Synthesis, Physical Properties, and Chemistry of Donor/Acceptor Substituted Pentacenes

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1. Synthetic Procedures for **S1** and **6b**

S1: To a solution of phenylacetylene (0.86 mL, 0.80 g, 7.8 mmol) in THF (5 mL) cooled to $-78\text{ }^{\circ}\text{C}$ was added dropwise HexLi (2.3 M in hexanes, 3.3 mL, 7.5 mmol). The solution was stirred for 30 min before being transferred via cannula into a suspension of 6,13-pentacenequinone (0.414 g, 1.34 mmol) in THF (5 mL) at $-78\text{ }^{\circ}\text{C}$. The reaction mixture was then placed in a $-15\text{ }^{\circ}\text{C}$ cooling bath, allowed to warm to rt, and stirred for 3 h. The reaction mixture was cooled to $-78\text{ }^{\circ}\text{C}$, quenched via the addition of satd. aq. NH_4Cl (15 mL), and warmed to rt. H_2O (100 mL) was added and the mixture was extracted with CH_2Cl_2 ($2 \times 70\text{ mL}$). The combined organic phase was washed with satd. aq. NaCl (100 mL), dried (MgSO_4), filtered, and the solvent removed *in vacuo*. Column chromatography (silica gel, CH_2Cl_2) afforded pure **S1** (0.414 g, 60%) as a pale yellow foamy solid. Note: **S1** slowly decomposes on silica affording a spot ca. $R_f = 0.10$ (CH_2Cl_2). The ^1H NMR spectrum of the crude product showed 100% conversion, no impurities except phenylacetylene. $R_f = 0.50$ (CH_2Cl_2). IR (CDCl_3 , cast): 3600–3100 (s, br), 3055 (s), 3032 (m), 2230 (m), 1598 (m), 1491 (s) cm^{-1} . ^1H NMR (500 MHz, CDCl_3): δ 8.68 (s, 4H), 7.95–7.89 (m, 4H), 7.55–7.47 (m, 8H), 7.33–7.26 (m, 6H), 3.60 (s, 2H). ^{13}C NMR (125 MHz, CDCl_3): δ 136.2, 133.2, 131.7, 128.8, 128.3, 128.2, 126.9, 126.0, 121.9, 91.1, 88.1, 69.8. ^{13}C NMR (APT, 100 MHz, CDCl_3): δ 136.2 (C), 133.2 (C), 131.7 (CH), 128.8 (CH), 128.3 (CH), 128.2 (CH), 126.9 (CH), 126.0 (CH), 121.9 (C), 91.1 (C), 88.1 (C), 69.8 (C).

6b: To a solution of **S1** (0.380 g, 0.741 mmol) in dry THF (5 mL) that had been deoxygenated by bubbling N_2 for 10 min was added a solution of $\text{SnCl}_2 \cdot 2\text{H}_2\text{O}$ (0.462 g, 2.05 mmol) in THF (6 mL). The solution was stirred at rt for 7 h in the dark before pouring the solution into MeOH (40 mL). The mixture was filtered and the solid was washed with MeOH ($4 \times 15\text{ mL}$), and CH_2Cl_2 ($3 \times 4\text{ mL}$) to afford the crude product **6b**. The solid was suspended in CH_2Cl_2 (12 mL) and stirred for 5 min after which hexanes (60 mL) was added and the suspension was filtered and the solid was washed with hexanes ($4 \times 15\text{ mL}$) to afford **6b** (0.348 g, 98%) as a blue solid. The reaction mixture was performed in the dark by wrapping the reaction flask in aluminum foil and the work-up was performed under dim lighting conditions. UV-vis (CH_2Cl_2) λ_{max} (ϵ): 253 (39 100), 312 (335 000), 357 (30 300), 370 (39 700), 416 (2 270), 441 (3 670), 564 (5 910), 607 (16 400), 660 (27 900) nm. IR (microscope): 3047 (m), 2186 (w), 1490 (s), 871 (s), 752 (s) cm^{-1} . ^1H NMR (300 MHz, CDCl_3): δ 9.30 (s, 4H), 8.10–8.00 (m, 4H), 7.85–7.95 (m, 4H), 7.60–7.46 (m, 6H), 7.46–7.38 (m, 4H). Due to low solubility, ^{13}C NMR: useful data was not obtained due to insolubility of the compound. MALDI HRMS m/z calcd. for $\text{C}_{38}\text{H}_{22}$ (M^+) 478.1716, found 478.1714. Anal. calcd. for $\text{C}_{38}\text{H}_{22}$: C, 95.37; H, 4.63. Found: C, 95.40; H, 4.58. TGA: $T_d \approx 490\text{ }^{\circ}\text{C}$. DSC: decomposition, $246\text{ }^{\circ}\text{C}$ (onset), $265\text{ }^{\circ}\text{C}$ (peak).

2. Solid-state Packing Diagrams for 1b and 6a

(a)

(b)

Figure S1. Solid-state packing of pentacene **1b**•0.5CH₂Cl₂ (a) viewed down the short molecular axis (b) viewed down the long molecular axis. Hydrogen atoms and co-crystallized solvent are not shown. Carbon = gray, nitrogen = purple, silicon = yellow.

Figure S2. Solid-state packing of pentacene **6a** (hexyl groups have been omitted for clarity) illustrating various C–H... π interactions and their associated non-covalent distances in Å. Carbon = gray, hydrogen = white, nitrogen = purple, oxygen = red.

3. Solution-State UV-vis Absorption data of Compounds 1a–e and 6a–b

Table S1. Summary of optical properties for **1a–e** and **6a–b** in the solution (measured in CH₂Cl₂) and solid state.

Compound	λ_{max} (CH ₂ Cl ₂) /nm ^a	λ_{max} (film) /nm ^b	Red Shift /nm ^c	λ_{edge} (CH ₂ Cl ₂) /nm ^d	$E_{\text{g}}^{\text{opt}}$ (CH ₂ Cl ₂) /eV ^d
1a	674	685	11	747	1.66
1b	668	683	15	739	1.68
1c	666	718	52	723	1.72
1d	655	668	13	695	1.78
1e	652	671	19	686	1.81
6a	689	823	134	834	1.49
6b	660	– ^e	– ^e	697	1.78

^a Lowest energy absorption maxima. ^b Thin film drop cast from CH₂Cl₂. ^c Red-shift for the longest wavelength UV-vis absorption λ_{max} measured between the solid-state and solution-state. ^d The wavelength used as the absorption edge for determining $E_{\text{g}}^{\text{opt}}$ corresponds to the lowest energy absorption wavelength that has a molar absorptivity (ϵ) $\geq$ to 1000 L·mol⁻¹·cm⁻¹. ^e Data not measured.

4. Solid-state UV-vis Absorption Spectra of Compounds 1a–e and 6a

Figure S3. Solid-state UV-vis absorption spectra (intensity normalized to unity for λ_{max}) of thin film (cast from CH_2Cl_2) of pentacene: (A) 1a, (B) 1b, (C) 1c, (D) 1d, (E) 1e, (F) 6a.

5. Cyclic Voltammetry Data for Compounds 1a–e and 6a–b

Figure S4. Cyclic voltammogram of 1 mM functionalized pentacenes in 0.1 M *n*-Bu₄NPF₆ solution of benzene/MeCN (3:1 v/v) at a scan rate of 150 mV/s with potentials plotted against the Ag/Ag⁺ reference electrode. Ferrocene/ferrocenium (Fc/Fc⁺) was used as an internal standard. The arrows indicate the direction of the scan. (A) **1a**, (B) **1b**, (C) **1c**, (D) **1d**, (E) **1e**.

Figure S5. Cyclic voltammogram of 1 mM functionalized pentacenes in 0.1 M $n\text{-Bu}_4\text{NPF}_6$ solution of benzene/MeCN (3:1 v/v) at a scan rate of 150 mV/s with potentials plotted against the Ag/Ag^+ reference electrode. Ferrocene/ferrocenium (Fc/Fc^+) was used as an internal standard. The arrows indicate the direction of the scan. (A) **6a**, (B) **6b** (due to limited solubility of **6b**, it was measured as a 0.1 mM solution of **6b** in 0.1 M $n\text{-Bu}_4\text{NPF}_6$ solution of CH_2Cl_2 measured at a scan rate of 200 mV/s).

6. ^1H and ^{13}C NMR Spectra of Compounds 1a–c, 3–6, 8a, 9 and S1

498.122 MHz H1 1D in CDCl₃ recorded on ibd5

Pulse Sequence: s2pul

Figure S6. ^1H NMR (500 MHz) spectrum of **1a** in CDCl_3 .

Figure S7. ¹³C NMR (100 MHz) spectrum of **1a** in CDCl₃.

Figure S8. ¹H NMR (500 MHz) spectrum of **1b** in CDCl₃ (**X** = CH₂Cl₂).

125.264 MHz C13[H1] 1D in cdcl3 (ref. to CDC13 @ 77.0 ppm), temp 27.2 C -> actual temp = 27.0 C, autotdb probe

Pulse Sequence: s2pul

Figure S9. ^{13}C NMR (125 MHz) spectrum of **1b** in CDCl_3 .

499.821 MHz H1 1D in cdcl3 (ref. to CDC13 @ 7.24 ppm), temp 26.1 C -> actual temp = 27.0 C, autoxdb probe

Pulse Sequence: s2pul

Figure S10. ¹H NMR (500 MHz) spectrum of **1c** in CDCl₃ (X = CH₂Cl₂).

125.691 MHz C13[H1] 1D in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 26.1 C -> actual temp = 27.0 C, autotdb probe

Pulse Sequence: s2pul

Figure S11. ¹³C NMR (125 MHz) spectrum of **1c** in CDCl₃.

Figure S12. ¹H NMR (400 MHz) spectrum of 3a in CDCl₃ (**X** = CH₂Cl₂).

Figure S13. ^{13}C NMR (100 MHz) spectrum of **3a** in CDCl_3 (**X** = CH_2Cl_2).

Figure S14. ¹H NMR (500 MHz) spectrum of **4a** in CDCl₃ (**X** = CH₂Cl₂).

Figure S15. ¹³C NMR (125 MHz) spectrum of 4a in CDCl₃ (X = CH₂Cl₂).

498.122 MHz ¹H 1D in cdcl3 (ref. to CDCl₃ @ 7.24 ppm), temp 27.2 C -> actual temp = 27.0 C, autoxdb probe

Pulse Sequence: s2pul

Figure S16. ¹H NMR (500 MHz) spectrum of **4b** in CDCl₃.

125.264 MHz C13[H1] 1D in cdcl3 (ref. to CDCl3 @ 77.0 ppm), temp 27.2 C -> actual temp = 27.0 C, autotxdb probe

Pulse Sequence: s2pul

Figure S17. ¹³C NMR (125 MHz) spectrum of **4b** in CDCl₃.

499.821 MHz H1 1D in cdcl3 (ref. to CDC13 @ 7.24 ppm), temp 26.1 C -> actual temp = 27.0 C, autotdb probe

Pulse Sequence: s2pul

Figure S18. ^1H NMR (500 MHz) spectrum of **4c** in CDCl_3 (**X** = CH_2Cl_2).

125.691 MHz C13[H1] 1D in cdcl3 (ref. to CDC13 @ 77.0 ppm), temp 26.1 C -> actual temp = 27.0 C, autoxdb probe

Pulse Sequence: s2pul

Figure S19. ^{13}C NMR (500 MHz) spectrum of **4c** in CDCl_3 .

Figure S20. ¹H NMR (500 MHz) spectrum of **4d** in CDCl₃.

Figure S21. ^{13}C NMR (125 MHz) spectrum of **4d** in CDCl_3 .

Figure S22. ^1H NMR (500 MHz) spectrum of **4e** in CDCl_3 (**X** = CH_2Cl_2).

Figure S23. ^{13}C NMR (125 MHz) spectrum of **4e** in CDCl_3 (**X** = CH_2Cl_2).

Figure S24. ^1H NMR (500 MHz) spectrum of **6a** in CDCl_3 .

125.267 MHz C13[H1] 1D in CDCl3 recorded on ibd5

Pulse Sequence: s2pul

Figure S25. ¹³C NMR (125 MHz) spectrum of 6a in CDCl₃.

299.971 MHz H1 1D in cdcl3 (ref. to CDC13 @ 7.24 ppm), temp 27.5 C -> actual temp = 27.0 C, id300 probe

Pulse Sequence: s2pul

Figure S26. ^1H NMR (300 MHz) spectrum of **6b** in CDCl_3 (**X** = CH_2Cl_2 ; ***** = H_2O).

498.122 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.24 ppm), temp 27.2 C -> actual temp = 27.0 C, autoxdb probe

Pulse Sequence: s2pul

Figure S27. ¹H NMR (500 MHz) spectrum of **8a** in CDCl₃.

125.264 MHz C13[H1] 1D in cdcl3 (ref. to CDCl3 @ 77.0 ppm), temp 27.2 C -> actual temp = 27.0 C, autotdb probe

Pulse Sequence: s2pul

Figure S28. ^{13}C NMR (125 MHz) spectrum of **8a** in CDCl_3 .

498.122 MHz H1 1D in cdcl3 (ref. to CDC13 @ 7.24 ppm), temp 27.2 C -> actual temp = 27.0 C, autotx probe

Pulse Sequence: s2pul

Figure S29. ^1H NMR (500 MHz) spectrum of **9** in CDCl_3 (**X** = CH_2Cl_2 ; **+** = EtOAc).

125.264 MHz C13[H1] 1D in cdcl3 (ref. to CDC13 @ 77.0 ppm), temp 27.2 C -> actual temp = 27.0 C, autoxdb probe

Pulse Sequence: s2pul

Figure S30. ¹³C NMR (125 MHz) spectrum of **9** in CDCl₃ (X = CH₂Cl₂; + = EtOAc).

499.821 MHz H1 1D in cdcl3 (ref. to CDC13 @ 7.24 ppm), temp 26.1 C -> actual temp = 27.0 C, autotx probe

Pulse Sequence: s2pul

Figure S31. ¹H NMR (500 MHz) spectrum of S1 in CDCl₃ (X = CH₂Cl₂; + = acetone).

125.691 MHz C13[H1] 1D in cdcl3 (ref. to CDC13 @ 77.0 ppm), temp 26.1 C -> actual temp = 27.0 C, autotdb probe

Pulse Sequence: s2pul

Figure S32. ^{13}C NMR (125 MHz) spectrum of S1 in CDCl_3 .

[2+2]/Retro[2+2] Reactivity**[4+2] Reactivity**

Figure S33. DFT calculated energy profile using B3LYP/6-31G(d) for reaction of TCNE with pentacene **1b'**/**1d'** illustrating the origin of the preference for the [4+2] reactivity versus the formal [2+2]/retro[2+2] reactivity.

[2+2]/Retro[2+2] Reactivity

[4+2] Reactivity

Figure S34. DFT calculated energy profile using B3LYP/6-31G(d) for reaction of TCNE with pentacene **4b'** illustrating the origin of the preference for the formal [2+2]/retro[2+2] pathway versus the [4+2] pathway.

Table S2. B3LYP/6-31G(d) optimized structures related to the [4+2] reactivity of **1d'** and **1b'** with TCNE. Electronic energies are relative to TCNE and the appropriate starting material **1d'** or **1b'**.

<p>1d' [1d' + TCNE = 0.0 kcal/mol, defined]</p>	<p>1b' [1b' + TCNE = 0.0 kcal/mol, defined]</p>	<p>TCNE</p>
<p>13d [−6.6 kcal/mol]</p>	<p>13b [−7.1 kcal/mol]</p>
<p>TS12d [+13.3 kcal/mol]</p>	<p>TS12b [+12.3 kcal/mol]</p>
<p>8d' [−10.4 kcal/mol]</p>	<p>8b' [−10.8 kcal/mol]</p>	

Table S3. B3LYP/6-31G(d) optimized structures related to the [2+2] reactivity of **1d'** and **1b'** with TCNE. Electronic energies are relative to TCNE and the appropriate starting material **1d'** or **1b'**.

<p>TS9d [+31.4 kcal/mol]</p>	<p>TS9b [NA] <i>Transition State Searches to Locate this Structure were Unsuccessful</i></p>
<p>10d [+28.0 kcal/mol]</p>	<p>10b [+22.3 kcal/mol]</p>
<p>11d [-17.7 kcal/mol]</p>	<p>11b [-18.7 kcal/mol]</p>

Table S3 (continued). B3LYP/6-31G(d) optimized structures related to the [2+2] reactivity of **1d'** and **1b'** with TCNE. Electronic energies are relative to TCNE and the appropriate starting material **1d'** or **1b'**.

Table S4. B3LYP/6-31G(d) optimized structures related to the [4+2] reactivity of **4b'** with TCNE. Electronic energies are relative to starting materials TCNE and **4b'**.

<p>4b' [4b' + TCNE = 0.0 kcal/mol, defined]</p>	<p>syn-16 [−4.7 kcal/mol]</p>	<p>anti-16 [−5.3 kcal/mol]</p>
	<p>syn-TS17 [−27.5 kcal/mol]</p>	<p>anti-TS17 [−26.8 kcal/mol]</p>
	<p>syn-15 [−11.1 kcal/mol]</p>	<p>anti-15 [−10.4 kcal/mol]</p>

Table S5. B3LYP/6-31G(d) optimized structures related to the [2+2] reactivity of **4b'** with TCNE. Electronic energies are relative to starting materials TCNE and **4b'**.

<p>TS18 [+18.5 kcal/mol]</p>	<p>19 [+16.2 kcal/mol]</p>
<p>TS20 [+20.3 kcal/mol]</p>	<p>21 [−26.5 kcal/mol]</p>
<p>TS22 [−5.2 kcal/mol]</p>	<p>14b' [−43.3 kcal/mol]</p>

Table S6. B3LYP/6-31G(d,p) calculated HOMO and LUMO of pentacenes **1b'** and **1d'** and their dipole moments.^a

Cmpd.	1b'	1d'
LUMO		
HOMO		
Structure		
Dipole /Debye	5.32	2.59

^a Calculated HOMO and LUMO using B3LYP/6-31G(d,p) for **1b'** and **1d'** where the structures of **1b** and **1d**, respectively, have been altered by formally replacing the *Si**i*-Pr₃ group with a SiMe₃ group to simplify the calculations.

Table S7. B3LYP/6-31G(d,p) calculated HOMO and LUMO of pentacenes **1b'** and **1d'** and their dipole moments.^a

Cmpd.	6a'	6c'
LUMO		
HOMO		
Structure		
Dipole /Debye	13.74	3.52

^a Calculated HOMO and LUMO using B3LYP/6-31G(d,p) for **6a'** and **6c'** where the structure of **6a** and **6c**, respectively, have been altered by formally replacing the Si*i*-Pr₃ group with a SiMe₃ group, the *n*-Hex₂N of **6a** was replaced with Me₂N group and the C₈H₁₇O group of **6c** was replaced with the MeO group to simplify the calculations.

8. Cartesian Coordinates for DFT Optimized Structures

8.1 [4+2] Reactivity of 1d' and 1b' with TCNE

Compound: TCNE
Charge: 0
Spin Multiplicity: 1
Computational Method/Basis Set: B3LYP/6-31G(d)
Solvation: gas phase
Electronic Energy (AU): -447.518338396

C	0.000114	0.686202	0.000000
C	-0.000114	-0.686202	0.000000
C	-1.218796	1.433523	0.000000
C	-1.218992	-1.433439	0.000000
C	1.218796	-1.433523	0.000000
C	1.218992	1.433439	0.000000
N	-2.198775	-2.059534	0.000000
N	2.198775	-2.059307	0.000000
N	2.198775	2.059534	0.000000
N	-2.198775	2.059307	0.000000

Compound: **1d'**
Charge: 0
Spin Multiplicity: 1
Computational Method/Basis Set: B3LYP/6-31G(d)
Solvation: gas phase
Electronic Energy (AU): -1753.38446788

C	0.075611	3.725410	0.003815
C	-0.631097	2.527429	0.004472
C	0.013025	1.273079	0.004494
C	1.463405	1.236360	0.003997
C	2.170526	2.457445	0.003128
C	1.524217	3.688860	0.003004
C	-0.728577	0.053477	0.004653
C	2.140702	-0.017336	0.004070
C	1.402139	-1.236010	0.004360
C	-0.048283	-1.201340	0.004870
C	-0.753779	-2.422248	0.005242
H	-1.838935	-2.392470	0.005751
C	-0.107275	-3.653821	0.004924
C	1.341361	-3.688514	0.004068
C	2.047850	-2.490666	0.003851
H	-1.716345	2.551954	0.004950
H	3.255694	2.426200	0.002320
H	3.133208	-2.513653	0.003048
C	-0.823336	-4.895997	0.005302
H	-1.910344	-4.866178	0.005998
C	-0.157761	-6.089825	0.004756
H	-0.711732	-7.024662	0.005035
C	1.273481	-6.124250	0.003722
C	1.996368	-4.964323	0.003381
H	1.781643	-7.084762	0.003136
H	3.083438	-4.987107	0.002417

C	-0.578579	5.001278	0.003799
H	-1.665710	5.025035	0.004446
C	0.144964	6.160855	0.002948
H	-0.362390	7.121769	0.002926
C	1.576172	6.124911	0.001994
H	2.130917	7.059292	0.001188
C	2.241212	4.930861	0.002013
H	3.328085	4.900154	0.001149
C	3.559758	-0.053278	0.003348
C	4.783775	-0.087057	0.002394
C	-2.142595	0.089011	0.003873
C	-3.362708	0.121229	0.002444
Si	6.622875	-0.144901	-0.005571
C	-4.782243	0.162549	0.000243
C	-5.543396	-1.021276	-0.001142
C	-5.474458	1.395935	-0.000969
C	-6.935597	-0.988404	-0.003734
H	-5.032107	-1.979041	-0.000251
C	-6.857807	1.436028	-0.003536
H	-4.907293	2.321590	0.000060
C	-7.602263	0.244462	-0.004985
H	-7.487590	-1.921198	-0.004783
H	-7.393056	2.380276	-0.004534
C	7.273792	1.330383	-0.992949
H	6.910618	1.308566	-2.026598
H	6.957567	2.280656	-0.547697
H	8.370576	1.324607	-1.022632
C	7.251458	-0.062917	1.775845
H	6.873365	-0.901430	2.371472
H	8.347757	-0.099664	1.802188
H	6.935397	0.864113	2.267391
C	7.172322	-1.762368	-0.816648
H	6.801543	-2.633130	-0.263828
H	6.802096	-1.836975	-1.845356
H	8.266974	-1.829293	-0.848776
C	-9.764852	-0.772527	-0.009442
H	-9.591710	-1.383506	0.885925
H	-10.797226	-0.418954	-0.011437
H	-9.588133	-1.383151	-0.904355
O	-8.955219	0.394394	-0.007597

Compound: **1b'**
 Charge: 0
 Spin Multiplicity: 1
 Computational Method/Basis Set: B3LYP/6-31G(d)
 Solvation: gas phase
 Electronic Energy (AU): -1772.83035930

C	-0.274946	-3.690802	0.004426
C	0.401089	-2.475013	0.004586
C	-0.274422	-1.237606	0.004627
C	-1.725156	-1.236398	0.004694
C	-2.400904	-2.475093	0.004291
C	-1.723827	-3.690051	0.004131
C	0.438467	0.000055	0.004083
C	-2.433919	0.000063	0.004701
C	-1.725149	1.236519	0.004701
C	-0.274415	1.237719	0.004632
C	0.401103	2.475122	0.004597
H	1.486690	2.471390	0.004645
C	-0.274927	3.690914	0.004441
C	-1.723808	3.690171	0.004147
C	-2.400891	2.475216	0.004304
H	1.486677	-2.471287	0.004631
H	-3.486543	-2.471514	0.003866
H	-3.486529	2.471640	0.003879
C	0.410924	4.949857	0.004414
H	1.498376	4.946040	0.004658
C	-0.283110	6.127507	0.004003
H	0.248144	7.075473	0.003943
C	-1.714661	6.127040	0.003529
C	-2.409293	4.949812	0.003592
H	-2.246160	7.074908	0.003034
H	-3.496634	4.946370	0.003054
C	0.410897	-4.949749	0.004395
H	1.498349	-4.945937	0.004638
C	-0.283143	-6.127395	0.003981
H	0.248107	-7.075363	0.003919
C	-1.714694	-6.126921	0.003506
H	-2.246198	-7.074785	0.003009
C	-2.409319	-4.949689	0.003571
H	-3.496660	-4.946240	0.003033
C	-3.853117	0.000059	0.004191
C	-5.077819	0.000036	0.003365
C	1.851326	0.000050	0.001546
C	3.072899	0.000038	-0.002607
Si	-6.916415	-0.000099	-0.003598
C	4.490158	0.000006	-0.010312
C	5.224984	1.204402	-0.012975
C	5.224930	-1.204423	-0.012749
C	6.610172	1.209731	-0.022133
H	4.689977	2.149462	-0.004995
C	6.610118	-1.209818	-0.021901
H	4.689882	-2.149459	-0.004579
C	7.347771	-0.000062	-0.035207
H	7.124260	2.163279	-0.018552
H	7.124163	-2.163389	-0.018109

C	-7.521362	-1.551145	-0.900694
H	-7.156342	-1.581564	-1.933492
H	-7.177689	-2.462438	-0.397897
H	-8.617757	-1.580359	-0.931282
C	-7.544648	0.001924	1.780367
H	-7.196656	0.887275	2.324416
H	-8.641630	0.002099	1.805485
H	-7.196881	-0.882303	2.326384
C	-7.521669	1.548767	-0.904243
H	-7.178311	2.461286	-0.403457
H	-7.156531	1.576973	-1.937061
H	-8.618071	1.577607	-0.935025
N	8.729002	-0.000099	-0.064767
C	9.456787	1.253332	0.038609
H	9.263500	1.774408	0.988657
H	10.527294	1.051859	-0.026508
H	9.195290	1.934753	-0.781070
C	9.456717	-1.253565	0.038624
H	9.194951	-1.935079	-0.780888
H	10.527223	-1.052186	-0.026811
H	9.263640	-1.774493	0.988798

Compound: **13d**

Charge: 0

Spin Multiplicity: 1

Computational Method/Basis Set: B3LYP/6-31G(d)

Solvation: gas phase

Electronic Energy (AU): -2200.91329013

C	-0.052073	-3.036147	-1.192588
C	0.711420	-1.898850	-0.919010
C	0.134589	-0.628001	-0.718359
C	-1.310359	-0.508683	-0.759459
C	-2.076057	-1.670466	-1.000764
C	-1.492968	-2.917048	-1.236587
C	0.939938	0.524425	-0.477085
C	-1.927251	0.757261	-0.557307
C	-1.126030	1.910542	-0.295037
C	0.318673	1.794544	-0.254637
C	1.082618	2.947979	-0.001797
H	2.163599	2.857155	0.031390
C	0.497021	4.194176	0.213733
C	-0.944788	4.309793	0.174365
C	-1.709618	3.172839	-0.078517
H	1.792979	-1.985930	-0.882539
H	-3.157447	-1.577716	-1.030063
H	-2.791596	3.254433	-0.104286
C	1.273387	5.368376	0.474798
H	2.356314	5.277751	0.505617
C	0.667044	6.577059	0.682943
H	1.266047	7.461586	0.881053
C	-0.757436	6.691320	0.644438
C	-1.536911	5.594151	0.398704
H	-1.217588	7.660815	0.814084
H	-2.620424	5.677259	0.370916

C	0.539971	-4.316915	-1.419042
H	1.621794	-4.406844	-1.376363
C	-0.243302	-5.412302	-1.676555
H	0.216222	-6.382528	-1.840489
C	-1.663455	-5.294826	-1.721691
H	-2.264533	-6.177455	-1.919342
C	-2.271588	-4.085039	-1.507317
H	-3.353932	-3.996214	-1.532356
C	-3.338635	0.877667	-0.638778
C	-4.555429	0.979010	-0.721162
C	2.347735	0.416514	-0.480388
C	3.564892	0.324871	-0.494974
Si	-6.393212	1.119142	-0.798313
C	4.979223	0.215822	-0.506997
C	5.794152	1.330556	-0.233147
C	5.611183	-1.017078	-0.792457
C	7.182358	1.231058	-0.240611
H	5.328055	2.285013	-0.008972
C	6.990337	-1.122886	-0.802027
H	5.001064	-1.889497	-1.004540
C	7.789896	-0.000202	-0.525802
H	7.777662	2.110151	-0.023046
H	7.480853	-2.066433	-1.018572
C	-7.128689	-0.616700	-0.673997
H	-6.787572	-1.256734	-1.495739
H	-6.848211	-1.100881	0.268078
H	-8.224182	-0.576285	-0.716192
C	-6.972691	2.187951	0.647352
H	-6.552698	3.198671	0.591446
H	-8.065984	2.279813	0.647966
H	-6.670334	1.753780	1.606694
C	-6.870224	1.918852	-2.443929
H	-6.430353	2.917421	-2.545270
H	-6.530960	1.316561	-3.294207
H	-7.959679	2.023715	-2.521255
C	9.999134	0.878847	-0.278807
H	9.837990	1.269185	0.734147
H	11.011937	0.480421	-0.355952
H	9.871685	1.690977	-1.006034
C	-1.572228	-2.537442	2.262135
C	-0.188991	-2.654222	2.318206
C	0.466633	-3.899322	2.097439
C	-2.406858	-3.657855	1.984427
C	-2.218747	-1.295767	2.529558
C	0.630957	-1.534136	2.641198
N	-2.751343	-0.284115	2.751124
N	-3.100606	-4.566055	1.759200
N	1.015331	-4.911323	1.919211
N	1.302004	-0.620158	2.906650
O	9.131942	-0.211619	-0.559486

Compound: **13b**

Charge: 0

Spin Multiplicity: 1

Computational Method/Basis Set: B3LYP/6-31G(d)

Solvation: gas phase
Electronic Energy (AU): -2220.35996795

C	-0.201497	-3.007357	-1.172307
C	0.529744	-1.849935	-0.891936
C	-0.080951	-0.595295	-0.697259
C	-1.528031	-0.512192	-0.751594
C	-2.261112	-1.693713	-0.998355
C	-1.644023	-2.924957	-1.229969
C	0.694844	0.578375	-0.451317
C	-2.179236	0.737662	-0.557838
C	-1.409272	1.912065	-0.291543
C	0.037113	1.833167	-0.236479
C	0.769193	3.004898	0.022822
H	1.851675	2.940518	0.068344
C	0.150818	4.237244	0.229457
C	-1.292411	4.316637	0.172964
C	-2.025936	3.159777	-0.085195
H	1.612898	-1.908719	-0.845705
H	-3.344209	-1.629062	-1.037427
H	-3.109280	3.214468	-0.122975
C	0.894944	5.430276	0.497079
H	1.979348	5.366097	0.541067
C	0.256796	6.624502	0.695073
H	0.831493	7.523902	0.898283
C	-1.169183	6.703233	0.639025
C	-1.918476	5.586338	0.386791
H	-1.655387	7.661373	0.800673
H	-3.003328	5.642693	0.345982
C	0.425293	-4.271811	-1.394072
H	1.508663	-4.333749	-1.340768
C	-0.326908	-5.387022	-1.660253
H	0.159002	-6.344983	-1.820346
C	-1.748793	-5.305714	-1.719329
H	-2.325320	-6.203120	-1.923697
C	-2.389787	-4.112021	-1.509459
H	-3.473742	-4.050870	-1.544707
C	-3.592202	0.821685	-0.652811
C	-4.810620	0.890269	-0.746973
C	2.101963	0.507494	-0.443354
C	3.322703	0.447348	-0.447581
Si	-6.649894	0.971770	-0.842126
C	4.735381	0.377781	-0.447190
C	5.526603	1.525759	-0.225351
C	5.410310	-0.843116	-0.663769
C	6.909044	1.462385	-0.219715
H	5.036922	2.479311	-0.051890
C	6.792193	-0.917286	-0.659862
H	4.830077	-1.745194	-0.833333
C	7.587327	0.236188	-0.438694
H	7.468805	2.372286	-0.040918
H	7.260135	-1.879689	-0.827310
C	-7.296404	-0.740909	-1.313100
H	-6.903753	-1.061769	-2.284742
H	-7.011365	-1.493858	-0.569581
H	-8.391400	-0.737147	-1.380509

C	-7.318399	1.490252	0.846701
H	-6.947730	2.480179	1.135500
H	-8.414750	1.532087	0.835020
H	-7.015537	0.782573	1.626193
C	-7.134571	2.236096	-2.161893
H	-6.748180	3.233366	-1.922820
H	-6.744586	1.954096	-3.146400
H	-8.226185	2.311525	-2.242802
N	8.963287	0.168055	-0.437366
C	9.752809	1.357531	-0.163161
H	9.546615	1.767614	0.835836
H	10.812535	1.103072	-0.211634
H	9.562193	2.148076	-0.901469
C	9.630439	-1.111148	-0.617018
H	9.376648	-1.566727	-1.583570
H	10.710304	-0.958462	-0.592442
H	9.369529	-1.826542	0.175893
C	-1.775444	-2.549863	2.258610
C	-0.391647	-2.661272	2.336715
C	0.273751	-3.901622	2.121215
C	-2.600745	-3.673282	1.966837
C	-2.430753	-1.312155	2.520119
C	0.417672	-1.539617	2.679769
N	-2.969535	-0.302394	2.736197
N	-3.286309	-4.585257	1.731334
N	0.832428	-4.909167	1.947541
N	1.080304	-0.625262	2.964751

Compound: **TS12d**
 Charge: 0
 Spin Multiplicity: 1
 Computational Method/Basis Set: B3LYP/6-31G(d)
 Solvation: gas phase
 Electronic Energy (AU): -2200.88162358

C	-0.063253	-2.999019	-1.184313
C	0.702467	-1.940649	-0.614469
C	0.179352	-0.634340	-0.455876
C	-1.251913	-0.496005	-0.438894
C	-2.014848	-1.771805	-0.335649
C	-1.477744	-2.880207	-1.156829
C	1.020152	0.496291	-0.309713
C	-1.847730	0.753148	-0.391335
C	-1.016046	1.940325	-0.310014
C	0.420787	1.805182	-0.241505
C	1.207498	2.958913	-0.127787
H	2.286261	2.851794	-0.073954
C	0.644830	4.239001	-0.083029
C	-0.789280	4.372002	-0.158938
C	-1.577039	3.215901	-0.270881
H	1.774982	-2.076889	-0.510787
H	-3.090364	-1.628104	-0.442980
H	-2.657017	3.314275	-0.317689
C	1.442777	5.418304	0.033020
H	2.523037	5.312117	0.092478
C	0.858188	6.656699	0.071535
H	1.472409	7.548205	0.161647
C	-0.559621	6.788688	-0.003745
C	-1.358879	5.679320	-0.115120
H	-1.004305	7.779390	0.029791
H	-2.439909	5.778391	-0.169843
C	0.533340	-4.152776	-1.736549
H	1.615485	-4.253905	-1.722399
C	-0.263332	-5.134628	-2.304284
H	0.192550	-6.019256	-2.739404
C	-1.658799	-4.994761	-2.309232
H	-2.276794	-5.769607	-2.754304
C	-2.265580	-3.883370	-1.722966
H	-3.347838	-3.807126	-1.687652
C	-3.265392	0.887876	-0.422416
C	-4.482173	1.001519	-0.455474
C	2.422151	0.352790	-0.284914
C	3.636507	0.228500	-0.261090
Si	-6.323682	1.138638	-0.387095
C	5.045456	0.079386	-0.226153
C	5.889915	1.204397	-0.163481
C	5.641379	-1.203795	-0.248546
C	7.273585	1.067070	-0.124975
H	5.450288	2.196728	-0.142815
C	7.015976	-1.347173	-0.210744
H	5.007180	-2.083765	-0.288711
C	7.846120	-0.213654	-0.148270
H	7.893422	1.954571	-0.075508
H	7.480090	-2.327976	-0.223411

C	-7.048357	-0.601268	-0.510912
H	-6.775604	-1.083490	-1.456620
H	-6.695973	-1.238999	0.307509
H	-8.143583	-0.567133	-0.458596
C	-6.788229	1.942332	1.256401
H	-6.379260	2.955998	1.334728
H	-7.878103	2.010981	1.362306
H	-6.400916	1.361852	2.100812
C	-6.905828	2.198470	-1.840214
H	-6.475621	3.205622	-1.799787
H	-6.623215	1.752239	-2.800404
H	-7.997978	2.301902	-1.828048
C	10.078277	0.634384	-0.027529
H	9.911491	1.216609	0.887375
H	11.077788	0.198022	-0.002257
H	9.990802	1.293473	-0.900584
C	-1.846888	-2.314813	1.358348
C	-0.417713	-2.572409	1.770981
C	0.108923	-3.883470	1.743603
C	-2.692710	-3.513076	1.430842
C	-2.478582	-1.261238	2.164894
C	0.301702	-1.569770	2.458141
N	-3.004502	-0.422902	2.771808
N	-3.398395	-4.435632	1.419672
N	0.559650	-4.960555	1.673994
N	0.902092	-0.711818	2.977014
O	9.179208	-0.464269	-0.113831

Compound: **TS12b**

Charge: 0

Spin Multiplicity: 1

Computational Method/Basis Set: B3LYP/6-31G(d)

Solvation: gas phase

Electronic Energy (AU): -2220.32912524

C	-0.184237	-2.961137	-1.201400
C	0.548760	-1.864403	-0.661531
C	-0.026620	-0.591058	-0.474790
C	-1.463736	-0.508437	-0.443538
C	-2.179488	-1.812184	-0.333239
C	-1.602137	-2.901695	-1.155014
C	0.773091	0.575499	-0.325412
C	-2.106637	0.716924	-0.396400
C	-1.321358	1.936350	-0.317283
C	0.119381	1.859985	-0.252455
C	0.859925	3.042895	-0.137253
H	1.942215	2.977869	-0.085322
C	0.246500	4.300507	-0.088934
C	-1.190367	4.376137	-0.162139
C	-1.932076	3.188967	-0.274744
H	1.628069	-1.955436	-0.584098
H	-3.258108	-1.704181	-0.455584
H	-3.015220	3.244882	-0.318554
C	0.998312	5.509714	0.028277
H	2.082045	5.445987	0.085751

C	0.364303	6.724360	0.070531
H	0.943914	7.639298	0.161667
C	-1.056306	6.799706	-0.001985
C	-1.811226	5.659267	-0.114406
H	-1.540362	7.771728	0.034574
H	-2.895467	5.715549	-0.166857
C	0.452744	-4.091638	-1.757098
H	1.537413	-4.146515	-1.758104
C	-0.308527	-5.110122	-2.309782
H	0.178783	-5.977651	-2.744451
C	-1.709124	-5.027280	-2.297304
H	-2.299281	-5.829237	-2.730549
C	-2.352869	-3.939843	-1.708570
H	-3.437088	-3.907357	-1.661093
C	-3.528527	0.797977	-0.423900
C	-4.747601	0.867474	-0.455365
C	2.174224	0.487903	-0.303401
C	3.394087	0.405573	-0.274936
Si	-6.592330	0.936711	-0.375708
C	4.801278	0.300249	-0.231544
C	5.623801	1.448178	-0.199725
C	5.439974	-0.959795	-0.207934
C	7.002052	1.348122	-0.148602
H	5.161106	2.430400	-0.213075
C	6.817091	-1.070456	-0.155292
H	4.833923	-1.860598	-0.221589
C	7.644546	0.082485	-0.124923
H	7.588045	2.258616	-0.122409
H	7.256879	-2.059852	-0.131660
C	-7.255357	-0.828608	-0.487685
H	-6.970433	-1.305451	-1.432552
H	-6.876176	-1.449541	0.331658
H	-8.350833	-0.833125	-0.429815
C	-7.076828	1.729956	1.267423
H	-6.707538	2.759353	1.337838
H	-8.167715	1.756152	1.381854
H	-6.659902	1.169387	2.111215
C	-7.225077	1.967698	-1.828890
H	-6.833090	2.990628	-1.795636
H	-6.932162	1.528310	-2.789184
H	-8.320307	2.029719	-1.809615
N	9.014614	-0.022955	-0.073744
C	9.838377	1.174288	-0.008491
H	9.629568	1.767558	0.892763
H	10.889675	0.884680	0.013731
H	9.684133	1.817691	-0.884789
C	9.645038	-1.332521	-0.004425
H	9.404793	-1.943585	-0.884658
H	10.727908	-1.206991	0.031225
H	9.336908	-1.888292	0.891989
C	-2.015320	-2.341313	1.348846
C	-0.589096	-2.563252	1.787451
C	-0.016041	-3.852654	1.742393
C	-2.831487	-3.562742	1.421063
C	-2.683820	-1.307291	2.153596
C	0.104772	-1.533716	2.458398

N	-3.236833	-0.488868	2.762372
N	-3.511474	-4.503773	1.412585
N	0.471535	-4.913542	1.665554
N	0.679952	-0.652914	2.968635

Compound: **8d'**

Charge: 0

Spin Multiplicity: 1

Computational Method/Basis Set: B3LYP/6-31G(d)

Solvation: gas phase

Electronic Energy (AU): -2200.91931942

C	-0.109675	-0.565057	0.122285
C	1.306762	-0.488218	0.129274
C	-0.904067	0.570329	0.107010
C	1.973331	0.724365	0.124188
C	1.189878	1.945080	0.123116
C	-0.252562	1.868616	0.113135
C	-0.993519	3.052216	0.108127
H	-2.077510	2.990523	0.095504
C	-0.380194	4.312677	0.114565
C	1.058620	4.388585	0.127032
C	1.802132	3.200552	0.130631
H	2.886716	3.253552	0.136655
C	-1.132644	5.526706	0.108165
H	-2.218094	5.465861	0.096474
C	-0.500752	6.743092	0.114889
H	-1.083018	7.660392	0.109158
C	0.922460	6.818169	0.128017
C	1.679068	5.675257	0.133608
H	1.404919	7.791667	0.132390
H	2.764864	5.728923	0.141961
C	3.395545	0.774668	0.126662
C	4.617833	0.806370	0.127080
C	-2.318924	0.470645	0.093406
C	-3.533804	0.370903	0.078103
Si	6.464422	0.851695	0.092158
C	-4.949585	0.247354	0.055452
C	-5.777714	1.359960	0.289588
C	-5.563811	-0.998943	-0.205146
C	-7.165179	1.245332	0.268867
H	-5.324290	2.325555	0.491370
C	-6.941902	-1.120029	-0.227708
H	-4.942678	-1.868422	-0.396506
C	-7.756208	0.000609	0.009618
H	-7.772317	2.123908	0.453440
H	-7.419357	-2.073285	-0.430275
C	7.106961	-0.856097	0.583420
H	6.775238	-1.133978	1.590370
H	6.760986	-1.629640	-0.111524
H	8.203836	-0.872102	0.578217
C	7.020281	1.294971	-1.656719
H	6.646635	2.280617	-1.955921
H	8.115327	1.317534	-1.720372
H	6.655534	0.564987	-2.387683

C	7.052043	2.155169	1.328030
H	6.673234	3.150736	1.070347
H	6.716969	1.922565	2.345079
H	8.147713	2.208657	1.340515
C	-9.977168	0.865887	0.189346
H	-9.840730	1.652687	-0.563562
H	-10.984855	0.456070	0.105332
H	-9.840905	1.293493	1.190968
C	1.971307	-1.849397	0.158520
C	-0.621677	-1.989980	0.151408
C	1.412888	-2.638816	1.323438
C	0.012459	-2.714138	1.320359
H	-1.711214	-2.036896	0.157605
H	3.059430	-1.776309	0.170029
C	-0.095656	-2.707724	-1.181848
C	1.532821	-2.616379	-1.178175
C	-0.659451	-3.407215	2.322792
H	-1.744158	-3.470776	2.316276
C	2.151586	-3.256108	2.328216
H	3.236836	-3.203260	2.324749
C	1.476365	-3.943344	3.341750
H	2.042470	-4.425294	4.133549
C	0.081771	-4.018074	3.339140
H	-0.432557	-4.557668	4.129077
C	-0.570356	-4.101864	-1.190647
C	2.158215	-3.949670	-1.188747
C	2.043741	-1.884886	-2.349848
C	-0.678779	-2.041344	-2.358498
N	2.707156	-4.971524	-1.177529
N	-1.007280	-5.176408	-1.177505
N	-1.190898	-1.524461	-3.261846
N	2.500818	-1.310000	-3.247642
O	-9.095517	-0.226057	-0.034147

Compound: **8b'**

Charge: 0

Spin Multiplicity: 1

Computational Method/Basis Set: B3LYP/6-31G(d)

Solvation: gas phase

Electronic Energy (AU): -2220.36594648

C	0.114854	-0.536583	0.142020
C	1.532256	-0.497572	0.137799
C	-0.650812	0.619682	0.134514
C	2.232455	0.696158	0.127006
C	1.481655	1.937411	0.133636
C	0.037616	1.899724	0.136916
C	-0.671238	3.102627	0.141093
H	-1.756563	3.069396	0.139341
C	-0.024597	4.346426	0.143572
C	1.415678	4.383825	0.141861
C	2.127090	3.176160	0.136778
H	3.212742	3.200122	0.132778
C	-0.744469	5.579988	0.146745
H	-1.831234	5.547785	0.146125

C	-0.080530	6.779278	0.149017
H	-0.638251	7.711757	0.150755
C	1.344192	6.816310	0.147834
C	2.070086	5.653540	0.144142
H	1.852589	7.776581	0.148859
H	3.156992	5.678232	0.141799
C	3.655254	0.707653	0.115043
C	4.878034	0.705569	0.101828
C	-2.065909	0.558929	0.131303
C	-3.284290	0.490582	0.121624
Si	6.723270	0.701154	0.039964
C	-4.699605	0.407411	0.103165
C	-5.504462	1.556860	0.244533
C	-5.357185	-0.828749	-0.067050
C	-6.886932	1.480079	0.220001
H	-5.027738	2.524156	0.372776
C	-6.738690	-0.916400	-0.093771
H	-4.765957	-1.731432	-0.189448
C	-7.549084	0.237500	0.053678
H	-7.458327	2.394018	0.327574
H	-7.192664	-1.889462	-0.235971
C	7.329148	-1.024702	0.515529
H	7.005648	-1.298023	1.526402
H	6.952674	-1.786333	-0.176741
H	8.425060	-1.068811	0.493412
C	7.267223	1.135276	-1.715244
H	6.915612	2.131373	-2.006473
H	8.361499	1.128908	-1.794419
H	6.872681	0.417564	-2.442905
C	7.366270	1.983484	1.270778
H	7.009394	2.989738	1.023469
H	7.042124	1.755399	2.292399
H	8.463036	2.008161	1.264936
N	-8.925374	0.153985	0.037268
C	-9.728245	1.364370	0.096402
H	-9.533683	2.034642	-0.753801
H	-10.785106	1.093942	0.080288
H	-9.540347	1.924945	1.021428
C	-9.573352	-1.120252	-0.228049
H	-9.300973	-1.871951	0.524067
H	-10.655392	-0.986588	-0.187912
H	-9.314418	-1.520188	-1.219386
C	2.159990	-1.876349	0.161303
C	-0.435471	-1.946830	0.172627
C	1.588911	-2.652069	1.329324
C	0.186951	-2.690320	1.335661
H	-1.525863	-1.963219	0.186442
H	3.249797	-1.832865	0.164969
C	0.061088	-2.676533	-1.165451
C	1.691335	-2.630770	-1.172409
C	-0.496001	-3.365997	2.342442
H	-1.582053	-3.400253	2.343409
C	2.317800	-3.289225	2.328844
H	3.404026	-3.264620	2.318159
C	1.631654	-3.958940	3.346798
H	2.190250	-4.455856	4.134708

C	0.235613	-3.996775	3.353604
H	-0.287445	-4.522742	4.147047
C	-0.452811	-4.056866	-1.174079
C	2.279136	-3.981139	-1.187121
C	2.215080	-1.914741	-2.348017
C	-0.510320	-1.992526	-2.337731
N	2.799208	-5.018040	-1.179938
N	-0.920743	-5.118299	-1.159928
N	-1.012335	-1.462999	-3.239421
N	2.682662	-1.355156	-3.250061

8.2 [2+2] Reactivity of 1d' and 1b' with TCNE

Compound: **TS9d**

Charge: 0

Spin Multiplicity: 1

Computational Method/Basis Set: B3LYP/6-31G(d)

Solvation: gas phase

Electronic Energy (AU): -2200.85898801

C	0.115054	-3.483490	0.055025
C	0.625406	-2.206483	0.254747
C	-0.182789	-1.048586	0.193452
C	-1.593654	-1.215921	-0.124649
C	-2.099819	-2.518675	-0.319411
C	-1.294191	-3.647680	-0.236297
C	0.325028	0.258162	0.418517
C	-2.430184	-0.071596	-0.247527
C	-1.896329	1.238466	-0.086215
C	-0.491577	1.406915	0.244710
C	0.010078	2.721639	0.372863
H	1.058518	2.868441	0.611230
C	-0.791574	3.845803	0.206985
C	-2.193914	3.672845	-0.111004
C	-2.701036	2.385219	-0.245847
H	1.683156	-2.108777	0.464638
H	-3.155032	-2.632917	-0.546268
H	-3.750831	2.249126	-0.485840
C	-0.278565	5.177525	0.342602
H	0.771960	5.306294	0.591427
C	-1.093395	6.262021	0.174327
H	-0.694156	7.266422	0.285045
C	-2.478668	6.091042	-0.142454
C	-3.009906	4.839098	-0.279338
H	-3.106598	6.968369	-0.270259
H	-4.062171	4.704347	-0.516863
C	0.944296	-4.651347	0.135458
H	1.997198	-4.521840	0.373021
C	0.414738	-5.895478	-0.061161
H	1.048311	-6.775281	0.009403
C	-0.978072	-6.058515	-0.352577
H	-1.374971	-7.058767	-0.502872
C	-1.803790	-4.972883	-0.436035
H	-2.862263	-5.093856	-0.652576
C	-3.808437	-0.235552	-0.549940
C	-4.996083	-0.375185	-0.809613
Si	-6.789494	-0.590357	-1.184751
C	3.779000	0.517816	-0.915409
C	4.101014	1.688937	-1.674798
C	4.606242	-0.638815	-1.057624
C	5.172165	1.689920	-2.531454
H	3.479329	2.571513	-1.568111
C	5.680550	-0.633416	-1.923525
H	4.402477	-1.509311	-0.441943
C	5.973211	0.529313	-2.668284
H	5.433373	2.565060	-3.116637
H	6.302999	-1.516152	-2.004357

C	-7.048646	-2.322241	-1.895150
H	-6.469874	-2.467665	-2.814272
H	-6.745042	-3.096100	-1.180964
H	-8.106130	-2.487398	-2.135786
C	-7.770801	-0.379686	0.415867
H	-7.612546	0.611952	0.854347
H	-8.845729	-0.496626	0.229574
H	-7.476930	-1.124918	1.163403
C	-7.298836	0.719256	-2.449173
H	-7.139012	1.732316	-2.062816
H	-6.726361	0.621166	-3.378408
H	-8.362630	0.621965	-2.699204
C	2.700609	0.504369	-0.065542
C	1.754069	0.457015	0.794433
C	2.266703	-0.899264	2.969638
C	2.192961	0.493683	2.457779
C	3.489551	1.189958	2.507051
C	1.197950	1.302930	3.173426
C	1.245246	-1.458799	3.760875
C	3.269424	-1.725827	2.436194
N	0.414059	-1.935876	4.430839
N	4.078304	-2.378057	1.893589
N	4.517543	1.728629	2.501708
N	0.432401	1.962932	3.742028
C	7.874987	-0.469692	-3.730637
H	7.329326	-1.333156	-4.126050
H	8.605500	-0.128632	-4.463902
H	8.384266	-0.741305	-2.799882
O	6.995315	0.641318	-3.525932

Compound: **10d**

Charge: 0

Spin Multiplicity: 1

Computational Method/Basis Set: B3LYP/6-31G(d)

Solvation: gas phase

Electronic Energy (AU): -2200.85823962

C	-0.053071	-3.552432	-0.073504
C	0.528156	-2.323059	0.216080
C	-0.207016	-1.117065	0.208770
C	-1.617776	-1.178456	-0.146071
C	-2.197151	-2.433290	-0.429417
C	-1.462262	-3.612612	-0.401115
C	0.373534	0.140934	0.524826
C	-2.381388	0.020360	-0.214879
C	-1.775000	1.283648	0.040968
C	-0.370875	1.346243	0.407550
C	0.203194	2.616724	0.632066
H	1.252252	2.684730	0.901198
C	-0.528066	3.796004	0.525982
C	-1.929893	3.727885	0.170648
C	-2.507939	2.483497	-0.058276
H	1.584151	-2.303710	0.453836
H	-3.252239	-2.469082	-0.681198
H	-3.558466	2.426124	-0.325218

C	0.058120	5.082299	0.760925
H	1.107958	5.131384	1.039293
C	-0.688692	6.222370	0.650178
H	-0.234726	7.191700	0.836587
C	-2.073240	6.155257	0.295781
C	-2.672947	4.948485	0.064824
H	-2.646228	7.074776	0.215319
H	-3.725465	4.892430	-0.201443
C	0.704180	-4.769930	-0.050760
H	1.757804	-4.718283	0.211685
C	0.106143	-5.965594	-0.334832
H	0.685099	-6.884533	-0.308909
C	-1.286920	-6.026046	-0.660638
H	-1.738806	-6.989525	-0.879966
C	-2.045355	-4.889444	-0.691808
H	-3.104013	-4.932684	-0.935137
C	-3.758516	-0.041111	-0.556840
C	-4.945118	-0.095732	-0.850980
Si	-6.738729	-0.187763	-1.276086
C	3.725209	0.295808	-0.902112
C	4.055675	1.502392	-1.590860
C	4.470800	-0.892667	-1.202345
C	5.058160	1.527519	-2.536379
H	3.496955	2.404438	-1.364345
C	5.463624	-0.862751	-2.150409
H	4.265462	-1.797635	-0.639475
C	5.769702	0.341023	-2.827515
H	5.291829	2.453746	-3.047004
H	6.048479	-1.745914	-2.384031
C	-7.084112	-1.879213	-2.044141
H	-6.492341	-2.033552	-2.953456
H	-6.846404	-2.690557	-1.346774
H	-8.143271	-1.972074	-2.314388
C	-7.744710	0.038149	0.306850
H	-7.537135	1.005189	0.778399
H	-8.819635	-0.006286	0.091627
H	-7.516428	-0.744899	1.038450
C	-7.132224	1.186753	-2.512445
H	-6.921212	2.176388	-2.091517
H	-6.541662	1.079935	-3.429299
H	-8.192753	1.162753	-2.792346
C	2.718127	0.280809	0.029143
C	1.808163	0.233029	0.933068
C	2.315337	-1.277528	2.970545
C	2.251952	0.155656	2.542461
C	3.562162	0.829736	2.636304
C	1.280955	0.924767	3.337371
C	1.323776	-1.856181	3.783144
C	3.262607	-2.089789	2.329852
N	0.513525	-2.350762	4.467036
N	4.022074	-2.723419	1.699233
N	4.597530	1.353366	2.662074
N	0.533410	1.553855	3.961829
C	7.171744	1.426559	-4.440804
H	7.985103	1.098627	-5.087736
H	6.351458	1.820584	-5.050839

H 7.534352 2.199647 -3.754759
O 6.761504 0.258206 -3.723973

Compound: **10b**

Charge: 0

Spin Multiplicity: 1

Computational Method/Basis Set: B3LYP/6-31G(d)

Solvation: gas phase

Electronic Energy (AU): -2220.31315976

C -0.184577 -3.533571 0.063743
C 0.354134 -2.288461 0.364414
C -0.403142 -1.097299 0.288253
C -1.788223 -1.193834 -0.150157
C -2.323726 -2.465356 -0.446729
C -1.568961 -3.628256 -0.350973
C 0.135107 0.175911 0.610649
C -2.568997 -0.012023 -0.285167
C -2.001977 1.266836 -0.019089
C -0.623481 1.363133 0.429659
C -0.086987 2.649297 0.664639
H 0.942150 2.741915 0.996227
C -0.830956 3.811447 0.491188
C -2.206986 3.709933 0.051240
C -2.748064 2.451491 -0.187253
H 1.392886 -2.243020 0.665315
H -3.359788 -2.527144 -0.764250
H -3.778818 2.369807 -0.517588
C -0.283366 5.113666 0.735611
H 0.746275 5.187386 1.077053
C -1.041061 6.236984 0.555346
H -0.616713 7.218231 0.749410
C -2.399963 6.136776 0.117048
C -2.962820 4.915023 -0.125422
H -2.982941 7.043671 -0.017751
H -3.995791 4.834208 -0.454731
C 0.593069 -4.735519 0.157236
H 1.626505 -4.656962 0.485433
C 0.038103 -5.947799 -0.141731
H 0.631572 -6.854333 -0.061096
C -1.330094 -6.042213 -0.554839
H -1.748490 -7.018400 -0.784620
C -2.106728 -4.922190 -0.655038
H -3.146784 -4.991468 -0.964030
C -3.924018 -0.106863 -0.701110
C -5.092439 -0.188578 -1.055704
Si -6.859663 -0.322953 -1.563759
C 3.588122 0.371292 -0.583633
C 3.971549 1.572263 -1.267238
C 4.375632 -0.807861 -0.811126
C 5.040783 1.592456 -2.121312
H 3.390437 2.473755 -1.102823
C 5.442041 -0.786264 -1.670273
H 4.138766 -1.707872 -0.252296
C 5.815332 0.410902 -2.358008
H 5.296689 2.518813 -2.619320

H	6.023034	-1.690375	-1.798710
C	-7.153362	-2.056274	-2.257699
H	-6.515844	-2.251933	-3.127365
H	-6.943274	-2.826859	-1.507259
H	-8.197037	-2.175155	-2.574133
C	-7.948694	-0.026945	-0.048414
H	-7.778277	0.968033	0.377841
H	-9.010858	-0.101108	-0.313362
H	-7.746309	-0.764190	0.736472
C	-7.206902	0.979448	-2.889559
H	-7.023286	1.992370	-2.513533
H	-6.572956	0.830004	-3.770852
H	-8.252924	0.929722	-3.216794
C	2.517770	0.352629	0.259601
C	1.542501	0.302743	1.098145
C	1.975327	-1.160823	3.182359
C	1.886276	0.264918	2.720553
C	3.164264	0.988001	2.892553
C	0.844691	1.010140	3.447884
C	0.976631	-1.749761	3.978461
C	2.973970	-1.955375	2.602824
N	0.160885	-2.253035	4.649518
N	3.781695	-2.580097	2.024282
N	4.178199	1.545236	2.985868
N	0.043771	1.623261	4.019743
N	6.879235	0.431126	-3.199240
C	7.664510	-0.781447	-3.433521
H	7.038003	-1.586021	-3.834375
H	8.445786	-0.563576	-4.161079
H	8.140792	-1.132884	-2.510581
C	7.284294	1.671863	-3.860087
H	8.162596	1.476699	-4.474586
H	6.489174	2.053985	-4.510928
H	7.542746	2.445971	-3.128199

Compound: **11d**

Charge: 0

Spin Multiplicity: 1

Computational Method/Basis Set: B3LYP/6-31G(d)

Solvation: gas phase

Electronic Energy (AU): -2200.93098389

C	-0.321227	3.694957	-0.469475
C	0.345571	2.486423	-0.630016
C	-0.310335	1.237794	-0.516446
C	-1.731081	1.234831	-0.204881
C	-2.396295	2.468710	-0.043540
C	-1.739112	3.686855	-0.167755
C	0.372479	0.004789	-0.685789
C	-2.418191	-0.003765	-0.066212
C	-1.724981	-1.238205	-0.211440
C	-0.304275	-1.232499	-0.523275
C	0.357599	-2.477310	-0.644214
H	1.419917	-2.493712	-0.863533
C	-0.303231	-3.689933	-0.490000

C	-1.721002	-3.690434	-0.187653
C	-2.384042	-2.476196	-0.056623
H	1.407968	2.509136	-0.848394
H	-3.456564	2.457112	0.188714
H	-3.444283	-2.470932	0.175987
C	0.371666	-4.949055	-0.620904
H	1.432873	-4.946200	-0.855910
C	-0.306449	-6.124447	-0.462959
H	0.213934	-7.072306	-0.568265
C	-1.706849	-6.125139	-0.162269
C	-2.389639	-4.949219	-0.029675
H	-2.223232	-7.073469	-0.041985
H	-3.452872	-4.945193	0.197161
C	0.347563	4.958055	-0.593191
H	1.408843	4.961655	-0.827855
C	-0.336374	6.129227	-0.429075
H	0.179407	7.080179	-0.529015
C	-1.736874	6.121414	-0.128952
H	-2.257921	7.066539	-0.003664
C	-2.413971	4.941465	-0.003131
H	-3.477247	4.930992	0.223274
C	-3.808783	-0.007688	0.228266
C	-5.005356	-0.010411	0.483829
Si	-6.809771	-0.012609	0.869302
C	3.414730	-0.001119	0.987553
C	2.475902	-0.009819	2.044248
C	4.780701	-0.000041	1.313002
C	2.893479	-0.016949	3.361316
H	1.414425	-0.011042	1.820883
C	5.211015	-0.007193	2.637144
H	5.530803	0.006518	0.528110
C	4.266232	-0.015694	3.672245
H	2.178473	-0.023673	4.177472
H	6.273583	-0.006087	2.848169
C	-7.249064	1.636621	1.680801
H	-6.681999	1.788940	2.606024
H	-7.036387	2.480118	1.014127
H	-8.316186	1.672109	1.932803
C	-7.772983	-0.233943	-0.741038
H	-7.508968	-1.173936	-1.238387
H	-8.852585	-0.249282	-0.546281
H	-7.570488	0.583094	-1.442498
C	-7.166950	-1.441205	2.053901
H	-6.907912	-2.407262	1.605868
H	-6.596574	-1.339889	2.984056
H	-8.232004	-1.469956	2.315497
C	5.937635	-0.022386	5.380806
H	6.453473	0.876740	5.021772
H	5.936142	-0.028959	6.471552
H	6.457548	-0.914780	5.010999
C	2.978232	0.006570	-0.395473
C	1.798339	0.009196	-1.058648
O	4.567894	-0.023161	4.993107
C	3.853955	0.014398	-1.667490
C	2.436694	0.017093	-2.475088
C	2.204711	-1.177995	-3.294005

C	2.202780	1.219345	-3.282863
C	4.667641	1.219679	-1.861600
C	4.670423	-1.186882	-1.874323
N	5.307126	2.181131	-1.977098
N	5.312087	-2.145632	-1.999776
N	2.010510	-2.131882	-3.925918
N	2.007388	2.178666	-3.906125

Compound: **11b**
Charge: 0
Spin Multiplicity: 1
Computational Method/Basis Set: B3LYP/6-31G(d)
Solvation: gas phase
Electronic Energy (AU): -2220.37854890

C	-0.458052	3.699988	-0.571443
C	0.200840	2.494637	-0.780115
C	-0.443531	1.243114	-0.634736
C	-1.842559	1.233850	-0.237016
C	-2.499860	2.464703	-0.026957
C	-1.854526	3.685562	-0.183011
C	0.232992	0.014410	-0.853650
C	-2.516459	-0.007801	-0.065002
C	-1.829105	-1.238708	-0.259461
C	-0.430259	-1.225444	-0.657927
C	0.226990	-2.467184	-0.827839
H	1.273695	-2.477292	-1.112303
C	-0.418796	-3.683128	-0.640823
C	-1.814797	-3.691028	-0.250542
C	-2.472941	-2.480210	-0.071537
H	1.247902	2.520761	-1.062204
H	-3.544031	2.448747	0.269327
H	-3.516964	-2.480576	0.225738
C	0.251230	-4.938789	-0.821921
H	1.295622	-4.929835	-1.122916
C	-0.411135	-6.117981	-0.629436
H	0.104992	-7.063091	-0.773504
C	-1.789876	-6.125964	-0.241421
C	-2.467381	-4.953631	-0.058850
H	-2.294458	-7.077079	-0.095289
H	-3.514504	-4.955464	0.233686
C	0.198685	4.965881	-0.728286
H	1.243391	4.973594	-1.028198
C	-0.476567	6.134114	-0.514832
H	0.029498	7.087230	-0.640705
C	-1.855771	6.120025	-0.128634
H	-2.370730	7.062786	0.034444
C	-2.520878	4.937315	0.031153
H	-3.568295	4.922557	0.322263
C	-3.887676	-0.018162	0.309284
C	-5.068436	-0.025657	0.630286
Si	-6.852015	-0.033272	1.099113
C	3.365897	-0.000478	0.645272
C	2.498316	-0.022094	1.757745
C	4.750591	0.001112	0.902507
C	2.983983	-0.040748	3.051572
H	1.424705	-0.024519	1.600183
C	5.249907	-0.017607	2.193545
H	5.458896	0.017563	0.079389
C	4.379980	-0.039108	3.312707
H	2.275242	-0.056912	3.870272
H	6.323600	-0.015226	2.333338
C	-7.265945	1.622740	1.910500
H	-6.661074	1.789147	2.809008

H	-7.086657	2.459422	1.225668
H	-8.321670	1.655327	2.207014
C	-7.886829	-0.278306	-0.463000
H	-7.641573	-1.223639	-0.959857
H	-8.956754	-0.294568	-0.220506
H	-7.718429	0.530274	-1.183032
C	-7.148593	-1.449589	2.315036
H	-6.903613	-2.419356	1.867122
H	-6.538311	-1.334316	3.217875
H	-8.200883	-1.481145	2.623716
C	2.851501	0.019407	-0.704662
C	1.636294	0.026064	-1.306158
C	3.654561	0.040606	-2.024514
C	2.195522	0.047529	-2.753159
C	1.921629	-1.140938	-3.570102
C	1.917151	1.255887	-3.538805
C	4.454143	1.249326	-2.252866
C	4.460370	-1.156858	-2.287636
N	5.083736	2.213529	-2.396584
N	5.094888	-2.113334	-2.458722
N	1.692645	-2.090373	-4.197186
N	1.685366	2.220360	-4.141437
N	4.866514	-0.057648	4.597522
C	6.302000	-0.055039	4.835384
H	6.780654	0.844160	4.424292
H	6.486773	-0.073608	5.910163
H	6.788750	-0.934506	4.392513
C	3.949855	-0.076438	5.727465
H	4.524985	-0.087504	6.654122
H	3.302380	0.810837	5.740846
H	3.308233	-0.967975	5.716118

Compound: **s-cis-7d'**

Charge: 0

Spin Multiplicity: 1

Computational Method/Basis Set: B3LYP/6-31G(d)

Solvation: gas phase

Electronic Energy (AU): -2200.95272492

C	-0.530363	3.950987	0.013917
C	0.252540	2.880200	-0.402926
C	-0.238083	1.555192	-0.452430
C	-1.631814	1.330403	-0.105115
C	-2.413562	2.422473	0.327471
C	-1.904425	3.713361	0.407352
C	-2.182305	0.024373	-0.226879
C	-1.383327	-1.059373	-0.687805
C	0.022003	-0.842257	-1.000246
C	0.789949	-1.963590	-1.395073
H	1.848162	-1.841185	-1.596333
C	0.243163	-3.233546	-1.533467
C	-1.162852	-3.436645	-1.249568
C	-1.925834	-2.354432	-0.831057
H	1.260023	3.091332	-0.740331
H	-3.451480	2.242056	0.588879

H	-2.976459	-2.500769	-0.601423
C	1.027390	-4.360265	-1.950114
H	2.081899	-4.207094	-2.165460
C	0.460664	-5.596493	-2.080501
H	1.063791	-6.441503	-2.400851
C	-0.930177	-5.796058	-1.802366
C	-1.714056	-4.751882	-1.400544
H	-1.356984	-6.788646	-1.915653
H	-2.770294	-4.897727	-1.188700
C	-0.022509	5.291670	0.058632
H	1.005267	5.467312	-0.248468
C	-0.815742	6.321971	0.478930
H	-0.421722	7.333832	0.511683
C	-2.170499	6.086266	0.878984
H	-2.779191	6.923287	1.209460
C	-2.697258	4.825953	0.842425
H	-3.727157	4.643705	1.138983
C	-3.545452	-0.198463	0.108513
C	-4.718869	-0.389421	0.397318
Si	-6.492642	-0.682547	0.820156
C	3.036011	-0.239527	1.030917
C	4.263768	-0.898236	1.203518
C	1.935857	-0.656023	1.807045
C	4.402188	-1.944027	2.112814
H	5.120481	-0.603337	0.605125
C	2.070515	-1.681696	2.727300
H	0.982019	-0.150614	1.712274
C	3.302447	-2.339350	2.886216
H	5.363037	-2.434944	2.210222
H	1.233635	-1.993256	3.343557
C	-6.730704	-0.356277	2.666071
H	-6.105795	-1.020738	3.273265
H	-6.472527	0.676266	2.926784
H	-7.775930	-0.522686	2.954819
C	-7.554789	0.497499	-0.203439
H	-7.405496	0.338790	-1.277232
H	-8.619436	0.345414	0.013295
H	-7.315855	1.544284	0.015809
C	-6.912130	-2.478161	0.408185
H	-6.761681	-2.689301	-0.656585
H	-6.289895	-3.175287	0.980850
H	-7.960826	-2.694825	0.646239
C	4.544982	-4.028563	4.032592
H	5.331689	-3.348438	4.381640
H	4.328507	-4.762835	4.809693
H	4.884289	-4.546292	3.126674
C	3.756095	1.965938	0.163864
C	4.619548	2.154116	1.295865
C	3.759147	3.059266	-0.764993
N	5.324689	2.359162	2.197835
N	3.750043	3.979571	-1.476996
C	0.569499	0.462951	-0.862632
C	2.023553	0.685660	-1.119370
C	2.949386	0.864707	0.042046
C	2.527765	0.618031	-2.389794
C	3.934235	0.628195	-2.681034

C	1.672742	0.466868	-3.533385
N	1.017106	0.354989	-4.487127
N	5.069262	0.597105	-2.932867
O	3.323128	-3.334718	3.806284

Compound: **s-cis-7b'**

Charge: 0

Spin Multiplicity: 1

Computational Method/Basis Set: B3LYP/6-31G(d)

Solvation: gas phase

Electronic Energy (AU): -2220.40046677

C	0.866688	3.970875	-0.250348
C	0.034314	2.988711	0.274301
C	0.442971	1.642634	0.414375
C	1.807185	1.302019	0.043664
C	2.639429	2.304545	-0.497785
C	2.208823	3.615482	-0.664460
C	2.279792	-0.023250	0.251712
C	1.433381	-1.013451	0.824595
C	0.057186	-0.681219	1.165046
C	-0.763487	-1.717554	1.671199
H	-1.804068	-1.512943	1.895587
C	-0.291824	-3.005764	1.891442
C	1.087163	-3.321454	1.579240
C	1.899472	-2.326314	1.051677
H	-0.944678	3.290188	0.625126
H	3.654521	2.038300	-0.774925
H	2.929684	-2.557053	0.799596
C	-1.129366	-4.043705	2.420291
H	-2.163341	-3.805590	2.656890
C	-0.637181	-5.300766	2.629630
H	-1.279696	-6.077268	3.035421
C	0.727252	-5.611481	2.323478
C	1.559739	-4.654713	1.815506
H	1.095324	-6.618052	2.501602
H	2.596393	-4.884881	1.582561
C	0.440788	5.333920	-0.385523
H	-0.562520	5.597496	-0.061116
C	1.280591	6.275799	-0.909701
H	0.948986	7.305404	-1.010371
C	2.603549	5.923101	-1.329986
H	3.250917	6.691357	-1.743676
C	3.052976	4.638287	-1.209449
H	4.058908	4.368505	-1.521261
C	3.612156	-0.359021	-0.112359
C	4.759069	-0.643227	-0.429790
Si	6.492433	-1.066872	-0.902518
C	-3.051644	0.007267	-0.792705
C	-4.369118	-0.463691	-0.973036
C	-2.025160	-0.661571	-1.488166
C	-4.650433	-1.542245	-1.792392
H	-5.184483	0.007742	-0.433502
C	-2.297791	-1.725409	-2.330736
H	-1.001998	-0.315906	-1.406616

C	-3.620345	-2.207469	-2.504373
H	-5.678257	-1.872527	-1.875907
H	-1.474567	-2.180579	-2.867166
C	6.712988	-0.717434	-2.746713
H	6.022098	-1.314993	-3.351971
H	6.533179	0.338370	-2.978644
H	7.734149	-0.960494	-3.065666
C	7.672310	-0.001819	0.118319
H	7.538921	-0.176064	1.191799
H	8.715316	-0.232413	-0.132051
H	7.512031	1.065945	-0.068814
C	6.778938	-2.899741	-0.542611
H	6.642833	-3.123882	0.521447
H	6.087469	-3.532091	-1.111022
H	7.800155	-3.191739	-0.816957
N	-3.891930	-3.274797	-3.324981
C	-5.267346	-3.699286	-3.541422
H	-5.880845	-2.890601	-3.960724
H	-5.277785	-4.531693	-4.246102
H	-5.738820	-4.039068	-2.609396
C	-2.813771	-3.942775	-4.038317
H	-2.053329	-4.327097	-3.346422
H	-3.222052	-4.789513	-4.591527
H	-2.317932	-3.273781	-4.755813
C	-3.534924	2.318679	-0.037899
C	-4.424984	2.538233	-1.141676
C	-3.402587	3.448214	0.834141
N	-5.142852	2.774554	-2.026450
N	-3.282242	4.398020	1.496500
C	-0.415806	0.641306	0.937716
C	-1.841840	0.976502	1.229135
C	-2.813119	1.155726	0.102092
C	-2.292547	1.017857	2.521536
C	-3.681032	1.134997	2.869414
C	-1.400273	0.882574	3.638326
N	-0.712652	0.787415	4.571260
N	-4.802278	1.189224	3.173751

Compound: **s-trans-7d'**

Charge: 0

Spin Multiplicity: 1

Computational Method/Basis Set: B3LYP/6-31G(d)

Solvation: gas phase

Electronic Energy (AU): -2200.95380294

C	-1.489101	3.842160	0.049300
C	-0.498073	2.869867	-0.040855
C	-0.782333	1.491731	-0.156852
C	-2.182295	1.099318	-0.116081
C	-3.182155	2.091598	-0.034492
C	-2.879550	3.444296	0.037636
C	-2.532979	-0.278238	-0.131698
C	-1.527526	-1.283226	-0.184035
C	-0.127746	-0.898743	-0.248977
C	0.821971	-1.936190	-0.371225

H	1.872418	-1.694610	-0.465549
C	0.474887	-3.285118	-0.372326
C	-0.919488	-3.657235	-0.280907
C	-1.873599	-2.650150	-0.198960
H	0.531918	3.204428	-0.007247
H	-4.219885	1.775536	-0.009789
H	-2.924467	-2.916403	-0.149688
C	1.455967	-4.324795	-0.469800
H	2.504752	-4.046230	-0.535043
C	1.081846	-5.640128	-0.473150
H	1.835044	-6.419959	-0.543280
C	-0.298081	-6.007765	-0.383632
C	-1.266532	-5.047432	-0.291662
H	-0.569203	-7.059681	-0.389410
H	-2.316697	-5.320069	-0.224307
C	-1.177280	5.237009	0.155605
H	-0.132533	5.536910	0.166666
C	-2.172244	6.170903	0.234853
H	-1.923937	7.225787	0.311559
C	-3.548299	5.776660	0.216873
H	-4.319909	6.538734	0.280463
C	-3.890239	4.457076	0.122680
H	-4.933218	4.150896	0.111606
C	-3.901220	-0.659103	-0.093434
C	-5.077373	-0.994318	-0.062558
Si	-6.849954	-1.516232	-0.017281
C	4.012519	0.075002	0.313140
C	5.106559	0.430574	1.121840
C	4.289440	-0.573417	-0.913387
C	6.414318	0.146306	0.747690
H	4.941305	0.975973	2.044010
C	5.583979	-0.881115	-1.286880
H	3.478018	-0.841689	-1.581897
C	6.663113	-0.523089	-0.459556
H	7.227180	0.459883	1.391394
H	5.793464	-1.388912	-2.222474
C	-7.635327	-0.827139	1.556066
H	-7.129333	-1.202603	2.452425
H	-7.589040	0.267399	1.580420
H	-8.691044	-1.118831	1.619681
C	-7.711889	-0.827241	-1.550419
H	-7.249483	-1.201586	-2.470513
H	-8.768968	-1.120636	-1.562901
H	-7.668771	0.267391	-1.576341
C	-6.905981	-3.404565	-0.016660
H	-6.434672	-3.817927	-0.915609
H	-6.388564	-3.818961	0.856046
H	-7.942807	-3.761821	0.010088
C	9.031638	-0.507654	-0.139459
H	9.004384	-0.990640	0.844838
H	9.893348	-0.872119	-0.699968
H	9.110137	0.578968	-0.014124
C	2.225807	0.222148	2.034553
C	3.038760	-0.433800	3.016836
C	0.977607	0.675836	2.572921
N	3.640266	-0.978420	3.851906

N	0.014368	1.037226	3.118451
C	0.232301	0.483673	-0.234140
C	1.660218	0.870893	-0.298461
C	2.628075	0.383920	0.721036
C	2.100911	1.702352	-1.315354
C	3.363334	2.381359	-1.331122
C	1.276359	2.014015	-2.444577
N	0.659102	2.272065	-3.397153
N	4.346720	3.002270	-1.389630
O	7.890619	-0.856420	-0.918295

Compound: **s-trans-7b'**
 Charge: 0
 Spin Multiplicity: 1
 Computational Method/Basis Set: B3LYP/6-31G(d)
 Solvation: gas phase
 Electronic Energy (AU): -2220.40243764

C	-1.830616	3.820571	0.029103
C	-0.802516	2.884746	-0.011618
C	-1.032223	1.495653	-0.122924
C	-2.417366	1.052310	-0.130025
C	-3.454937	2.008329	-0.101110
C	-3.204226	3.371697	-0.033828
C	-2.715949	-0.337288	-0.139406
C	-1.672442	-1.303923	-0.131697
C	-0.285859	-0.868532	-0.149191
C	0.705154	-1.873068	-0.208461
H	1.749555	-1.595429	-0.258697
C	0.406958	-3.233202	-0.195266
C	-0.975454	-3.655273	-0.153778
C	-1.967749	-2.683013	-0.131847
H	0.212836	3.255548	0.061446
H	-4.480865	1.655201	-0.112772
H	-3.009488	-2.986813	-0.118474
C	1.428737	-4.237639	-0.228316
H	2.468325	-3.920588	-0.254776
C	1.103462	-5.565713	-0.218540
H	1.886817	-6.318337	-0.239253
C	-0.264928	-5.982757	-0.178814
C	-1.270649	-5.057623	-0.148386
H	-0.497057	-7.044007	-0.172463
H	-2.312105	-5.367969	-0.118567
C	-1.574068	5.226948	0.134023
H	-0.542055	5.564421	0.184783
C	-2.604350	6.124497	0.163523
H	-2.397896	7.188409	0.239840
C	-3.963446	5.679760	0.093691
H	-4.764159	6.413623	0.118323
C	-4.253413	4.347874	-0.000434
H	-5.283399	4.003680	-0.049877
C	-4.069855	-0.768450	-0.151277
C	-5.233933	-1.144668	-0.162075
Si	-6.989502	-1.719505	-0.172278
C	3.788480	0.229740	0.449016
C	4.885739	0.560602	1.273890
C	4.088879	-0.388687	-0.786444
C	6.187791	0.287433	0.904032
H	4.718676	1.088680	2.205523
C	5.384271	-0.689947	-1.160476
H	3.287102	-0.647650	-1.470493
C	6.482467	-0.361346	-0.323572
H	6.987268	0.601330	1.563291
H	5.547867	-1.175075	-2.114598
C	-7.844878	-1.052009	1.373881
H	-7.354783	-1.409179	2.286418
H	-7.833613	0.043499	1.396099

H	-8.892396	-1.376590	1.406347
C	-7.824656	-1.058917	-1.732775
H	-7.324859	-1.422383	-2.637574
H	-8.872442	-1.381398	-1.775769
H	-7.810887	0.036437	-1.760878
C	-6.993157	-3.608969	-0.168312
H	-6.480416	-4.011385	-1.049368
H	-6.494567	-4.007038	0.722771
H	-8.020192	-3.994407	-0.175493
C	8.881291	-0.259984	0.170329
H	8.779176	-0.700051	1.169578
H	9.813313	-0.624736	-0.263010
H	8.956894	0.830987	0.279374
C	1.992832	0.418009	2.162828
C	2.787735	-0.211728	3.174295
C	0.745652	0.907527	2.667186
N	3.377359	-0.737335	4.030400
N	-0.223096	1.307275	3.175720
C	0.021731	0.526813	-0.153366
C	1.435172	0.969192	-0.196208
C	2.408409	0.531950	0.844182
C	1.862739	1.803450	-1.214987
C	3.106181	2.517850	-1.221029
C	1.050575	2.074579	-2.364046
N	0.447651	2.300116	-3.333874
N	4.071460	3.166525	-1.280317
C	8.051233	-1.208289	-2.005158
H	9.127398	-1.348986	-2.111968
H	7.569159	-2.185753	-2.135206
H	7.710698	-0.545908	-2.812605
N	7.771799	-0.647453	-0.690462

8.3 [4+2] Reactivity of 4b' with TCNE

Compound: 4b'

Charge: 0

Spin Multiplicity: 1

Computational Method/Basis Set: B3LYP/6-31G(d)

Solvation: gas phase

Electronic Energy (AU): -2003.04228636

C	-1.284734	-1.234661	-0.422022
C	-1.955265	-2.406762	-0.135259
C	-1.698000	-3.610634	-0.838823
C	-0.700101	-3.604847	-1.863620
C	-0.031721	-2.388594	-2.149074
C	-0.316222	-1.224424	-1.466894
H	-3.143912	-4.821203	0.226412
H	-2.703038	-2.414851	0.652221
C	-2.385761	-4.820955	-0.553344
C	-0.425284	-4.810793	-2.563901
H	0.714850	-2.364397	-2.937684
C	-1.107375	-5.968107	-2.263397
C	-2.097751	-5.973417	-1.248998
H	0.333858	-4.802670	-3.342460
H	-0.889295	-6.884909	-2.804603
H	-2.629434	-6.893838	-1.023045
C	-1.463649	0.023137	0.436059
C	-1.999121	2.447142	-0.077939
H	-2.732295	2.425004	0.722419
C	-2.744215	-0.001037	1.171353
C	-3.773314	-0.026137	1.823824
Si	-5.349888	-0.052004	2.780957
C	-5.277168	1.293832	4.105684
H	-5.152601	2.287377	3.660310
H	-6.199943	1.306264	4.698952
H	-4.439352	1.129480	4.792647
C	-5.537295	-1.750952	3.589364
H	-4.702637	-1.965552	4.266403
H	-6.463814	-1.802397	4.174647
H	-5.573068	-2.548729	2.838627
C	-6.782510	0.266512	1.590431
H	-6.685612	1.242086	1.100850
H	-6.823970	-0.497192	0.805658
H	-7.741505	0.252487	2.123143
O	-0.362812	0.140371	1.375177
C	-0.196385	-0.915049	2.311251
H	0.038244	-1.869959	1.824259
H	0.648481	-0.616414	2.936531
H	-1.086889	-1.042324	2.942112
C	-1.765622	3.670132	-0.754687
C	-0.774197	3.704909	-1.785714
C	-2.204811	6.035762	-1.105279
H	-2.748452	6.942307	-0.853032
C	-1.221723	6.070347	-2.126450
H	-1.021488	7.003298	-2.646621
C	2.821753	0.058088	-0.650196
C	1.747292	0.067434	-1.213889

C	4.084974	0.054582	0.009564
C	4.831884	-1.129584	0.154583
C	4.630719	1.234416	0.549611
C	6.060255	-1.138795	0.799650
H	4.432916	-2.057205	-0.245268
C	5.857664	1.236366	1.197258
H	4.072636	2.161744	0.461036
C	6.615603	0.048689	1.333060
H	6.590216	-2.079497	0.888879
H	6.226887	2.171218	1.601593
N	7.854198	0.049761	1.956598
C	8.309529	1.245180	2.644847
H	7.644695	1.540661	3.472069
H	9.304706	1.064029	3.055406
H	8.386329	2.093636	1.953786
C	8.515826	-1.212025	2.239900
H	9.477867	-1.012174	2.715550
H	7.928581	-1.860039	2.909885
H	8.713033	-1.770950	1.316778
C	0.426254	0.062615	-1.860428
O	0.697428	0.076718	-3.280719
C	-0.433150	0.074452	-4.149096
H	-0.020741	0.096318	-5.161241
H	-1.043513	-0.828769	-4.030091
H	-1.068594	0.955610	-4.001449
C	-0.084181	2.508803	-2.101439
H	0.664704	2.518042	-2.888181
C	-0.347102	1.324242	-1.445681
C	-1.314112	1.295610	-0.402290
C	-0.523612	4.931698	-2.458828
H	0.230958	4.954421	-3.241563
C	-2.469895	4.862735	-0.435818
H	-3.221553	4.832642	0.349574

Compound: **syn-16**
 Charge: 0
 Spin Multiplicity: 1
 Computational Method/Basis Set: B3LYP/6-31G(d)
 Solvation: gas phase
 Electronic Energy (AU): -2450.56810649

C	0.412882	2.127270	0.429224
C	0.359532	3.506983	0.456264
C	0.956586	4.261953	1.496767
C	1.644855	3.566034	2.539879
C	1.675029	2.150363	2.501281
C	1.067361	1.437148	1.489207
H	0.379720	6.207058	0.738270
H	-0.155429	4.036381	-0.339907
C	0.905075	5.681715	1.532424
C	2.258802	4.315870	3.579671
H	2.175260	1.606891	3.297713
C	2.193477	5.690729	3.585497
C	1.509489	6.380471	2.552674
H	2.780529	3.783437	4.371305
H	2.666348	6.254918	4.384864
H	1.464337	7.466032	2.571247
C	-0.102165	1.338865	-0.780291
C	-1.567778	-0.689437	-1.144018
H	-2.020849	-0.163896	-1.978409
C	-1.142753	2.093373	-1.507354
C	-1.993222	2.705466	-2.129309
Si	-3.358834	3.587129	-3.006364
C	-4.621016	2.303745	-3.577929
H	-5.004473	1.726712	-2.728960
H	-5.473176	2.788823	-4.070100
H	-4.178430	1.601555	-4.293999
C	-2.630587	4.505764	-4.489842
H	-2.142647	3.813314	-5.185243
H	-3.416820	5.035068	-5.042509
H	-1.885765	5.246832	-4.177939
C	-4.154329	4.801563	-1.797853
H	-4.559695	4.277308	-0.925358
H	-3.431055	5.542331	-1.438409
H	-4.978907	5.343863	-2.277055
O	0.998100	1.016050	-1.669361
C	1.695085	2.107598	-2.253798
H	2.210835	2.720389	-1.503756
H	2.436313	1.655779	-2.917410
H	1.023868	2.747879	-2.842067
C	-1.964110	-2.021782	-0.877788
C	-1.362149	-2.710706	0.223305
C	-3.269324	-4.012981	-1.402972
H	-3.990273	-4.528473	-2.030953
C	-2.689311	-4.688099	-0.301404
H	-2.974381	-5.714485	-0.088650
C	3.472812	-0.920402	0.560646
C	2.410362	-0.554755	1.019220
C	4.720431	-1.358218	0.030057
C	5.871340	-0.550867	0.102092

C	4.848795	-2.614925	-0.591260
C	7.087941	-0.973813	-0.413007
H	5.801580	0.427020	0.569409
C	6.060335	-3.047854	-1.109562
H	3.975835	-3.256118	-0.669559
C	7.221693	-2.242579	-1.026663
H	7.940501	-0.309612	-0.336478
H	6.101197	-4.021082	-1.583849
N	8.440436	-2.681149	-1.519036
C	8.503799	-3.911028	-2.289589
H	7.900618	-3.868362	-3.210332
H	9.540947	-4.104015	-2.570078
H	8.156565	-4.766456	-1.697144
C	9.564283	-1.762425	-1.577561
H	10.436025	-2.288567	-1.971004
H	9.368179	-0.891130	-2.222285
H	9.824484	-1.392158	-0.578320
C	1.113912	-0.096701	1.542401
O	1.061331	-0.568601	2.903609
C	-0.104205	-0.230909	3.657855
H	0.028374	-0.719804	4.626252
H	-0.195008	0.850565	3.811528
H	-1.023563	-0.602769	3.193946
C	-0.381784	-2.037700	0.989284
H	0.093770	-2.550179	1.820083
C	-0.000686	-0.740434	0.700791
C	-0.610990	-0.050627	-0.380006
C	-1.762652	-4.048817	0.497010
H	-1.308648	-4.569394	1.336804
C	-2.923023	-2.704264	-1.676328
H	-3.363460	-2.183302	-2.523149
C	-4.981429	-2.815779	1.667390
C	-5.525392	-2.335970	0.498915
C	-5.344600	-0.980018	0.084775
C	-6.349283	-3.156916	-0.332828
C	-4.201815	-1.983145	2.526436
C	-5.203858	-4.161020	2.096638
N	-5.234106	0.123535	-0.265260
N	-7.039695	-3.799796	-1.013021
N	-3.585445	-1.316309	3.252995
N	-5.389613	-5.246021	2.472118

Compound: *anti*-16
Charge: 0
Spin Multiplicity: 1
Computational Method/Basis Set: B3LYP/6-31G(d)
Solvation: gas phase
Electronic Energy (AU): -2450.56902222

C	-1.127649	-1.825531	0.626447
C	-0.680757	-3.024315	1.145428
C	-1.410634	-3.734784	2.131524
C	-2.653970	-3.193708	2.587062
C	-3.085207	-1.952931	2.056072
C	-2.343858	-1.268726	1.115961
H	-0.011055	-5.376764	2.323764
H	0.258113	-3.439997	0.791631
C	-0.957975	-4.969544	2.670258
C	-3.401630	-3.909170	3.561290
H	-4.015965	-1.518155	2.409181
C	-2.938307	-5.104866	4.061736
C	-1.704237	-5.639451	3.613135
H	-4.346514	-3.494806	3.904647
H	-3.517655	-5.644713	4.805914
H	-1.349403	-6.583016	4.018891
C	-0.412957	-1.156169	-0.553034
C	0.414396	1.176785	-1.075063
H	1.309393	0.723235	-1.488400
C	1.000609	-1.563937	-0.638222
O	-1.113026	-1.475351	-1.786240
C	-1.142092	-2.842442	-2.169145
H	-1.680396	-3.465969	-1.443884
H	-1.672429	-2.866016	-3.124452
H	-0.129484	-3.245310	-2.306774
C	0.255577	2.580430	-1.156883
C	-0.928428	3.171669	-0.611599
C	1.023339	4.784242	-1.863849
H	1.760983	5.411837	-2.355658
C	-0.138561	5.371512	-1.307466
H	-0.281930	6.446313	-1.371941
C	-4.710399	-0.312353	-1.282449
C	-3.877640	-0.122793	-0.414788
C	-2.855118	0.094434	0.625871
O	-3.541537	0.801167	1.674446
C	-2.779257	1.123697	2.839695
H	-3.465802	1.674068	3.487563
H	-2.431986	0.226217	3.363797
H	-1.918405	1.760114	2.611062
C	-1.901554	2.325755	-0.028710
H	-2.811748	2.757381	0.376444
C	-1.729344	0.955423	0.027097
C	-0.547246	0.370107	-0.498713
C	-1.088667	4.583377	-0.688841
H	-1.986757	5.031612	-0.270669
C	1.221611	3.420141	-1.778042
H	2.110477	2.964805	-2.208339
C	1.500300	5.012893	1.788795
C	2.585493	4.460988	1.148737

C	2.891280	3.068633	1.249674
C	3.497691	5.265796	0.397111
C	0.618680	4.219770	2.584325
C	1.227881	6.414517	1.721393
N	3.177397	1.944538	1.333228
N	4.265002	5.904099	-0.199904
N	-0.097010	3.597334	3.257241
N	1.001395	7.555006	1.694560
C	2.166602	-1.891005	-0.728368
C	3.548482	-2.238034	-0.801882
C	3.990857	-3.347718	-1.544744
C	4.520583	-1.469874	-0.132281
C	5.335457	-3.681895	-1.615315
H	3.264075	-3.952695	-2.079301
C	5.866843	-1.797453	-0.197099
H	4.207779	-0.602194	0.441528
C	6.315181	-2.921001	-0.933119
H	5.623689	-4.541818	-2.207657
H	6.575567	-1.170894	0.330776
N	7.655857	-3.265021	-0.978331
C	8.647652	-2.370419	-0.405985
H	9.638010	-2.815059	-0.519472
H	8.656979	-1.381585	-0.890663
H	8.472816	-2.219957	0.666514
C	8.098533	-4.321783	-1.871530
H	9.173834	-4.464929	-1.750644
H	7.608768	-5.273622	-1.631330
H	7.899022	-4.094672	-2.930659
Si	-5.947805	-0.612898	-2.609988
C	-6.509382	1.049584	-3.313587
H	-6.963725	1.676910	-2.538294
H	-5.665987	1.604440	-3.740006
H	-7.253110	0.906688	-4.107494
C	-5.130244	-1.650180	-3.962785
H	-4.257015	-1.135995	-4.379745
H	-4.793427	-2.616619	-3.570708
H	-5.830714	-1.846423	-4.784160
C	-7.421618	-1.540721	-1.874428
H	-8.182278	-1.735955	-2.640661
H	-7.113603	-2.504765	-1.454015
H	-7.894724	-0.963020	-1.072282

Compound: ***syn*-TS17**
 Charge: 0
 Spin Multiplicity: 1
 Computational Method/Basis Set: B3LYP/6-31G(d)
 Solvation: gas phase
 Electronic Energy (AU): -2450.51681132

C	0.265794	2.303812	0.298419
C	0.200698	3.682079	0.224390
C	0.866521	4.517538	1.155072
C	1.633447	3.906861	2.197060
C	1.671940	2.493127	2.266627
C	1.001837	1.701340	1.357086
H	0.219289	6.396182	0.292185
H	-0.382381	4.146476	-0.565366
C	0.805038	5.935747	1.084273
C	2.313432	4.737316	3.129129
H	2.227951	2.014985	3.067948
C	2.236783	6.108003	3.032648
C	1.474828	6.713292	2.001140
H	2.894552	4.270142	3.920523
H	2.760265	6.734265	3.749955
H	1.421644	7.796802	1.939088
C	-0.339908	1.434370	-0.807785
C	-1.698988	-0.689332	-0.997386
H	-2.218615	-0.228433	-1.830173
C	-1.502432	2.101803	-1.428109
C	-2.473936	2.627069	-1.942900
Si	-4.028291	3.365661	-2.621554
C	-5.207391	1.953535	-3.046186
H	-5.404439	1.331406	-2.165781
H	-6.167671	2.343063	-3.406241
H	-4.793690	1.311379	-3.832645
C	-3.595196	4.362509	-4.168614
H	-3.141090	3.727997	-4.938262
H	-4.495894	4.816980	-4.599504
H	-2.890263	5.170500	-3.941822
C	-4.776464	4.482314	-1.296111
H	-5.006554	3.912581	-0.389123
H	-4.092637	5.292866	-1.019847
H	-5.708879	4.937125	-1.652906
O	0.662640	1.114532	-1.805992
C	1.207300	2.201321	-2.542712
H	1.766136	2.896314	-1.903636
H	1.892314	1.748254	-3.263380
H	0.427202	2.755572	-3.081771
C	-1.980806	-2.009279	-0.639995
C	-1.326490	-2.588263	0.469554
C	-2.746544	-4.263576	-1.327746
H	-3.180354	-4.864899	-2.119556
C	-2.133361	-4.817327	-0.246969
H	-2.045418	-5.890768	-0.116771
C	3.393996	-0.705216	0.527463
C	2.348003	-0.311557	1.000996
C	4.627787	-1.165366	-0.016114
C	5.765762	-0.337121	-0.049337

C	4.755747	-2.463806	-0.544463
C	6.969624	-0.779339	-0.577181
H	5.695490	0.672200	0.345305
C	5.954554	-2.916570	-1.074838
H	3.892918	-3.123337	-0.538911
C	7.103208	-2.088875	-1.099095
H	7.812402	-0.098630	-0.583412
H	5.996394	-3.923153	-1.473299
N	8.308134	-2.543351	-1.606201
C	8.371287	-3.835171	-2.267601
H	7.726395	-3.886695	-3.158770
H	9.399310	-4.027147	-2.579881
H	8.074416	-4.643721	-1.587802
C	9.422443	-1.622748	-1.752436
H	10.284632	-2.164204	-2.145790
H	9.197447	-0.790852	-2.437962
H	9.712936	-1.194525	-0.784862
C	1.067061	0.178663	1.532942
O	1.058655	-0.182719	2.926756
C	-0.092988	0.205190	3.682768
H	0.095176	-0.156169	4.696406
H	-0.217925	1.293649	3.706230
H	-1.012890	-0.256634	3.308365
C	-0.380246	-1.846400	1.180192
H	0.132806	-2.273607	2.035531
C	-0.060034	-0.547450	0.782038
C	-0.736495	0.041780	-0.301454
C	-1.775321	-3.925090	0.829495
H	-1.375888	-4.359006	1.743318
C	-2.995137	-2.839863	-1.277399
H	-3.559608	-2.393865	-2.093277
C	-3.750567	-3.434842	1.431507
C	-4.413563	-2.858213	0.229501
C	-4.759495	-1.456202	0.272278
C	-5.450228	-3.656680	-0.387684
C	-3.471972	-2.534827	2.521578
C	-4.197498	-4.734294	1.873626
N	-5.028135	-0.325656	0.242728
N	-6.263823	-4.284843	-0.930344
N	-3.201992	-1.827078	3.403600
N	-4.508749	-5.794559	2.235291

Compound: *anti*-TS17
 Charge: 0
 Spin Multiplicity: 1
 Computational Method/Basis Set: B3LYP/6-31G(d)
 Solvation: gas phase
 Electronic Energy (AU): -2450.51793165

C	-0.951609	-2.083121	0.393398
C	-0.468034	-3.345651	0.677396
C	-1.161862	-4.242985	1.526928
C	-2.403420	-3.822664	2.100221
C	-2.871580	-2.517252	1.813745
C	-2.168567	-1.657226	0.995865
H	0.273932	-5.858645	1.386913
H	0.477021	-3.661566	0.245545
C	-0.671922	-5.544279	1.821532
C	-3.112079	-4.720172	2.944444
H	-3.799177	-2.174861	2.263549
C	-2.613370	-5.975493	3.207947
C	-1.381323	-6.391205	2.642248
H	-4.055116	-4.397118	3.378735
H	-3.162548	-6.654873	3.854167
H	-0.998575	-7.384146	2.861959
C	-0.256210	-1.196068	-0.645159
C	0.423889	1.231100	-0.869962
H	1.326264	0.884100	-1.361308
C	1.186373	-1.486902	-0.723600
O	-0.898278	-1.357476	-1.938726
C	-0.784376	-2.633309	-2.552639
H	-1.277400	-3.420950	-1.968531
H	-1.285823	-2.537669	-3.518942
H	0.265826	-2.910816	-2.714965
C	0.165822	2.598468	-0.757144
C	-0.996768	3.038740	-0.087058
C	0.470211	4.882890	-1.668753
H	0.986250	5.501247	-2.395454
C	-0.639577	5.309881	-1.007969
H	-1.069450	6.292619	-1.170446
C	-4.658459	-0.354381	-1.098542
C	-3.793954	-0.303410	-0.242716
C	-2.726399	-0.245165	0.773582
O	-3.363763	0.260602	1.957969
C	-2.539095	0.398068	3.120540
H	-3.199836	0.798212	3.892854
H	-2.139219	-0.566429	3.452041
H	-1.712179	1.098748	2.964366
C	-1.891209	2.101849	0.435894
H	-2.788803	2.420851	0.955358
C	-1.654981	0.736498	0.271299
C	-0.483863	0.296615	-0.371666
C	-1.117181	4.479947	0.071468
H	-1.939841	4.851322	0.678203
C	1.070256	3.650493	-1.206399
H	2.003516	3.336273	-1.668458
C	0.534151	4.780327	1.379555
C	1.736260	4.329258	0.625400

C	2.413441	3.147379	1.108015
C	2.666576	5.356929	0.210065
C	0.121132	3.974246	2.499527
C	0.397382	6.196496	1.621011
N	2.973717	2.183398	1.435821
N	3.419444	6.157299	-0.168732
N	-0.258361	3.324645	3.386026
N	0.239325	7.334207	1.801524
C	2.383882	-1.683320	-0.776052
C	3.798011	-1.866276	-0.796400
C	4.399127	-2.909238	-1.524333
C	4.641979	-0.992552	-0.082566
C	5.775744	-3.079047	-1.541049
H	3.772313	-3.593277	-2.089446
C	6.018726	-1.156355	-0.093334
H	4.205701	-0.175203	0.485030
C	6.628306	-2.210182	-0.817222
H	6.189999	-3.893892	-2.122495
H	6.624174	-0.455598	0.468595
N	8.000167	-2.386036	-0.813854
C	8.853986	-1.398788	-0.174794
H	9.894122	-1.718758	-0.257412
H	8.763781	-0.402368	-0.633958
H	8.619409	-1.302155	0.892632
C	8.601552	-3.388584	-1.676018
H	9.682715	-3.387043	-1.527179
H	8.234290	-4.394124	-1.433794
H	8.402069	-3.202283	-2.742698
Si	-5.955651	-0.432529	-2.403088
C	-6.726537	1.282822	-2.596341
H	-7.177477	1.623991	-1.657576
H	-5.977387	2.024336	-2.896355
H	-7.512940	1.272927	-3.361342
C	-5.141315	-0.970721	-4.021663
H	-4.355589	-0.268957	-4.323025
H	-4.683707	-1.961696	-3.924099
H	-5.878742	-1.019655	-4.832571
C	-7.273384	-1.683390	-1.883111
H	-8.061619	-1.755881	-2.642797
H	-6.843480	-2.682494	-1.749444
H	-7.745455	-1.393977	-0.937414

Compound: ***syn-15***
 Charge: 0
 Spin Multiplicity: 1
 Computational Method/Basis Set: B3LYP/6-31G(d)
 Solvation: gas phase
 Electronic Energy (AU): -2450.54304100

C	0.299857	2.365789	0.269664
C	0.275583	3.745259	0.190104
C	0.988788	4.564060	1.100178
C	1.758841	3.934745	2.128745
C	1.756903	2.520875	2.203540
C	1.044765	1.745639	1.311580
H	0.381382	6.457974	0.241620
H	-0.313742	4.224154	-0.586368
C	0.969492	5.983204	1.023465
C	2.483372	4.748161	3.042209
H	2.315430	2.029252	2.994882
C	2.446857	6.120086	2.940399
C	1.682231	6.743873	1.921918
H	3.066686	4.266747	3.823403
H	3.004385	6.733194	3.643285
H	1.661128	7.828228	1.855310
C	-0.371799	1.511451	-0.810026
C	-1.798932	-0.578530	-0.945814
H	-2.339165	-0.101910	-1.756857
C	-1.544463	2.208884	-1.378562
C	-2.524118	2.756239	-1.853823
Si	-4.085117	3.526487	-2.476887
C	-5.405839	2.178439	-2.555081
H	-5.536608	1.688226	-1.583595
H	-6.374345	2.599177	-2.852571
H	-5.140926	1.407450	-3.288272
C	-3.763603	4.241346	-4.196885
H	-3.440846	3.463744	-4.898497
H	-4.675085	4.698338	-4.601705
H	-2.986357	5.013682	-4.172399
C	-4.594252	4.892400	-1.276241
H	-4.761367	4.491967	-0.270206
H	-3.825367	5.670021	-1.204496
H	-5.524781	5.371310	-1.605303
O	0.577328	1.171871	-1.853207
C	1.111620	2.246252	-2.614645
H	1.711898	2.930210	-2.001726
H	1.755657	1.778781	-3.363458
H	0.321078	2.816403	-3.121214
C	-2.109265	-1.869221	-0.552378
C	-1.417507	-2.470294	0.507222
C	-2.636951	-4.125435	-1.435236
H	-2.800251	-4.590135	-2.401354
C	-1.990112	-4.696259	-0.416055
H	-1.553425	-5.688610	-0.439119
C	3.382703	-0.716897	0.497989
C	2.341806	-0.300481	0.963040
C	4.612032	-1.202686	-0.033684
C	5.785489	-0.426301	0.014624

C	4.701259	-2.475065	-0.628978
C	6.986395	-0.893750	-0.498027
H	5.745847	0.562555	0.461843
C	5.896805	-2.952654	-1.145099
H	3.810691	-3.093868	-0.687913
C	7.080786	-2.178343	-1.086146
H	7.857819	-0.252623	-0.439899
H	5.907957	-3.936906	-1.597747
N	8.282376	-2.659758	-1.576888
C	8.312588	-3.916269	-2.305014
H	7.700219	-3.891278	-3.220062
H	9.342117	-4.139429	-2.590615
H	7.954679	-4.744591	-1.680764
C	9.437753	-1.781411	-1.642556
H	10.289594	-2.339332	-2.035463
H	9.269518	-0.908396	-2.292287
H	9.713432	-1.413645	-0.646256
C	1.072729	0.222287	1.491409
O	1.061052	-0.128487	2.891351
C	-0.089704	0.271154	3.638421
H	0.108585	-0.045840	4.664959
H	-0.233796	1.357616	3.619025
H	-1.005020	-0.219467	3.286357
C	-0.407618	-1.783692	1.159649
H	0.137532	-2.228798	1.986039
C	-0.079652	-0.477603	0.758623
C	-0.781447	0.129866	-0.286916
C	-1.937379	-3.851846	0.842303
H	-1.399817	-4.325427	1.665244
C	-3.197366	-2.749655	-1.128533
H	-3.718427	-2.292302	-1.971067
C	-3.470575	-3.648250	1.302289
C	-4.267291	-2.972961	0.055416
C	-4.869863	-1.676898	0.409490
C	-5.349051	-3.839630	-0.442289
C	-3.502765	-2.795643	2.502049
C	-4.031320	-4.958655	1.671053
N	-5.352369	-0.641292	0.610639
N	-6.197722	-4.487655	-0.895830
N	-3.473551	-2.152757	3.467273
N	-4.411365	-6.007657	1.988831

Compound: **anti-15**
 Charge: 0
 Spin Multiplicity: 1
 Computational Method/Basis Set: B3LYP/6-31G(d)
 Solvation: gas phase
 Electronic Energy (AU): -2450.54407524

C	-0.937594	-2.168044	0.307987
C	-0.469382	-3.452031	0.512746
C	-1.160400	-4.384639	1.325428
C	-2.381426	-3.977212	1.949792
C	-2.833713	-2.651307	1.745017
C	-2.135746	-1.759106	0.957273
H	0.244599	-6.012591	1.064425
H	0.463802	-3.757587	0.048652
C	-0.685828	-5.707643	1.537455
C	-3.085439	-4.908465	2.760941
H	-3.744199	-2.318525	2.235271
C	-2.602040	-6.183849	2.944118
C	-1.390375	-6.587075	2.327466
H	-4.012848	-4.594960	3.234165
H	-3.147588	-6.888922	3.565421
H	-1.019429	-7.596380	2.483791
C	-0.237113	-1.234422	-0.685842
C	0.437623	1.203357	-0.836977
H	1.323969	0.873761	-1.368614
C	1.209386	-1.515976	-0.751791
O	-0.859155	-1.348964	-1.994264
C	-0.716221	-2.593461	-2.663018
H	-1.212739	-3.412586	-2.126945
H	-1.196815	-2.459913	-3.635512
H	0.340507	-2.852241	-2.814361
C	0.197286	2.550269	-0.625380
C	-0.940472	2.962755	0.080900
C	0.259885	4.767934	-1.734860
H	0.566561	5.177009	-2.691193
C	-0.814086	5.163766	-1.047162
H	-1.502396	5.938112	-1.367471
C	-4.697038	-0.327292	-0.952106
C	-3.794896	-0.324258	-0.134389
C	-2.676902	-0.329616	0.827298
O	-3.246615	0.124684	2.069223
C	-2.352552	0.214394	3.181242
H	-2.970490	0.538196	4.021831
H	-1.898451	-0.754035	3.419393
H	-1.559167	0.953101	3.016962
C	-1.846019	2.027788	0.551811
H	-2.734075	2.326609	1.099667
C	-1.615519	0.660044	0.327450
C	-0.467236	0.244719	-0.352722
C	-0.997548	4.461450	0.283899
H	-1.882224	4.788023	0.832671
C	1.087343	3.700912	-1.043544
H	1.958144	3.381904	-1.618339
C	0.300566	4.837814	1.165520
C	1.612452	4.377444	0.321644

C	2.437524	3.401059	1.052978
C	2.478970	5.518745	-0.017914
C	0.213489	4.151328	2.464921
C	0.292085	6.287041	1.424532
N	3.122675	2.612908	1.558022
N	3.189048	6.378747	-0.337379
N	0.080529	3.618844	3.486992
N	0.216552	7.425358	1.635134
C	2.409676	-1.700079	-0.784113
C	3.825717	-1.868972	-0.780932
C	4.447202	-2.926456	-1.470004
C	4.653039	-0.968481	-0.081195
C	5.825325	-3.084253	-1.462252
H	3.834636	-3.632183	-2.023882
C	6.031136	-1.119267	-0.066826
H	4.203301	-0.139270	0.457926
C	6.660108	-2.187884	-0.751318
H	6.254805	-3.911746	-2.014074
H	6.621893	-0.397668	0.484137
N	8.032915	-2.351430	-0.722497
C	8.868974	-1.340125	-0.097717
H	9.913023	-1.651998	-0.158727
H	8.775592	-0.357005	-0.583922
H	8.619623	-1.217937	0.963832
C	8.655239	-3.377905	-1.540470
H	9.733652	-3.364083	-1.373558
H	8.289922	-4.377277	-1.271226
H	8.472946	-3.228365	-2.615948
Si	-6.047784	-0.342340	-2.203136
C	-5.425147	0.513277	-3.769457
H	-5.151232	1.555645	-3.570880
H	-4.540094	0.007497	-4.171382
H	-6.197145	0.511738	-4.549051
C	-6.510926	-2.135862	-2.578241
H	-5.652448	-2.695062	-2.967025
H	-6.864323	-2.651630	-1.678220
H	-7.310487	-2.184004	-3.328038
C	-7.537331	0.582274	-1.496503
H	-8.367280	0.589720	-2.214018
H	-7.895802	0.111149	-0.574351
H	-7.287122	1.623385	-1.263172

8.4 [2+2] Reactivity of 4b' with TCNE

Compound: **TS18**

Charge: 0

Spin Multiplicity: 1

Computational Method/Basis Set: B3LYP/6-31G(d)

Solvation: gas phase

Electronic Energy (AU): -2450.53115306

C	4.136725	0.340602	-0.462863
C	4.906162	-0.852925	-0.613123
C	4.800854	1.587203	-0.660898
C	6.237086	-0.800876	-0.947472
H	4.433818	-1.810280	-0.418581
C	6.130893	1.642192	-0.995819
H	4.235566	2.505802	-0.541990
C	6.897731	0.447329	-1.150878
H	6.788202	-1.728877	-1.029526
H	6.596476	2.609669	-1.133815
C	2.801153	0.287892	-0.131722
C	1.475577	-1.690006	2.383675
C	1.642674	-0.261251	2.219225
C	2.962798	0.238139	2.600014
C	0.621489	0.578627	2.831531
C	0.266120	-2.276090	2.817266
C	2.521125	-2.539006	1.954933
N	-0.701537	-2.800309	3.208209
N	3.386913	-3.204870	1.537620
N	4.010143	0.629936	2.911443
N	-0.134993	1.283587	3.358381
N	8.220010	0.498699	-1.472932
C	8.895346	1.783975	-1.629999
H	8.855897	2.373730	-0.705852
H	9.942201	1.608230	-1.877220
H	8.448444	2.373586	-2.439691
C	8.996751	-0.731137	-1.608924
H	10.018167	-0.477346	-1.892230
H	9.030340	-1.292038	-0.666679
H	8.578593	-1.380874	-2.386703
C	-1.849043	-1.155754	0.013372
C	-2.510503	-2.367706	-0.078330
C	-1.848384	-3.569900	-0.422180
C	-0.447567	-3.522131	-0.705067
C	0.201724	-2.268024	-0.657777
C	-0.462327	-1.105689	-0.305835
H	-3.588212	-4.853097	-0.280512
H	-3.579310	-2.404901	0.107803
C	-2.523420	-4.818379	-0.497437
C	0.233938	-4.724089	-1.040320
H	1.252173	-2.216816	-0.927967
C	-0.446597	-5.918001	-1.099184
C	-1.838330	-5.964791	-0.828042
H	1.302148	-4.683447	-1.237480
H	0.081240	-6.833937	-1.350207
H	-2.361484	-6.915904	-0.877697
C	-2.610222	0.075508	0.520826

C	-2.563518	2.572481	0.501623
H	-3.605301	2.522207	0.803001
C	-3.952896	0.123316	-0.103220
C	-5.068702	0.162522	-0.593007
Si	-6.738150	0.242734	-1.369337
C	-7.661705	1.738074	-0.674110
H	-7.129197	2.671074	-0.890961
H	-8.664304	1.815283	-1.112903
H	-7.777304	1.664327	0.413173
C	-7.675183	-1.348328	-0.964270
H	-7.792758	-1.477595	0.117646
H	-8.677649	-1.333534	-1.409829
H	-7.151024	-2.229598	-1.351322
C	-6.522268	0.416473	-3.239225
H	-5.967671	1.327027	-3.492700
H	-5.974378	-0.435610	-3.657233
H	-7.496819	0.467000	-3.740624
O	-2.717732	0.064317	1.960438
C	-3.489367	-0.959199	2.581527
H	-3.007546	-1.939362	2.510469
H	-3.539407	-0.671956	3.634379
H	-4.506587	-1.002678	2.168930
C	-1.952320	3.839101	0.370864
C	-0.577016	3.897388	-0.021931
C	-2.021130	6.266950	0.466074
H	-2.563596	7.189566	0.653843
C	-0.658397	6.324758	0.072890
H	-0.173299	7.291001	-0.036493
C	0.303489	0.205457	-0.450464
O	0.780334	0.317664	-1.822418
C	-0.222986	0.378971	-2.830761
H	0.320753	0.472797	-3.774133
H	-0.834262	-0.531400	-2.858346
H	-0.877701	1.250259	-2.705454
C	0.106848	2.683621	-0.251807
H	1.147477	2.720186	-0.560830
C	-0.509221	1.452482	-0.106547
C	-1.877602	1.396638	0.262684
C	0.046213	5.168290	-0.165091
H	1.091208	5.209036	-0.463654
C	-2.652411	5.053978	0.610998
H	-3.695223	5.005304	0.914590
C	1.624724	0.184602	0.322855

Compound: **19**
 Charge: 0
 Spin Multiplicity: 1
 Computational Method/Basis Set: B3LYP/6-31G(d)
 Solvation: gas phase
 Electronic Energy (AU): -2450.53480628

C	4.095113	0.321224	-0.343931
C	4.859254	-0.883743	-0.504872
C	4.746896	1.566335	-0.626588
C	6.159782	-0.840086	-0.933901
H	4.400694	-1.830662	-0.237006
C	6.048867	1.608014	-1.046337
H	4.187645	2.487713	-0.501696
C	6.804477	0.403393	-1.218234
H	6.707649	-1.769354	-1.022545
H	6.505228	2.568978	-1.246439
C	2.800206	0.280590	0.075385
C	1.419191	-1.582156	2.453876
C	1.558308	-0.102671	2.196047
C	2.827146	0.412332	2.768265
C	0.491115	0.687039	2.841807
C	0.269422	-2.142746	3.031952
C	2.440307	-2.409393	1.964265
N	-0.671122	-2.635273	3.525448
N	3.301637	-3.044303	1.483147
N	3.832807	0.793931	3.204385
N	-0.275646	1.351645	3.402497
N	8.098220	0.444430	-1.627546
C	8.766780	1.724219	-1.858831
H	8.767843	2.341968	-0.953240
H	9.801629	1.537907	-2.144514
H	8.284396	2.286261	-2.667439
C	8.860788	-0.791416	-1.805203
H	9.852663	-0.545265	-2.183327
H	8.976416	-1.330832	-0.857374
H	8.374031	-1.454621	-2.528885
C	-1.811674	-1.169046	0.001813
C	-2.465820	-2.380581	-0.131474
C	-1.785392	-3.579645	-0.449836
C	-0.372128	-3.527863	-0.659663
C	0.272057	-2.274096	-0.572173
C	-0.409987	-1.114455	-0.245517
H	-3.526847	-4.867813	-0.403778
H	-3.542243	-2.419881	0.003181
C	-2.452271	-4.829313	-0.564602
C	0.330664	-4.727120	-0.959119
H	1.337175	-2.226996	-0.775405
C	-0.342705	-5.922477	-1.057005
C	-1.747042	-5.972881	-0.861883
H	1.408587	-4.682694	-1.090879
H	0.200300	-6.837177	-1.278357
H	-2.264357	-6.925197	-0.941441
C	-2.596160	0.057377	0.482253
C	-2.574083	2.555341	0.398685
H	-3.631122	2.502519	0.640394

C	-3.927733	0.087623	-0.167199
C	-5.038182	0.112768	-0.669847
Si	-6.701637	0.168745	-1.461322
C	-7.690833	1.587161	-0.698538
H	-7.197969	2.551735	-0.865365
H	-8.694068	1.643574	-1.139085
H	-7.807331	1.454400	0.382997
C	-7.576676	-1.477849	-1.151181
H	-7.699575	-1.667400	-0.078784
H	-8.574277	-1.481821	-1.607770
H	-7.011936	-2.315534	-1.576106
C	-6.474851	0.451864	-3.316593
H	-5.945718	1.391223	-3.513069
H	-5.897919	-0.358836	-3.775806
H	-7.445978	0.501784	-3.824658
O	-2.734027	0.059417	1.917321
C	-3.470854	-0.992892	2.534494
H	-2.947882	-1.952301	2.474741
H	-3.542090	-0.704168	3.585286
H	-4.480707	-1.077713	2.110062
C	-1.966641	3.824915	0.274149
C	-0.571597	3.888145	-0.039717
C	-2.060926	6.253264	0.311882
H	-2.620964	7.174384	0.448148
C	-0.678346	6.315871	-0.002747
H	-0.195665	7.284147	-0.104340
C	0.363307	0.195157	-0.321201
O	0.983633	0.305003	-1.630035
C	0.099799	0.352869	-2.745346
H	0.744275	0.456624	-3.621761
H	-0.489643	-0.566815	-2.838974
H	-0.576917	1.214308	-2.692309
C	0.133973	2.675776	-0.202624
H	1.189966	2.716465	-0.453850
C	-0.479176	1.441921	-0.064279
C	-1.866960	1.381073	0.227665
C	0.048459	5.161304	-0.174683
H	1.108771	5.205745	-0.412661
C	-2.689564	5.037532	0.446428
H	-3.747598	4.985459	0.690830
C	1.623411	0.180503	0.591812

Compound: **TS20**
Charge: 0
Spin Multiplicity: 1
Computational Method/Basis Set: B3LYP/6-31G(d)
Solvation: gas phase
Electronic Energy (AU): -2450.52833737

C	3.918133	0.173756	-0.572708
C	4.643705	-0.876475	-1.236588
C	4.539195	1.469551	-0.490066
C	5.880323	-0.639740	-1.775112
H	4.204796	-1.866378	-1.273469
C	5.776722	1.696540	-1.021854
H	4.017530	2.264335	0.032434
C	6.495021	0.648250	-1.688211
H	6.398419	-1.456353	-2.261103
H	6.217980	2.679925	-0.922891
C	2.704116	-0.034808	-0.008842
C	2.287252	-1.963504	2.295225
C	1.677730	-0.563142	2.134378
C	2.542918	0.481838	2.756810
C	0.375852	-0.510409	2.846525
C	2.932886	-2.625956	1.251912
C	2.212956	-2.592766	3.552763
N	3.440583	-3.212187	0.366767
N	2.159287	-3.112866	4.599850
N	3.265315	1.277227	3.198338
N	-0.585821	-0.513137	3.495033
N	7.723104	0.874177	-2.215070
C	8.351127	2.192063	-2.111039
H	8.515677	2.474099	-1.064494
H	9.317373	2.165255	-2.613664
H	7.737372	2.962207	-2.591667
C	8.461555	-0.207698	-2.869104
H	9.419269	0.176600	-3.218425
H	8.653556	-1.033413	-2.174510
H	7.910949	-0.595922	-3.733470
C	-2.035508	-1.166144	0.142046
C	-2.779823	-2.319611	-0.030626
C	-2.187160	-3.570769	-0.328324
C	-0.767891	-3.632267	-0.483328
C	-0.028842	-2.432268	-0.377957
C	-0.626282	-1.222780	-0.068850
H	-4.026659	-4.717203	-0.359283
H	-3.861213	-2.271732	0.050128
C	-2.946381	-4.763208	-0.474644
C	-0.148113	-4.881656	-0.758963
H	1.038627	-2.475367	-0.564089
C	-0.910568	-6.019997	-0.885711
C	-2.321179	-5.958806	-0.747015
H	0.934529	-4.917388	-0.849437
H	-0.433758	-6.974913	-1.088787
H	-2.908597	-6.867088	-0.851612
C	-2.747956	0.120020	0.581854
C	-2.453242	2.582636	0.802686
H	-3.521656	2.612460	0.992964

C	-3.956564	0.321055	-0.251231
C	-4.967764	0.484139	-0.912923
Si	-6.473033	0.741437	-1.944689
C	-7.614610	1.964535	-1.065618
H	-7.126012	2.935095	-0.923056
H	-8.528048	2.132440	-1.649684
H	-7.912486	1.592791	-0.078690
C	-7.346821	-0.919916	-2.167708
H	-7.656311	-1.339144	-1.203486
H	-8.245908	-0.808061	-2.786423
H	-6.693743	-1.651839	-2.656387
C	-5.938267	1.432350	-3.620858
H	-5.411412	2.386591	-3.507592
H	-5.267293	0.739576	-4.141281
H	-6.808309	1.604688	-4.266615
O	-3.109106	0.099063	1.980272
C	-3.971928	-0.918272	2.463697
H	-3.491028	-1.902988	2.465833
H	-4.192197	-0.634856	3.495388
H	-4.909863	-0.964423	1.892035
C	-1.714666	3.785056	0.866210
C	-0.304471	3.732867	0.627905
C	-1.560654	6.185328	1.213142
H	-2.029860	7.138585	1.440653
C	-0.162084	6.133539	0.976665
H	0.423525	7.047441	1.026981
C	0.240554	0.026347	-0.148208
O	0.731337	0.187841	-1.504709
C	-0.248465	0.408363	-2.512286
H	0.309845	0.492105	-3.447876
H	-0.951537	-0.429818	-2.587207
H	-0.808352	1.336268	-2.342639
C	0.280623	2.481009	0.335259
H	1.346763	2.444978	0.133753
C	-0.459544	1.311234	0.286444
C	-1.859287	1.367477	0.519394
C	0.451077	4.936403	0.691143
H	1.523383	4.892893	0.515472
C	-2.318479	5.039052	1.159451
H	-3.389155	5.073592	1.344728
C	1.576661	-0.172030	0.616628

Compound: **21**
Charge: 0
Spin Multiplicity: 1
Computational Method/Basis Set: B3LYP/6-31G(d)
Solvation: gas phase
Electronic Energy (AU): -2450.60283127

C	-4.011448	-0.120898	0.078800
C	-4.102908	0.386250	-1.234317
C	-5.227021	-0.462689	0.709306
C	-5.320069	0.532301	-1.876389
H	-3.195560	0.668026	-1.749953
C	-6.450798	-0.327599	0.075773
H	-5.230916	-0.854768	1.720710
C	-6.537816	0.172475	-1.245708
H	-5.325348	0.937146	-2.881395
H	-7.344811	-0.610653	0.617406
C	-2.761243	-0.255306	0.812084
C	-2.683590	-0.502005	2.339048
C	-1.072695	-0.389648	2.148251
C	-0.350152	-1.601732	2.561933
C	-0.508685	0.788149	2.825216
C	-3.289081	0.537732	3.180102
C	-3.135934	-1.825672	2.786587
N	-3.791389	1.364195	3.821235
N	-3.521538	-2.868707	3.118426
N	0.167480	-2.577211	2.917031
N	-0.107701	1.732508	3.367141
N	-7.748201	0.305038	-1.887233
C	-8.983794	0.006567	-1.179720
H	-9.126272	0.655436	-0.303617
H	-9.827725	0.156778	-1.854580
H	-9.007651	-1.036462	-0.838954
C	-7.808963	0.896471	-3.214178
H	-8.844004	0.896263	-3.559042
H	-7.446115	1.934614	-3.222995
H	-7.214699	0.321781	-3.936335
C	1.764988	1.305129	-0.048753
C	2.406980	2.529214	-0.051038
C	1.717244	3.743497	-0.287954
C	0.308080	3.695058	-0.526687
C	-0.326645	2.430746	-0.544682
C	0.368529	1.257045	-0.324381
H	3.443822	5.039056	-0.104432
H	3.476919	2.568403	0.129897
C	2.372615	5.004629	-0.287586
C	-0.397303	4.908292	-0.752350
H	-1.390393	2.385779	-0.761724
C	0.264971	6.114221	-0.742814
C	1.663014	6.162584	-0.509503
H	-1.469384	4.867038	-0.928682
H	-0.282124	7.037465	-0.912506
H	2.172187	7.122431	-0.504598
C	2.511599	0.038544	0.381783
C	2.648317	-2.392227	-0.262961
H	3.702146	-2.352029	-0.005686

C	3.942093	0.123908	0.024600
C	5.127690	0.195382	-0.248326
Si	6.912060	0.283895	-0.715865
C	7.834708	-1.114969	0.156311
H	7.441878	-2.095480	-0.135697
H	8.901846	-1.093549	-0.097232
H	7.747973	-1.031942	1.245539
C	7.595373	1.960406	-0.173020
H	7.497324	2.100292	0.909498
H	8.659588	2.046142	-0.425277
H	7.068835	2.785286	-0.666648
C	7.039936	0.096726	-2.591515
H	6.626744	-0.861670	-2.925480
H	6.493392	0.893781	-3.108119
H	8.086586	0.142246	-2.917054
O	2.346069	-0.142795	1.815243
C	3.001324	0.784971	2.676645
H	2.608847	1.802304	2.565116
H	2.789261	0.435103	3.688735
H	4.085305	0.784702	2.508076
C	2.093512	-3.630314	-0.662908
C	0.699719	-3.686688	-0.982567
C	2.291252	-6.004008	-1.142983
H	2.891417	-6.907547	-1.206655
C	0.909479	-6.059104	-1.460510
H	0.466965	-7.004181	-1.763144
C	-0.402004	-0.062861	-0.471843
O	-1.200907	-0.028822	-1.665817
C	-0.496186	0.080301	-2.900607
H	-1.265662	0.094747	-3.676234
H	0.088298	1.006059	-2.953447
H	0.164436	-0.778144	-3.064446
C	-0.059557	-2.498331	-0.888646
H	-1.116306	-2.527352	-1.140042
C	0.507779	-1.297035	-0.503518
C	1.890283	-1.240486	-0.185456
C	0.131766	-4.927522	-1.382576
H	-0.928269	-4.966634	-1.621043
C	2.869449	-4.818314	-0.753533
H	3.926967	-4.773458	-0.505205
C	-1.409173	-0.213089	0.656545

Compound: **TS22**
Charge: 0
Spin Multiplicity: 1
Computational Method/Basis Set: B3LYP/6-31G(d)
Solvation: gas phase
Electronic Energy (AU): -2450.56883620

C	-3.748121	-0.504473	0.251561
C	-3.946538	0.883694	0.363733
C	-4.809479	-1.270516	-0.268974
C	-5.126371	1.483390	-0.046285
H	-3.178033	1.494439	0.825752
C	-5.986854	-0.684012	-0.701322
H	-4.696932	-2.347806	-0.357579
C	-6.180323	0.717459	-0.608052
H	-5.241535	2.551097	0.095180
H	-6.764732	-1.318811	-1.106914
C	-2.555566	-1.162734	0.784504
C	-2.723480	-2.269861	1.752110
C	-0.587900	-1.612421	1.818647
C	0.455873	-2.590745	1.818788
C	-0.754544	-0.954002	3.083687
C	-3.657912	-2.151327	2.830269
C	-2.417889	-3.612243	1.357343
N	-4.364354	-2.023128	3.747993
N	-2.198710	-4.702708	1.009847
N	1.199438	-3.483557	1.905462
N	-0.855295	-0.395910	4.101123
N	-7.346019	1.309982	-1.038972
C	-8.458191	0.485411	-1.487378
H	-8.828881	-0.180140	-0.694392
H	-9.278816	1.132277	-1.800762
H	-8.172934	-0.133578	-2.347228
C	-7.557702	2.734924	-0.836288
H	-8.512841	3.020619	-1.279269
H	-7.578474	3.007441	0.229163
H	-6.772809	3.325717	-1.324786
C	1.260031	1.435557	-0.036240
C	1.566377	2.780255	0.026039
C	0.621636	3.785472	-0.299077
C	-0.684774	3.381229	-0.712585
C	-0.976182	1.995944	-0.775276
C	-0.048169	1.031431	-0.438277
H	1.922979	5.474992	0.079468
H	2.567559	3.082910	0.317113
C	0.927972	5.171251	-0.236587
C	-1.638962	4.376814	-1.056630
H	-1.954680	1.686214	-1.124641
C	-1.313645	5.712460	-0.984891
C	-0.018599	6.113494	-0.570387
H	-2.630501	4.064367	-1.376002
H	-2.049670	6.467561	-1.247273
H	0.224117	7.171307	-0.519184
C	2.270290	0.372352	0.400251
C	3.189789	-1.732281	-0.666294
H	4.178710	-1.423675	-0.342883

C	3.655174	0.876649	0.334953
C	4.802052	1.288001	0.324354
Si	6.549653	1.887038	0.276466
C	7.125282	2.194639	2.048862
H	7.072157	1.279244	2.648869
H	8.165022	2.544221	2.063345
H	6.510561	2.954947	2.543920
C	6.605638	3.486818	-0.728126
H	5.988178	4.268725	-0.271425
H	7.632043	3.868574	-0.793592
H	6.242364	3.327846	-1.749703
C	7.613378	0.558373	-0.543576
H	7.582965	-0.380637	0.020699
H	7.273220	0.348138	-1.563886
H	8.660770	0.879833	-0.599862
O	1.953227	-0.046089	1.758395
C	2.160191	0.913617	2.793895
H	1.565651	1.822167	2.636711
H	1.828444	0.428138	3.712566
H	3.220107	1.182031	2.876270
C	3.048422	-2.979685	-1.322490
C	1.742203	-3.401051	-1.724783
C	3.978569	-5.038097	-2.215876
H	4.831949	-5.682067	-2.409969
C	2.682803	-5.457089	-2.610937
H	2.556784	-6.418428	-3.101246
C	-0.427536	-0.454130	-0.596741
O	-1.375746	-0.611864	-1.662270
C	-0.956780	-0.258723	-2.979244
H	-1.835634	-0.413285	-3.609723
H	-0.644888	0.789460	-3.046025
H	-0.140467	-0.898207	-3.332261
C	0.647053	-2.544546	-1.461114
H	-0.349710	-2.855617	-1.760269
C	0.812203	-1.323707	-0.835937
C	2.110367	-0.910485	-0.421719
C	1.589312	-4.657218	-2.371409
H	0.593339	-4.978202	-2.665836
C	4.157418	-3.827929	-1.585911
H	5.148650	-3.506297	-1.276131
C	-1.195591	-1.002487	0.622427

Compound: **14b'**
 Charge: 0
 Spin Multiplicity: 1
 Computational Method/Basis Set: B3LYP/6-31G(d)
 Solvation: gas phase
 Electronic Energy (AU): -2450.62962545

C	-3.248969	-0.863354	-0.468042
C	-2.715045	0.153873	-1.298301
C	-4.580553	-0.675008	-0.024734
C	-3.458038	1.248569	-1.691843
H	-1.688413	0.095299	-1.641985
C	-5.329647	0.421589	-0.402104
H	-5.041493	-1.387256	0.645947
C	-4.800423	1.416218	-1.265597
H	-2.989133	1.984696	-2.332713
H	-6.338730	0.509556	-0.018837
C	-2.436926	-2.020026	-0.113243
C	-2.887306	-3.233915	0.377361
C	-0.525477	-2.404206	-1.570997
C	0.816719	-2.516307	-2.075287
C	-1.483404	-2.859464	-2.549769
C	-4.255444	-3.575775	0.611812
C	-1.986344	-4.315150	0.649905
N	-5.352229	-3.905265	0.825740
N	-1.292411	-5.225986	0.861732
N	1.816950	-2.684166	-2.645001
N	-2.214817	-3.220267	-3.378445
N	-5.549508	2.494004	-1.659058
C	-6.919538	2.645842	-1.189595
H	-6.966935	2.746871	-0.096770
H	-7.351548	3.544414	-1.631639
H	-7.541936	1.790753	-1.482753
C	-4.969264	3.513276	-2.522097
H	-5.723011	4.271996	-2.735776
H	-4.111285	4.008037	-2.047300
H	-4.635304	3.088172	-3.477415
C	2.283328	-0.567068	0.062972
C	3.630154	-0.811833	-0.102863
C	4.203002	-2.082169	0.162707
C	3.350781	-3.140004	0.607658
C	1.971850	-2.869176	0.781791
C	1.438542	-1.621112	0.526752
H	6.236558	-1.533465	-0.341623
H	4.280353	-0.011184	-0.441860
C	5.589976	-2.338914	-0.001900
C	3.911674	-4.418973	0.867903
H	1.316958	-3.667409	1.121043
C	5.259830	-4.637638	0.696930
C	6.106165	-3.588107	0.259695
H	3.257064	-5.220801	1.199775
H	5.681411	-5.619216	0.894752
H	7.168378	-3.775971	0.128875
C	1.656708	0.771850	-0.345885
C	0.182655	2.438459	0.859594
H	0.823107	3.226472	0.476442

C	2.660895	1.852238	-0.358870
C	3.489443	2.744370	-0.407241
Si	4.757096	4.088766	-0.446604
C	4.041998	5.559366	-1.393958
H	3.135972	5.943388	-0.911512
H	4.768475	6.380003	-1.440988
H	3.782090	5.284394	-2.422431
C	6.298766	3.430992	-1.318477
H	6.074883	3.117060	-2.344252
H	7.076187	4.203375	-1.367885
H	6.719446	2.568732	-0.788711
C	5.160195	4.580380	1.332020
H	4.271947	4.951486	1.855636
H	5.552064	3.730254	1.901544
H	5.916759	5.374554	1.352082
O	1.032609	0.636345	-1.656863
C	1.910333	0.597407	-2.782987
H	2.646321	-0.209567	-2.703389
H	1.268864	0.402969	-3.645279
H	2.422820	1.557479	-2.915763
C	-0.930323	2.794767	1.659370
C	-1.763128	1.752566	2.172580
C	-2.332124	4.446369	2.760484
H	-2.562505	5.481528	2.997697
C	-3.158018	3.412004	3.269796
H	-4.012948	3.665376	3.890764
C	-0.048557	-1.398206	0.792403
O	-0.499392	-2.195512	1.896823
C	0.122750	-2.000880	3.167849
H	-0.403922	-2.675985	3.845541
H	1.184722	-2.265058	3.146185
H	0.015218	-0.969695	3.521485
C	-1.440452	0.411760	1.854730
H	-2.065743	-0.380938	2.251103
C	-0.353714	0.084936	1.066154
C	0.481812	1.123975	0.568018
C	-2.879650	2.095179	2.983059
H	-3.510617	1.298964	3.370207
C	-1.243534	4.144968	1.973950
H	-0.607018	4.935678	1.583988
C	-0.950037	-1.940763	-0.364401