21152000	-0.18993400
H	2.15611600	1.89744800	-0.45916200
H	-0.22129600	-2.41424700	0.42054200
H	2.21927200	-2.36080500	0.21787400
H	3.39819400	-0.22472000	-0.36013400
Si	-2.25108800	-0.45526700	-0.19464400
C	-0.37864800	2.23287700	0.30744900
H	-1.39728400	2.31033200	0.67662800
H	0.17505100	3.16108000	0.18742600
H	-3.14690400	0.68941300	-0.50178900
H	-2.91224600	-1.73817900	0.16409700

2-TS(S_0)
Absolute energy: -560.917359000 a.u
Point group: C_1

C	-1.42801	1.16097	0.29991
C	-0.05246	0.94322	-0.06947
C	0.40177	-0.43718	-0.15209
C	-0.55407	-1.47454	-0.31141
C	-1.89502	-1.19957	-0.12112
C	-2.31758	0.11417	0.24224
H	-1.77202	2.17279	0.50799
H	-0.22456	-2.49932	-0.47846
H	-2.62814	-2.00247	-0.17098
H	-3.37199	0.29182	0.44861
Si	2.16661	-0.53697	0.20262
C	0.82015	1.96420	-0.42596
H	1.62195	1.77380	-1.13256
H	0.63888	3.00103	-0.14669
H	2.65590	0.16971	1.41348
H	2.89879	-1.81748	-0.05060

2a(T_1)
Absolute energy: -560.85447074 a.u
Point group: C_1

C	0.99828700	-1.47359800	0.23685300
C	-0.21962100	-0.67228200	0.10600100
C	-0.11733000	0.71310700	0.17167000
C	1.16187900	1.35726000	0.11142100
C	2.32990400	0.54928400	-0.15339200
C	2.25613700	-0.81570500	-0.19591600
H	1.08151200	-2.08583300	1.14732400
H	1.22975000	2.44158500	0.04881100
H	3.26698700	1.04919900	-0.39991300
H	3.12405500	-1.41302200	-0.47416900
C	-1.52458000	1.29477900	0.08658300
H	-1.85809100	1.77742300	1.01369100
H	-1.68339900	1.99135300	-0.74653300
Si	-2.06231000	-0.53202600	-0.15366400
H	-2.63161900	-0.88501900	-1.49834400
H	-2.96491800	-1.14439500	0.88110400

2b(T_1)
Absolute energy: -560.91176754 a.u
Point group: C_1

C	1.64209500	1.00717700	-0.00947000
C	0.21410600	0.99688100	0.00829400
C	-0.45334100	-0.28732400	0.00492000
C	0.32630400	-1.45058900	-0.00069700
C	1.73087400	-1.40735700	-0.01235900
C	2.38347700	-0.16813500	-0.01765200
H	2.15393200	1.96835800	-0.01546300
H	-0.16248100	-2.42400300	0.00254000
H	2.30298400	-2.33303100	-0.01499000
H	3.47121200	-0.12263900	-0.02623400
Si	-2.32751500	-0.45987300	0.07202700
C	-0.49081700	2.21820600	0.02697000
H	-1.57520200	2.26238300	0.01815700
H	0.04277200	3.16480700	0.04761100
H	-3.05652900	0.37083900	-0.94190300
H	-2.70766300	-1.90164500	-0.07813300

2-TS(T_1)
Absolute energy: -560.845870188 a.u
Point group: C_1

C	-1.21590	1.36809	0.11767
C	0.04484	0.86111	-0.22492
C	0.25925	-0.64781	-0.29795
C	-0.87574	-1.49489	-0.19681
C	-2.12086	-0.94101	0.00544
C	-2.30703	0.50993	0.18094
H	-1.34718	2.44053	0.26369
H	-0.76389	-2.57760	-0.24779
H	-2.99660	-1.58485	0.07276
H	-3.31218	0.89626	0.32668
Si	2.02950	-0.53549	0.21285
C	1.37318	1.43856	-0.13625
H	1.93837	1.44346	-1.08007
H	1.52527	2.36811	0.41697
H	2.48123	-1.37612	1.39338
H	3.11562	-0.67682	-0.81417

3a(S_0)
Absolute energy: -638.31953673 a.u
Point group: C_1

C	-0.30719700	-1.59442900	-0.69453500
C	-1.59900600	-1.67817700	-0.31160700
C	-0.52081000	1.62796400	-0.63285300
C	-2.31779700	-0.81559800	0.64051600
C	-1.80846600	1.51769800	-0.24806500
C	-2.40461700	0.53023100	0.66891200
C	0.67809100	-0.60657400	-0.25735700
C	0.59651100	0.75887400	-0.22464900
Si	2.46674700	-0.53261800	0.30468800
H	-0.24461200	2.48565100	-1.25131900
H	-2.49554400	2.30125200	-0.57974300
H	-3.06488200	0.96328900	1.42545900
H	-2.91626400	-1.35797900	1.37790000
H	-2.17406900	-2.53321700	-0.67653900
H	0.07113300	-2.38028200	-1.35300300
C	1.94853400	1.30434400	0.24826100
H	2.45283400	1.94133000	-0.49059300
H	1.89790600	1.85223100	1.19750300
H	3.51378700	-0.96086700	-0.68302100
H	2.83379900	-1.12075900	1.63599200

3b(S_0)
Absolute energy: -638.28184883 a.u
Point group: C_1

C	-0.30818900	1.54808600	-0.06091000
C	1.00479900	1.87153300	0.18670500
C	0.66633900	-1.42827500	-0.78131600
C	2.21180800	1.11443600	0.44593400
C	1.96353300	-1.06654900	-0.83596200
C	2.64698000	-0.10260600	0.00953300
C	-1.02013500	0.29551300	-0.02555500
C	-0.32327700	-0.99006900	0.24660600
Si	-2.77268400	0.26884900	-0.25878700
H	0.28973800	-2.12777900	-1.53125100
H	2.59149000	-1.56595700	-1.57862700
H	3.68599700	-0.34641300	0.24077400
H	2.95862900	1.69215100	0.99587700
H	1.18268300	2.94851500	0.22984000
H	-0.94598800	2.41887500	-0.22799300
C	-0.59731700	-1.76058200	1.31683000
H	-0.09570000	-2.71456700	1.46637400

H	-1.30324400	-1.44065000	2.07923200
H	-3.51156100	-1.01331300	-0.37864300
H	-3.50170200	1.49631400	-0.68375700

3-TS(S_0)
Absolute energy: -638.267667072 a.u
Point group: C_1

C	0.02820	1.67008	-0.29169
C	1.36260	1.81249	-0.03604
C	0.54339	-1.52996	-0.68922
C	2.35411	0.89602	0.51525
C	1.87039	-1.34699	-0.59844
C	2.58012	-0.42186	0.29141
C	-0.83995	0.53867	-0.07601
C	-0.49875	-0.84122	0.12671
Si	-2.63134	0.41691	-0.09899
H	0.16313	-2.27288	-1.39456
H	2.51079	-1.98645	-1.21182
H	3.46881	-0.84405	0.76753
H	3.08878	1.39447	1.15350
H	1.75420	2.82051	-0.19245
H	-0.47255	2.57468	-0.64021
C	-1.35292	-1.57431	0.94698
H	-1.40269	-2.66274	0.88930
H	-1.76924	-1.12685	1.84384
H	-3.27229	-0.58276	-0.99237
H	-3.51327	1.63176	0.02939

3a(T_1)
Absolute energy: -638.29897471 a.u
Point group: C_1

C	-0.19241600	-1.69366800	0.00008300
C	-1.59957600	-1.78562000	-0.00008200
C	-0.43187800	1.74066100	-0.00023300
C	-2.65421700	-0.85390400	-0.00017100
C	-1.83481800	1.62509300	0.00019400
C	-2.74898000	0.55357500	0.00013200
C	0.71574200	-0.62027800	0.00024100
C	0.63002000	0.81182600	-0.00010800
Si	2.59446700	-0.53891400	0.00002900
H	-0.08991600	2.77723100	-0.00052200
H	-2.33319300	2.59578400	0.00045500
H	-3.78511800	0.89590200	0.00031600
H	-3.63378000	-1.33430300	-0.00036900
H	-1.95313900	-2.81815300	-0.00019800
H	0.29116000	-2.67263100	0.00011700
C	2.08899600	1.29618800	-0.00005400
H	2.35715500	1.88383700	-0.88784900
H	2.35687500	1.88354000	0.88804600
H	3.31471800	-1.05479900	-1.21197100
H	3.31546500	-1.05483700	1.21155600

3b(T_1)
Absolute energy: -638.25523640 a.u
Point group: C_1

C	0.14187900	-1.53966700	0.20476300
C	-1.23837800	-1.76106200	0.57418300
C	-0.58463100	1.70275600	-0.32125700
C	-2.38322000	-1.05839600	0.26452300
C	-1.84143300	1.28475700	-0.73481600
C	-2.62069000	0.14246300	-0.46135800
C	0.87984600	-0.39819000	0.06296800
C	0.47594600	1.00417800	0.39888700
Si	2.65132600	-0.52129600	-0.53960700
H	-0.37527800	2.75836700	-0.49880200
H	-2.39699700	2.05774200	-1.26926300
H	-3.65504500	0.24054500	-0.79402700
H	-3.30442300	-1.56771500	0.55556400
H	-1.41145500	-2.72781500	1.05146600
H	0.67969700	-2.47693200	0.03290800
C	1.22678600	1.69733400	1.29622600
H	1.01369500	2.74009000	1.52391700
H	2.03403700	1.22474700	1.85058900
H	2.97232100	0.50631500	-1.58019900
H	2.98825900	-1.90223800	-1.02236600

3-TS(T_1)
Absolute energy: -638.247928446 a.u
Point group: C_1

C	-0.06842	-1.65531	0.10265
C	-1.47045	-1.77749	0.34700
C	-0.42401	1.73140	-0.19447
C	-2.53633	-0.89463	0.19116
C	-1.76481	1.51028	-0.48833
C	-2.65758	0.43595	-0.27272
C	0.77902	-0.56942	0.06004
C	0.59442	0.86904	0.34598
Si	2.56653	-0.52957	-0.44918
H	-0.10230	2.76839	-0.30608
H	-2.26938	2.40422	-0.85874
H	-3.69412	0.71384	-0.47031
H	-3.50535	-1.35855	0.38372
H	-1.77703	-2.79490	0.59665
H	0.41937	-2.61966	-0.06211
C	1.69045	1.43931	0.99317
H	1.82178	2.52152	1.02961
H	2.26624	0.87039	1.71649
H	2.77297	0.23144	-1.71970
H	3.28266	-1.85763	-0.52788

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Gaussian 09 full reference

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