# Supporting Information

**Silaiminyl-silylene-derived unsymmetrical diradicaloid silacycles isolated in three different charge and spin states**

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**Content:**



## I. Experimental section

See the main manuscript for experimental details.

## II. X-Ray crystallographic details

Crystallographic data were collected on a Smart Apex Ⅱ DUO system. During measurements a graphite-monochromatic Mo-$K_\alpha$ radiation ($\lambda$ = 0.71073 Å) was applied. Absorption corrections were all employed using the spherical harmonics

program (multi-scan type). All the structures were solved by direct methods (SHELXT)[S1] and refined against $F^2$ using SHELXL.[S2] In general, the non-hydrogen atoms were located by difference Fourier synthesis and refined anisotropically, and hydrogen atoms were included using a riding mode with $U_{iso}$ tied to the $U_{iso}$ of the parent atoms unless otherwise specified. A summary of cell parameters, data collection, and structure solution and refinements is given in Table S1.

**Table S1 Crystal data and refinements**

| | **2a** | **2b** | **3a** | **3c** | **4** |
|---|---|---|---|---|---|
| CCDC No. | 2410295 | 2410300 | 2410302 | 2410298 | 2410301 |
| Empirical formula | $C_{63}H_{81}N_5Si_2$ | $C_{66.5}H_{83}F_2N_5Si_2$ | $C_{63}H_{81}N_5Si_2$ | $C_{63}H_{79}Br_2N_5Si_2$ | $C_{53}H_{78}N_5PSi_2$ |
| formula weight | 964.50 | 1046.55 | 964.50 | 1122.31 | 872.35 |
| crystal system | triclinic | monoclinic | triclinic | monoclinic | monoclinic |
| space group | *P*-1 | $P2_1/n$ | *P*-1 | $P2_1/c$ | $P2_1/n$ |
| *a*/Å | 12.9066(15) | 13.5778(8) | 17.1143(12) | 15.9414(8) | 10.1000(6) |
| *b*/Å | 13.4149(15) | 33.8254(19) | 17.5158(12) | 13.0360(6) | 35.961(2) |
| c/Å | 18.373(2) | 13.7432(7) | 19.4003(13) | 31.7917(17) | 14.8678(9) |
| *α*/deg | 81.913(3) | 90 | 90.648(2) | 90 | 90 |
| *β*/deg | 75.751(3) | 109.099(2) | 91.284(2) | 95.634(2) | 101.002(2) |
| *γ*/deg | 84.616(4) | 90 | 101.493(2) | 90 | 90 |
| *V*/Å$^3$ | 3046.8(6) | 5964.5(6) | 5696.9(7) | 6574.8(6) | 5300.8(5) |
| *Z* | 2 | 4 | 4 | 4 | 4 |
| $\rho_{calcd}$/g·cm$^{-3}$ | 1.051 | 1.165 | 1.125 | 1.134 | 1.093 |
| $\mu$/mm$^{-1}$ | 0.531 | 0.110 | 0.568 | 1.446 | 0.761 |
| *F*(000) | 1044.0 | 2252.0 | 2088.0 | 2360.0 | 1896.0 |
| crystal size/mm$^3$ | 0.18x0.13x0.1 | 0.35x0.08x0.04 | 0.18x0.12x0.07 | 0.1x0.08x0.06 | 0.06x0.03x0.02 |
| index ranges | $-16 \le h \le 16$ | $-17 \le h \le 17$ | $-22 \le h \le 22$ | $-19 \le h \le 19$ | $-13 \le h \le 13$ |
| | $-17 \le k \le 17$ | $-43 \le k \le 43$ | $-22 \le k \le 22$ | $-15 \le k \le 16$ | $-46 \le h \le 46$ |
| | $-23 \le l \le 23$ | $-17 \le l \le 15$ | $-25 \le l \le 25$ | $-39 \le l \le 39$ | $-19 \le l \le 19$ |
| collected data | 62454 | 130553 | 82337 | 84130 | 68900 |
| unique data | 13979 ($R_{int}$ = 0.0468) | 13738 ($R_{int}$ = 0.1355) | 25929 ($R_{int}$ = 0.1067) | 13448 ($R_{int}$ = 0.1089) | 12198 ($R_{int}$ = 0.1022) |
| data/restraints/parameters | 13979/0/648 | 13738/285/783 | 25929/949/1525 | 13448/0/666 | 12198/0/566 |
| GOF on $F^2$ | 1.058 | 1.086 | 1.087 | 1.067 | 1.068 |
| final *R* indices [$I > 2(I)$] | $R_1$ = 0.0418 | $R_1$ = 0.0766 | $R_1$ = 0.0829 | $R_1$ = 0.0543 | $R_1$ = 0.0557 |
| | $wR_2$ = 0.1081 | $wR_2$ = 0.1446 | $wR_2$ = 0.1976 | $wR_2$ = 0.1281 | $wR_2$ = 0.1437 |
| *R* indices (all data) | $R_1$ = 0.0530 | $R_1$ = 0.1270 | $R_1$ = 0.1351 | $R_1$ = 0.0919 | $R_1$ = 0.0823 |
| | $wR_2$ = 0.1147 | $wR_2$ = 0.1689 | $wR_2$ = 0.2259 | $wR_2$ = 0.1443 | $wR_2$ = 0.1564 |
| Largest diff peak/hole (e·Å$^{-3}$) | 0.28/-0.33 | 0.58/-0.34 | 0.77/-0.51 | 0.37/-0.65 | 0.36/-0.33 |

[a] $R_1 = \sum(||F_o|-|F_c||)/\sum|F_o|$, $wR_2 = [\sum w(F_o^2-F_c^2)^2/\sum w(F_o^2)]^{1/2}$, GOF = $[\sum w(F_o^2-F_c^2)^2/(N_o-N_p)]^{1/2}$.

| | **5** | **6** | **7** |
|---|---|---|---|
| CCDC No. | 2410297 | 2410296 | 2410299 |
| Empirical formula | $C_{56}H_{76}Cl_3N_5Si_2$ | $C_{59}H_{77}Cl_4F_3N_5O_3SSi_2$ | $C_{109}H_{132}Cl_2F_{12}N_{10}O_{12}S_4Si_4$ |
| formula weight | 981.74 | 1191.29 | 2313.74 |
| crystal system | monoclinic | triclinic | monoclinic |
| space group | $P2_1/c$ | $P$-1 | $C2/c$ |
| $a$/Å | 16.0898(18) | 11.6274(15) | 25.8060(14) |
| $b$/Å | 11.0161(12) | 15.135(2) | 12.0502(5) |
| c/Å | 31.208(3) | 18.541(3) | 36.794(2) |
| $\alpha$/deg | 90 | 107.552(4) | 90 |
| $\beta$/deg | 90.671(5) | 97.235(4) | 91.991(2) |
| $\gamma$/deg | 90 | 91.871(4) | 90 |
| $V$/Å$^3$ | 5531.1(10) | 3077.5(7) | 11434.9(10) |
| $Z$ | 4 | 2 | 4 |
| $\rho_{calcd}$/g·cm$^{-3}$ | 1.179 | 1.286 | 1.344 |
| $\mu$/mm$^{-1}$ | 1.459 | 1.907 | 0.254 |
| $F$(000) | 2104.0 | 1258.0 | 4856.0 |
| crystal size/mm$^3$ | 0.12x0.05x0.03 | 0.13x0.1x0.05 | 0.38x0.28x0.03 |
| index ranges | $-18 \le h \le 19$ | $-14 \le h \le 14$ | $-33 \le h \le 33$ |
| | $-12 \le h \le 13$ | $-18 \le k \le 18$ | $-15 \le h \le 13$ |
| | $-37 \le l \le 37$ | $-23 \le l \le 23$ | $-47 \le l \le 47$ |
| collected data | 41951 | 40569 | 89679 |
| unique data | 10178 | 12513 | 13173 |
| | ($R_{int}$ = 0.1388) | ($R_{int}$ = 0.1102) | ($R_{int}$ = 0.0668) |
| data/restraints/parameters | 10178/0/612 | 12513/51/729 | 13173/247/776 |
| GOF on $F^2$ | 1.041 | 1.077 | 1.071 |
| final $R$ indices [$I > 2\sigma(I)$] | $R_1$ = 0.0954 | $R_1$ = 0.0881 | $R_1$ = 0.0765 |
| | $wR_2$ = 0.2591 | $wR_2$ = 0.2109 | $wR_2$ = 0.1609 |
| $R$ indices (all data) | $R_1$ = 0.1692 | $R_1$ = 0.1561 | $R_1$ = 0.1097 |
| | $wR_2$ = 0.3146 | $wR_2$ = 0.2453 | $wR_2$ = 0.1820 |
| Largest diff peak/hole (e·Å$^{-3}$) | 0.36/-0.33 | 1.03/-0.64 | 0.75/-0.48 |

[a] $R_1 = \sum(||F_o|-|F_c||)/\sum|F_o|$, $wR_2 = [\sum w(F_o^2-F_c^2)^2/\sum w(F_o^2)]^{1/2}$, GOF = $[\sum w(F_o^2-F_c^2)^2/(N_o-N_p)]^{1/2}$.

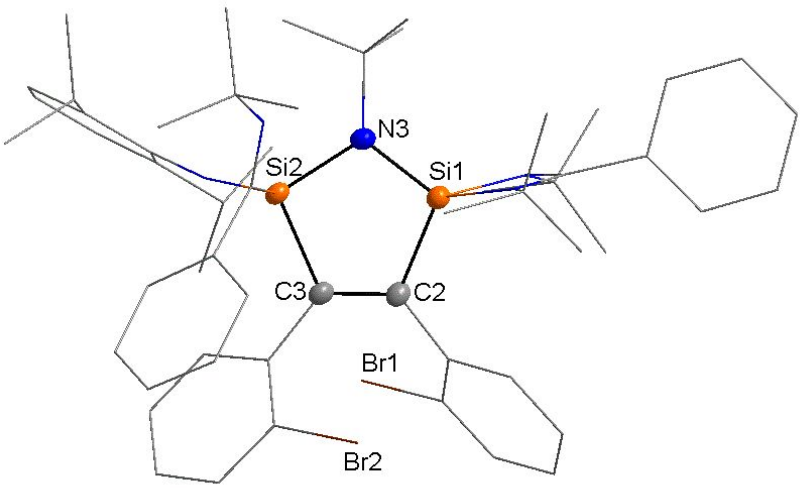



**Fig. S1** Molecular structures of **3c**. H atoms are omitted for clarity.

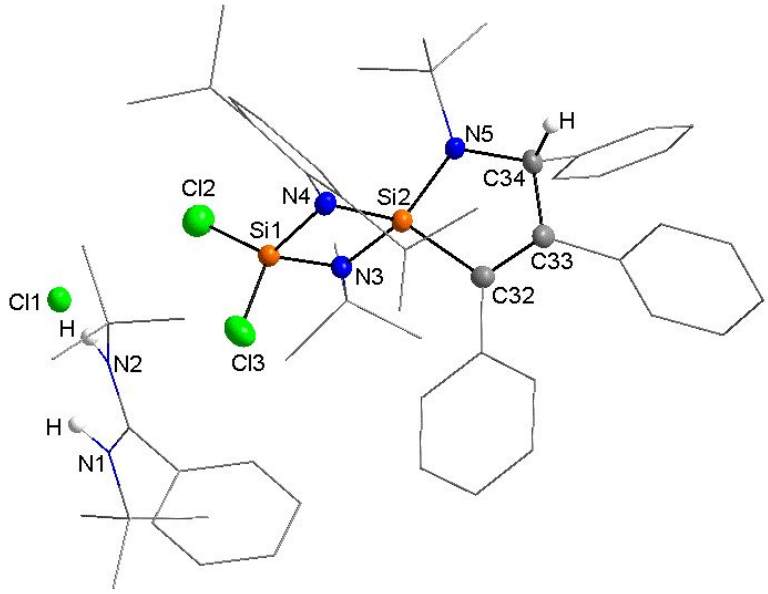



**Fig. S2** Molecular structures of **5**. H atoms are omitted for clarity except for C34*H*, N1*H* and N2*H*.

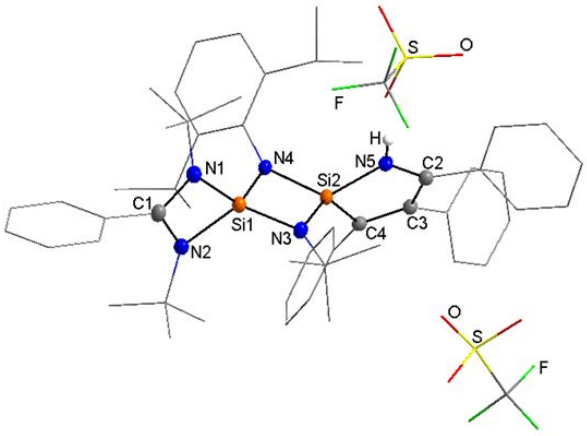



**Fig. S3** Molecular structures of **7**. H atoms are omitted for clarity.

## III. Theoretical calculations

Geometry optimizations and vibrational frequencies calculations of compounds **2a** in singlet, and triplet electronic states and **6** in doublet electronic state have been carried out at the BP86-D3(BJ)/def2-TZVPP level in the gas phase.[S3] The computation of **2a** in singlet diradical state is carried out by reoptimizing the **2a** (singlet state) with spin-unrestricted DFT (UBP86-D3(BJ)/def2-TZVPP) and a single point is performed on the unrestricted geometry by transpositioning the α and β orbitals to check the singlet diradical state and confirm. The singlet diradical geometry is then optimized by reading the single point check point file at UBP86-D3(BJ)/def2-TZVPP level. All the calculations were carried out using gaussian 16 program package.[S4] The absence of imaginary frequencies assures the minima on the potential energy surface except for one imaginary frequency for transition state. We have performed natural bonding orbital (NBO) [S5] calculation using NBO 6.0[S6] program to estimate natural bond orbitals, Mulliken spin densities, partial charges and Wiberg bond indices (WBI).[S7] The electron density distribution was analyzed by the quantum theory of atoms in molecules (QTAIM) using AIMALL,[S8] and the g-iso value from electron paramagnetic spectroscopy was calculated at UB3LYP-6-311G(d,p) level.[S9] The free energy profiles of compounds **2a**, **3a** and **3c** were carried out through the DFT method under B3LYP-D3(BJ)/def2-SVP level of theory using Gaussian 16 B.01 program.[S10-S14] The maximum forces of all structures were calculated to be less than 0.000450 Hartree/Bohr.

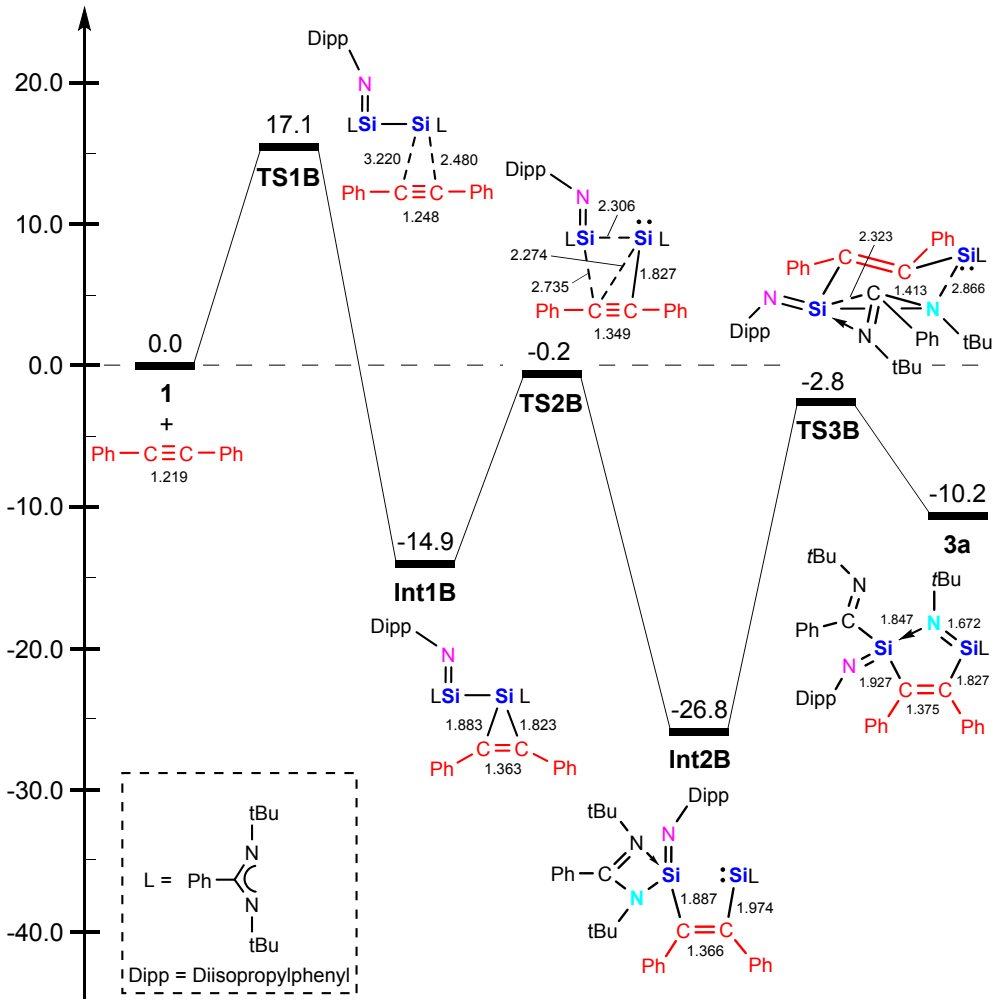



**Fig. S4** The free energy profile for the formation of **3a** at the B3LYP-D3(BJ)/def2-SVP level of theory.

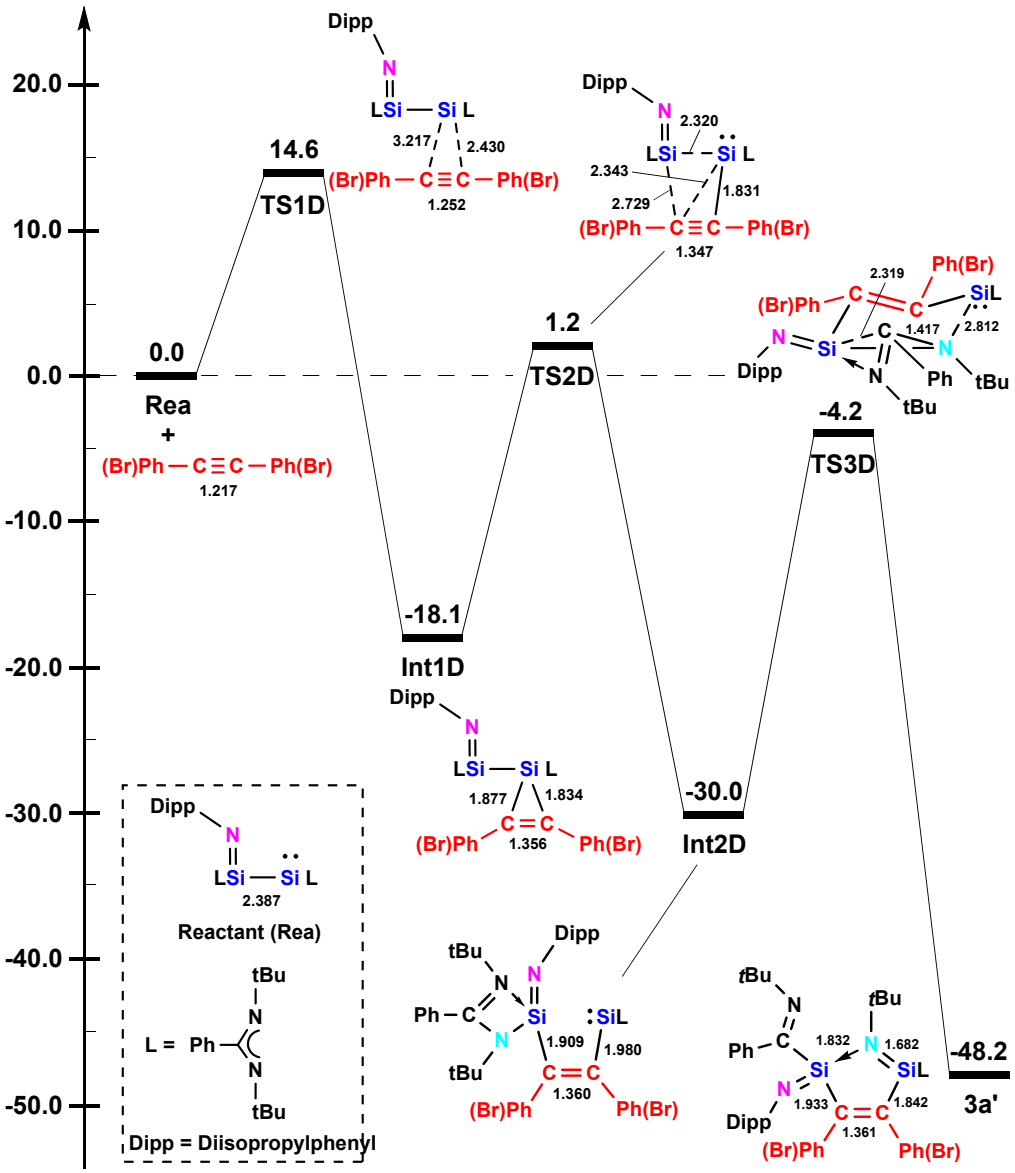
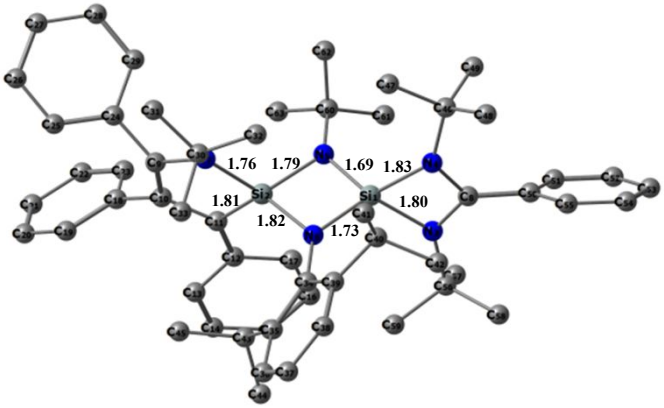
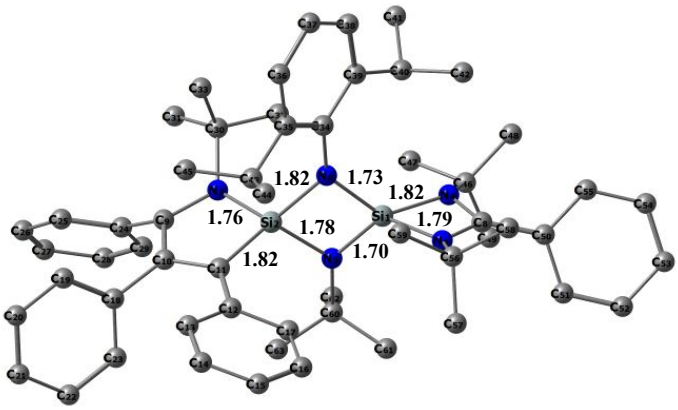


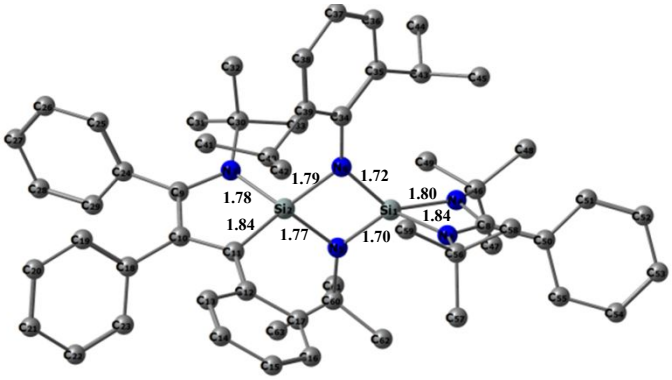

**Fig. S5** The free energy profile for the formation of **3c** at the B3LYP-D3(BJ)/def2-SVP level of theory.



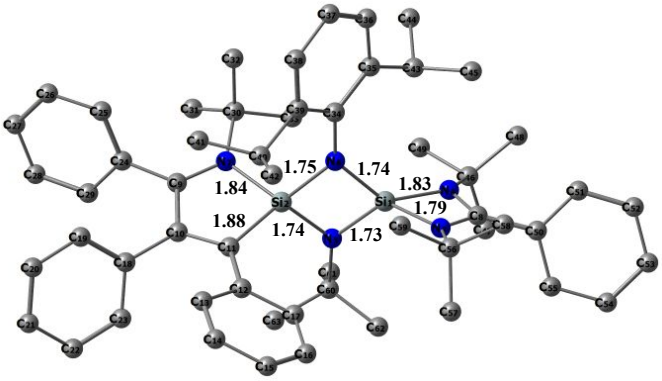

**2a (Singlet)**




**2a (Singlet Diradical)**

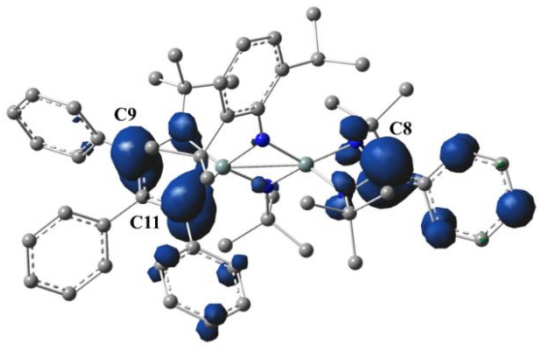



**6**

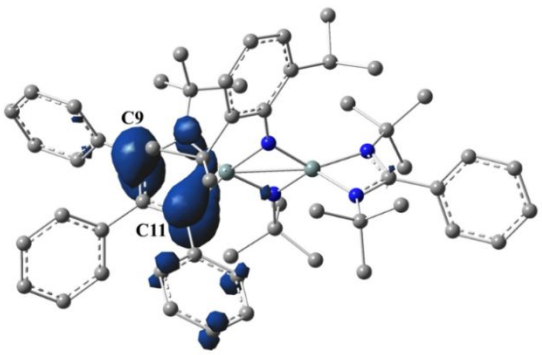



**7**

**Figure S6.** Optimized geometries of compounds **2a** (singlet, singlet diradical), **6** (cationic doublet) and **7** (dicationic singlet) at BP86-D3(BJ)/def2-TZVPP level of theory. Bond lengths in Å.

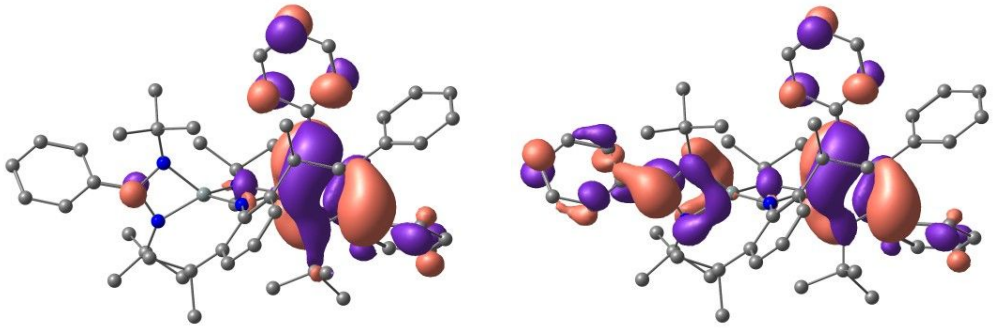



**2a**




**6**

**Figure S7.** Mulliken spin densities of compound **2a** (triplet diradical) and **6** (cationic doublet) at BP86-D3(BJ)/def2-TZVPP level at room temperature. Isodensity values at 0.03.



α-SOMO (-3.23 eV) (**2a**) β-SOMO (-3.10 eV) **(2a)**

**Figure S8.** The α-SOMO and β-SOMO orbitals of the singlet biradical state of compound **2a** at UBP86-D3(BJ)/def2-TZVPP level at Isodensity values at 0.03.

**Table S2.** NBO results of compounds **2a** (non-radical singlet)) **6** (cationic doublet) and **7** (dicationic singlet) at the BP86-D3(BJ)/def2-TZVPP level of theory. Occupation number ON, polarization and hybridization of the Si–N/C bonds, and partial charges q.

| Compound | Bond | ON | polarization and hybridization (%) | | *WBI* | qSi1 | qSi2 |
|---|---|---|---|---|---|---|---|
| **2a** | $Si_1$-N3 | 1.88 | $Si_1$: 12.6 | $N_3$: 87.4 | 0.49 | 2.23 | 2.30 |
| **(Singlet)** | | | s(22.2),p(54.0),d(22.4) | s(31.5), p(68.3), d(0.2) | | | |
| | $Si_1$-N4 | 1.88 | $Si_1$: 12.4 | $N_4$: 87.6 | 0.47 | | |
| | | | s(20.9),p(55.1),d(23.0) | s(31.0), p(68.8), d(0.2) | | | |
| | $Si_1$-N5 | 1.94 | $Si_1$: 16.0 | $N_5$: 84.0 | 0.68 | | |
| | | | s(28.6),p(68.1),d(3.3) | s(32.9), p(66.9), d(0.2) | | | |
| | $Si_1$-N6 | 1.93 | $Si_1$: 16.2 | $N_6$: 83.8 | 0.65 | | |
| | | | s(27.5),p(71.0),d(1.5) | s(31.5), p(68.4), d(0.1) | | | |
| | $Si_2$-N5 | 1.93 | $Si_2$: 14.0 | $N_5$: 86.0 | 0.49 | | |
| | | | s(22.3),p(76.3),d(1.3) | s(33.5), p(66.2), d(0.2) | | | |
| | $Si_2$-N6 | 1.92 | $Si_2$: 14.4 | $N_6$: 85.6 | 0.50 | | |
| | | | s(22.1),p(76.3),d(1.6) | s(33.5), p(66.4), d(0.1) | | | |
| | $Si_2$-N7 | 1.87 | $Si_2$: 12.5 | $N_7$: 87.5 | 0.59 | | |
| | | | s(25.0),p(51.5),d(23.5) | s(34.4), p(65.4), d(0.2) | | | |
| | $Si_2$-C11 | 1.85 | $Si_2$: 22.1 | $C_{11}$: 77.9 | 0.77 | | |
| | | | s(30.9),p(56.3),d(12.8) | s(31.4), p(68.4), d(0.2) | | | |
| **6** | $Si_1$-N3 | 0.96 | $Si_1$: 15.3 | $N_3$: 84.7 | 0.47 | 2.24 | 2.32 |
| | | | s(24.5),p(74.1),d(1.4) | s(30.4), p(69.4), d(0.2) | | | |
| | $Si_1$-N4 | 0.96 | $Si_1$: 15.4 | $N_4$: 84.6 | 0.46 | | |
| | | | s(18.9),p(79.6),d(1.5) | s(29.9), p(69.9), d(0.2) | | | |
| | $Si_1$-N5 | 0.97 | $Si_1$: 16.0 | $N_5$: 84.0 | 0.68 | | |
| | | | s(29.2),p(69.3),d(1.5) | s(33.3), p(66.5), d(0.2) | | | |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | $Si_1$-N6 | 0.97 | $Si_1$: 16.2 s(27.3),p(71.4),d(1.3) | $N_6$: 83.8 s(31.7), p(68.1), d(0.2) | 0.65 | | |
| | $Si_2$-N5 | 0.96 | $Si_2$: 14.8 s(23.2),p(75.5),d(1.3) | $N_5$: 85.2 s(33.0), p(66.8), d(0.2) | 0.52 | | |
| | $Si_2$-N6 | 0.95 | $Si_2$: 14.7 s(23.9),p(75.5),d(1.6) | $N_6$: 85.3 s(33.3), p(66.5), d(0.2) | 0.51 | | |
| | $Si_2$-N7 | 0.94 | $Si_2$: 12.4 s(25.0),p(50.9),d(24.1) | $N_7$: 87.6 s(33.5), p(66.3), d(0.2) | 0.55 | | |
| | $Si_2$-C11 | 0.91 | $Si_2$: 21.6 s(29.4),p(53.5),d(15.6) | $C_{11}$: 78.4 s(30.6), p(69.1), d(0.3) | 0.72 | | |
| **7** | $Si_1$-N3 | 1.92 | $Si_1$: 15.3 s(23.1),p(75.5),d(1.4) | $N_3$: 84.7 s(30.2), p(69.6), d(0.2) | 0.48 | 2.34 | 2.29 |
| | $Si_1$-N4 | 1.92 | $Si_1$: 16.0 s(22.3),p(76.3),d(1.4) | $N_4$: 84.0 s(29.1), p(70.7), d(0.2) | 0.47 | | |
| | $Si_1$-N5 | 1.93 | $Si_1$: 15.6 s(27.7),p(70.9),d(1.4) | $N_5$: 84.4 s(32.3), p(67.5), d(0.2) | 0.64 | | |
| | $Si_1$-N6 | 1.93 | $Si_1$: 15.7 s(26.9),p(71.7),d(1.4) | $N_6$: 84.3 s(31.8), p(68.0), d(0.2) | 0.62 | | |
| | $Si_2$-N5 | 1.93 | $Si_2$: 15.0 s(24.9),p(73.8),d(1.3) | $N_5$: 85.0 s(33.5), p(66.3), d(0.2) | 0.57 | | |
| | $Si_2$-N6 | 1.92 | $Si_2$: 15.0 s(25.4),p(73.3),d(1.3) | $N_6$: 85.0 s(33.0), p(66.8), d(0.2) | 0.56 | | |
| | $Si_2$-N7 | 1.93 | $Si_2$: 14.8 s(21.1),p(77.6),d(1.3) | $N_7$: 85.2 s(30.3), p(69.5), d(0.1) | 0.46 | | |
| | $Si_2$-C11 | 1.90 | $Si_2$: 24.5 s(28.6),p(70.8),d(0.6) | $C_{11}$: 75.5 s(29.0), p(70.7), d(0.3) | 0.65 | | |

**Table S3.** NBO charges of Si and coordinating N and C atoms of the compounds **2a** (non-radical singlet)) **6** (cationic doublet) and **7** (dicationic singlet).

| Atom | **2a** (Singlet) | **2a** (Triplet) | **6** (Doublet) | **7** (Singlet) |
|---|---|---|---|---|
| Si (1) | 2.23 | 2.25 | 2.25 | 2.34 |
| Si (2) | 2.3 | 2.32 | 2.32 | 2.29 |
| Ni(3) | -0.75 | -0.84 | -0.73 | -0.75 |
| Ni(4) | -0.74 | -0.82 | -0.71 | -0.73 |
| Ni(5) | -1.37 | -1.37 | -1.36 | -1.38 |
| Ni(6) | -1.31 | -1.32 | -1.31 | -1.33 |

| | | | | |
|---|---|---|---|---|
| Ni(7) | -0.85 | -0.79 | -0.80 | -0.69 |
| C (9) | -0.69 | -0.54 | -0.56 | -0.42 |

**Table S3a.** Mulliken charges of Si and coordinating N and C atoms of the compounds **2a** (non-radical singlet)) **6** (cationic doublet) and **7** (dicationic singlet).

| Atom | **2a** (Singlet) | **2a** (Triplet) | **6** (Doublet) | **7** (Singlet) |
|---|---|---|---|---|
| Si (1) | 0.11 | 0.21 | 0.18 | 0.20 |
| Si (2) | 0.11 | 0.14 | 0.14 | 0.18 |
| Ni(3) | -0.005 | -0.09 | 0.03 | 0.04 |
| Ni(4) | -0.07 | -0.13 | -0.04 | -0.02 |
| Ni(5) | -0.10 | -0.11 | -0.08 | -0.07 |
| Ni(6) | 0.009 | 0.005 | 0.05 | 0.09 |
| Ni(7) | -0.03 | 0.04 | 0.04 | 0.07 |
| C (11) | 0.20 | 0.22 | 0.24 | 0.30 |

**Table S4.** AIM results of the compounds **2a** (non-radical singlet)) **6** (cationic doublet) and **7** (dicationic singlet).

| Compound | Bond | $\rho$(r) | $\nabla^2\rho$(r) | *H* | *V* | *G* | ε |
|---|---|---|---|---|---|---|---|
| **2a** | Si1-N3 | 0.116 | 0.371 | -0.057 | -0.206 | 0.149 | 0.109 |
| | Si1-N4 | 0.108 | 0.311 | -0.053 | -0.184 | 0.131 | 0.079 |
| | Si1-N5 | 0.139 | 0.572 | -0.069 | -0.280 | 0.211 | 0.185 |
| | Si1-N6 | 0.131 | 0.496 | -0.064 | -0.253 | 0.189 | 0.177 |
| | Si2-N5 | 0.117 | 0.394 | -0.054 | -0.210 | 0.154 | 0.090 |
| | Si2-N6 | 0.108 | 0.329 | -0.051 | -0.184 | 0.133 | 0.077 |
| | Si2-N7 | 0.124 | 0.422 | -0.062 | -0.229 | 0.167 | 0.211 |
| | Si2-C11 | 0.133 | 0.220 | -0.085 | -0.224 | 0.139 | 0.221 |
| **6** | Si1-N3 | 0.115 | 0.347 | -0.057 | -0.201 | 0.144 | 0.076 |
| | Si1-N4 | 0.106 | 0.278 | -0.053 | -0.175 | 0.122 | 0.040 |
| | Si1-N5 | 0.138 | 0.552 | -0.069 | -0.276 | 0.207 | 0.199 |
| | Si1-N6 | 0.132 | 0.506 | -0.066 | -0.258 | 0.192 | 0.178 |
| | Si2-N5 | 0.120 | 0.412 | -0.058 | -0.219 | 0.161 | 0.110 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | Si2-N6 | 0.115 | 0.373 | -0.055 | -0.204 | 0.149 | 0.097 |
| | Si2-N7 | 0.121 | 0.400 | -0.06 | -0.219 | 0.159 | 0.178 |
| | Si2-C11 | 0.130 | 0.188 | -0.083 | -0.213 | 0.130 | 0.160 |
| **7** | Si1-N3 | 0.118 | 0.36 | -0.060 | -0.210 | 0.150 | 0.081 |
| | Si1-N4 | 0.110 | 0.288 | -0.056 | -0.184 | 0.128 | 0.047 |
| | Si1-N5 | 0.133 | 0.500 | -0.067 | -0.258 | 0.191 | 0.189 |
| | Si1-N6 | 0.128 | 0.467 | -0.064 | -0.244 | 0.180 | 0.167 |
| | Si2-N5 | 0.128 | 0.470 | -0.063 | -0.244 | 0.181 | 0.142 |
| | Si2-N6 | 0.125 | 0.446 | -0.062 | -0.235 | 0.173 | 0.126 |
| | Si2-N7 | 0.109 | 0.287 | -0.055 | -0.181 | 0.126 | 0.062 |
| | Si2-C11 | 0.124 | 0.133 | -0.079 | -0.192 | 0.113 | 0.170 |

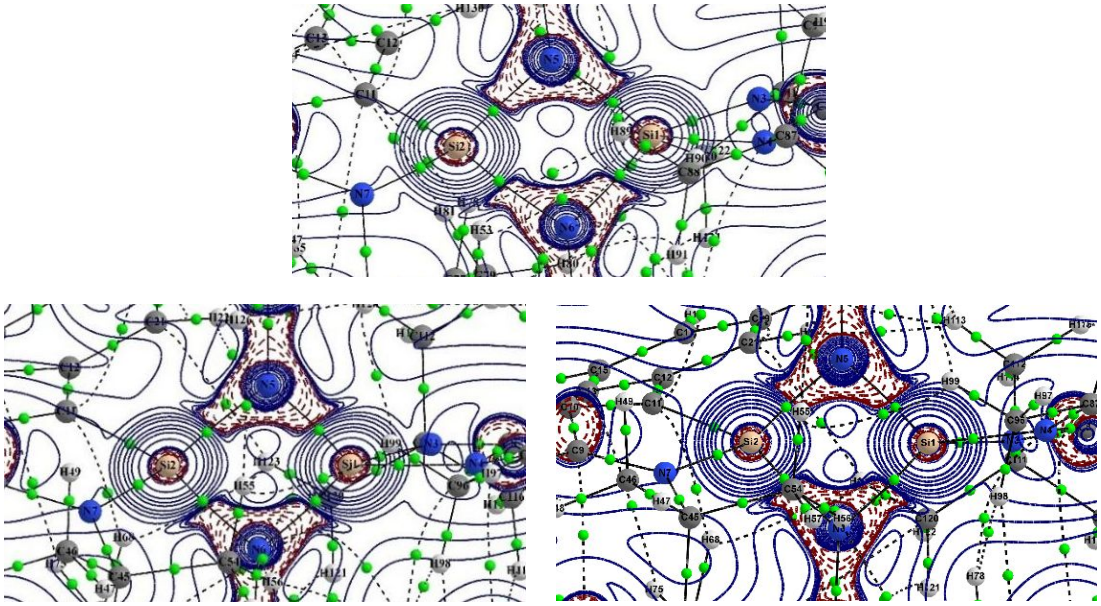
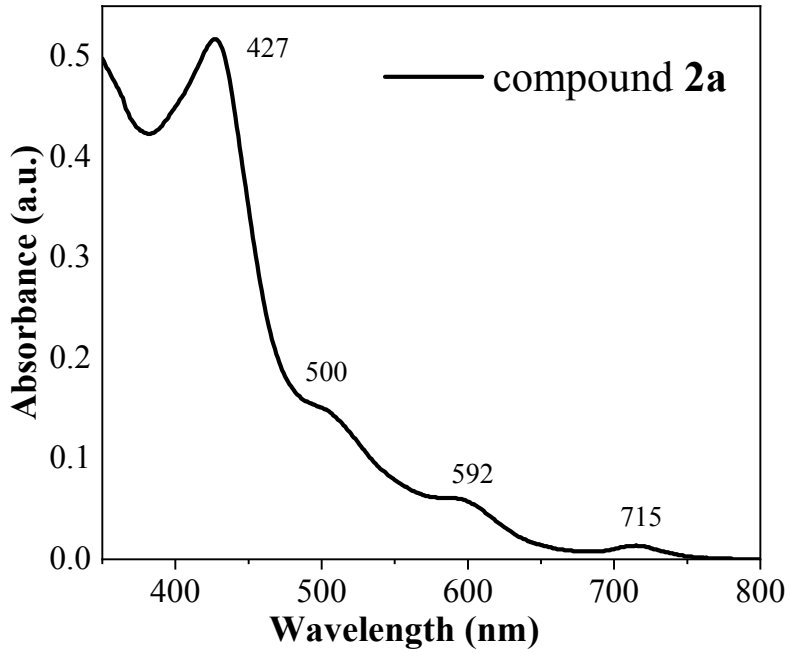


**Figure S9.** Contour plot of Laplacian distribution [$\nabla^2\rho$(r)] in compound **2a** in Si1-N5-Si2 plane in closed-shell singlet state. Contour plot of Laplacian distribution [$\nabla^2\rho$(r)] in compounds **6** (bottom, left) and **7** (bottom, right) in Si1-N5-Si2 plane. Solid blue lines indicate the areas of charge concentration ($\nabla^2\rho$(r) < 0), while dotted purple lines denote charge depletion ($\nabla^2\rho$(r) > 0). Solid lines connecting atomic nuclei (black) are the bond paths and small green spheres along the bond path are bond critical points (BCP). Those thick, solid blue lines separating the atomic basins indicate the zero-flux surface crossing the molecular plane.

Mulliken charges support the NBO charge distribution, however, with some exceptions (**Table S3a**). Quantum theory of atoms in molecules (QTAIM) analysis forecasts positive Laplacian ($\nabla^2\rho$(r)) and negative total energy density (H) at (3, -1) bond critical point (BCP) with electron density ρ<0.2 along the Si-N and Si-C bond paths (**Table**

**S4**) suggesting closed shell nature of the bonds in compounds **2a 6**, and **7** (**Figures S9** and **S9**). However, the negative Laplacian for a covalent bond does not always stand up for bonds with heavier elements like Si. Nevertheless, another parameter, which weighs the balance between potential energy density (V) and kinetic energy density (G), $|V|<2G$,[8] also denotes the closed shell nature of the Si-N and Si-C bonding interactions. Furthermore, the contour plots of compounds **2a**, **6**, and **7** along the Si1-N5-Si2 plane (**Figure S9**) indicate charge concentration on nitrogen atoms and charge depletion from Si atoms, which agrees well with the high positive charges on the Si atoms from NBO analysis. Interestingly, a slight deviation of ellipticity (ε) values from zero (The ε close to zero indicates a single or triple bond) is observed along some of the Si-N and Si-C bond paths of compounds **2a**, **6**, and **7** (**Table S4**), stipulating the possibility of partial multiple bond character.



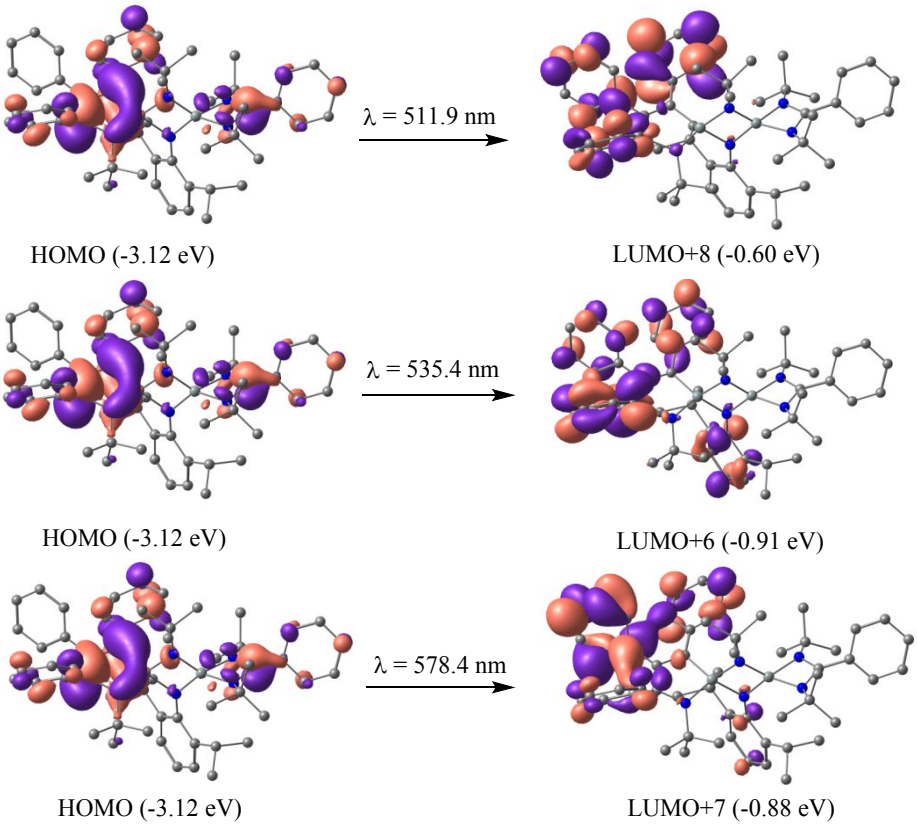
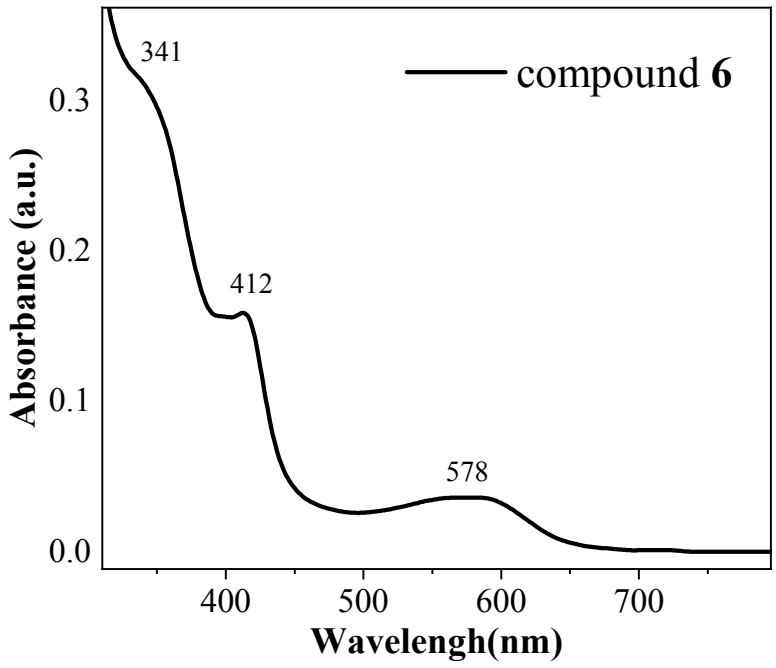



**Figure S10.** UV-VIS spectrum of **6** in DCM (top). The computed transitions and corresponding molecular orbitals of compound **2a** from TD-DFT at BP86-D3(BJ)/def2-TZVPP level (bottom).



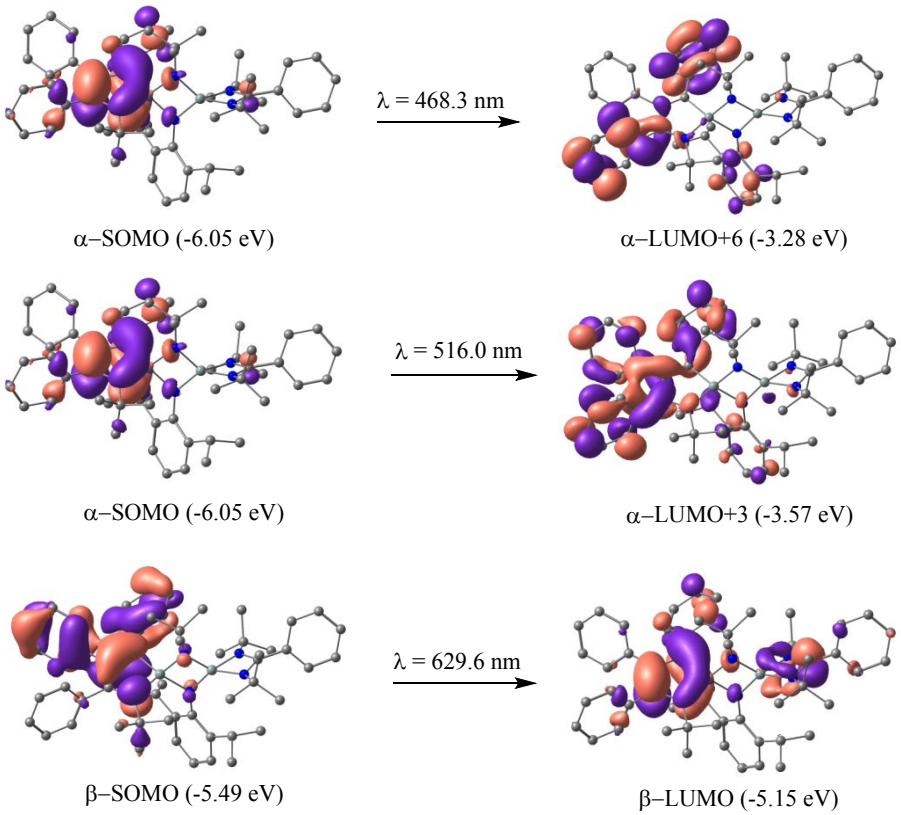



**Figure S11.** UV-VIS spectrum of **6** in DCM (top). The computed transitions and corresponding molecular orbitals of compound **6** from TD-DFT at BP86-D3(BJ)/def2-TZVPP level (bottom).

**Table S5.** NICS Results of Compounds **3a** and **4** at the BP86/def2-TZVPP Level

| Compound | NICS (0) | NICS (1) |
|---|---|---|
| **3** | -2.428 | -1.700 |
| **4** | -6.867 | -1.844 |
| **4-NMe** | -7.669 | -3.466 |

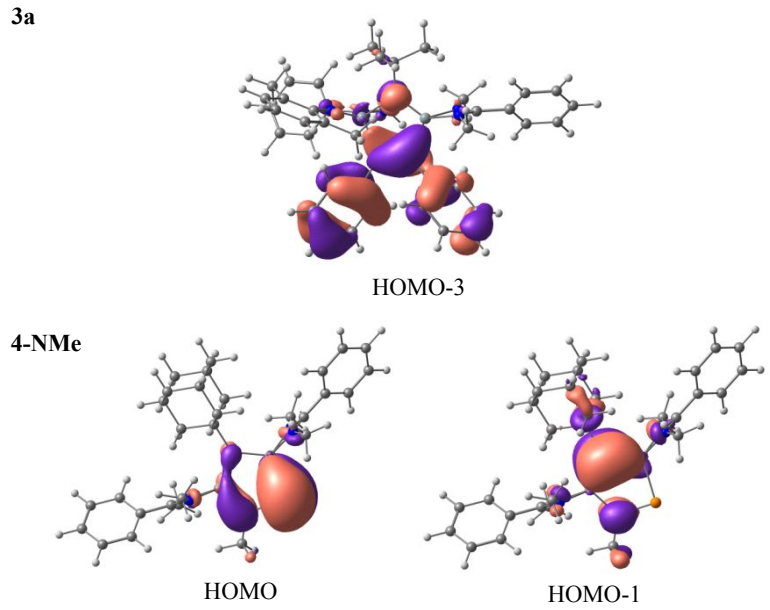



**Figure S12.** Molecular orbitals of compounds **3a** and **4**-NMe exhibiting Möbius topology.

Optimized Coordinates

**2a (Singlet)**

BP86-D3(BJ)/def2-TZVPP

G = -3032.0668374 Hartree

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| Si | 12.402940000 | 8.499705000 | 12.079933000 |
| Si | 11.661083000 | 6.512744000 | 13.496279000 |
| N | 12.682769000 | 8.908333000 | 10.352426000 |
| N | 12.797067000 | 10.288808000 | 12.030472000 |
| N | 10.945247000 | 7.992285000 | 12.790126000 |
| N | 13.218119000 | 7.143999000 | 12.780141000 |
| N | 11.563869000 | 6.261870000 | 15.243604000 |
| C | 12.857381000 | 10.229315000 | 10.663190000 |
| C | 10.783766000 | 5.087382000 | 15.473229000 |
| C | 10.452206000 | 4.365953000 | 14.313918000 |
| C | 10.855168000 | 4.940800000 | 13.069757000 |
| C | 10.594268000 | 4.398644000 | 11.751664000 |
| C | 10.424435000 | 3.011080000 | 11.493553000 |
| H | 10.464862000 | 2.307166000 | 12.321191000 |
| C | 10.226914000 | 2.522812000 | 10.205673000 |
| H | 10.108720000 | 1.447364000 | 10.058785000 |

| | | | |
|---|---|---|---|
| C | 10.191473000 | 3.386432000 | 9.103184000 |
| H | 10.037494000 | 2.999697000 | 8.095353000 |
| C | 10.356932000 | 4.756729000 | 9.325376000 |
| H | 10.329043000 | 5.449526000 | 8.482426000 |
| C | 10.548592000 | 5.249311000 | 10.614525000 |
| H | 10.653450000 | 6.325024000 | 10.767440000 |
| C | 9.501156000 | 3.224757000 | 14.379578000 |
| C | 9.912680000 | 1.963633000 | 14.837822000 |
| H | 10.948844000 | 1.832114000 | 15.153809000 |
| C | 9.022525000 | 0.887578000 | 14.868890000 |
| H | 9.360669000 | -0.086946000 | 15.225342000 |
| C | 7.702520000 | 1.058637000 | 14.442443000 |
| H | 7.004749000 | 0.220289000 | 14.466918000 |
| C | 7.282379000 | 2.310512000 | 13.981632000 |
| H | 6.253225000 | 2.451980000 | 13.647421000 |
| C | 8.176522000 | 3.381409000 | 13.945605000 |
| H | 7.855191000 | 4.355149000 | 13.574968000 |
| C | 9.924593000 | 5.000612000 | 16.672339000 |
| C | 9.811503000 | 3.837954000 | 17.456474000 |
| H | 10.439813000 | 2.979817000 | 17.224520000 |
| C | 8.922553000 | 3.779172000 | 18.531348000 |
| H | 8.855930000 | 2.864756000 | 19.123434000 |
| C | 8.128935000 | 4.882502000 | 18.857659000 |
| H | 7.437221000 | 4.835575000 | 19.699757000 |
| C | 8.232008000 | 6.049162000 | 18.089520000 |
| H | 7.610094000 | 6.915186000 | 18.324704000 |
| C | 9.115935000 | 6.105436000 | 17.014879000 |
| H | 9.188776000 | 7.009787000 | 16.408243000 |
| C | 12.602258000 | 6.675724000 | 16.247390000 |
| C | 12.126110000 | 6.622639000 | 17.708359000 |
| H | 11.245432000 | 7.253256000 | 17.877471000 |
| H | 12.945567000 | 6.996512000 | 18.339705000 |
| H | 11.884066000 | 5.606259000 | 18.036513000 |
| C | 12.988396000 | 8.125334000 | 15.955585000 |
| H | 13.383063000 | 8.237016000 | 14.940354000 |
| H | 13.762917000 | 8.459209000 | 16.659645000 |
| H | 12.112990000 | 8.777477000 | 16.069535000 |
| C | 13.824312000 | 5.748368000 | 16.113181000 |
| H | 13.512484000 | 4.705304000 | 16.264990000 |
| H | 14.586869000 | 5.993986000 | 16.867193000 |
| H | 14.287693000 | 5.830298000 | 15.122495000 |
| C | 14.563860000 | 6.660169000 | 12.800684000 |
| C | 14.856394000 | 5.293012000 | 12.522466000 |
| C | 16.169972000 | 4.826234000 | 12.660559000 |

| | | | |
|---|---|---|---|
| H | 16.365904000 | 3.771343000 | 12.463401000 |
| C | 17.218191000 | 5.660783000 | 13.025203000 |
| H | 18.232515000 | 5.273909000 | 13.130192000 |
| C | 16.945051000 | 7.007085000 | 13.231461000 |
| H | 17.761320000 | 7.685676000 | 13.483479000 |
| C | 15.647905000 | 7.525131000 | 13.126452000 |
| C | 15.509821000 | 9.026804000 | 13.289425000 |
| H | 14.444596000 | 9.273465000 | 13.359653000 |
| C | 16.173420000 | 9.568329000 | 14.564389000 |
| H | 15.810548000 | 9.036685000 | 15.453339000 |
| H | 15.949832000 | 10.638861000 | 14.688097000 |
| H | 17.267322000 | 9.465997000 | 14.532231000 |
| C | 16.070678000 | 9.720842000 | 12.034781000 |
| H | 17.130615000 | 9.463274000 | 11.897159000 |
| H | 15.995107000 | 10.814585000 | 12.110092000 |
| H | 15.532456000 | 9.398926000 | 11.132517000 |
| C | 13.824320000 | 4.279622000 | 12.072915000 |
| H | 12.891313000 | 4.811126000 | 11.875603000 |
| C | 14.214790000 | 3.573831000 | 10.763205000 |
| H | 14.485900000 | 4.293877000 | 9.980389000 |
| H | 13.361259000 | 2.981601000 | 10.403593000 |
| H | 15.066831000 | 2.891619000 | 10.902567000 |
| C | 13.549648000 | 3.242065000 | 13.172964000 |
| H | 14.461807000 | 2.668968000 | 13.399716000 |
| H | 12.773920000 | 2.538139000 | 12.842592000 |
| H | 13.200154000 | 3.716077000 | 14.097780000 |
| C | 12.533523000 | 11.486286000 | 12.878934000 |
| C | 12.365349000 | 10.974606000 | 14.312670000 |
| H | 11.636868000 | 10.160307000 | 14.368011000 |
| H | 12.023598000 | 11.790987000 | 14.962187000 |
| H | 13.320312000 | 10.605420000 | 14.706622000 |
| C | 13.716509000 | 12.469591000 | 12.874566000 |
| H | 14.652745000 | 11.958038000 | 13.127150000 |
| H | 13.535704000 | 13.240021000 | 13.637246000 |
| H | 13.830503000 | 12.974788000 | 11.909922000 |
| C | 11.271719000 | 12.227577000 | 12.405063000 |
| H | 11.405245000 | 12.629530000 | 11.392844000 |
| H | 11.063741000 | 13.069620000 | 13.079809000 |
| H | 10.395929000 | 11.569038000 | 12.402633000 |
| C | 12.951916000 | 11.332521000 | 9.711064000 |
| C | 11.889802000 | 11.552732000 | 8.808465000 |
| H | 10.997200000 | 10.931338000 | 8.876201000 |
| C | 11.966520000 | 12.575854000 | 7.866981000 |
| H | 11.131865000 | 12.744304000 | 7.185364000 |

| | | | |
|---|---|---|---|
| C | 13.104331000 | 13.389865000 | 7.799614000 |
| H | 13.165603000 | 14.186034000 | 7.057501000 |
| C | 14.164963000 | 13.171965000 | 8.687839000 |
| H | 15.062017000 | 13.789581000 | 8.629178000 |
| C | 14.092312000 | 12.156350000 | 9.638629000 |
| H | 14.937457000 | 11.957970000 | 10.295480000 |
| C | 13.022127000 | 8.184632000 | 9.096628000 |
| C | 11.752816000 | 8.043389000 | 8.241452000 |
| H | 10.944250000 | 7.586676000 | 8.825261000 |
| H | 11.953037000 | 7.403190000 | 7.371287000 |
| H | 11.412449000 | 9.020489000 | 7.876055000 |
| C | 14.124567000 | 8.899013000 | 8.299691000 |
| H | 13.791637000 | 9.847655000 | 7.865749000 |
| H | 14.435923000 | 8.241012000 | 7.477033000 |
| H | 15.004531000 | 9.089657000 | 8.929520000 |
| C | 13.542645000 | 6.800595000 | 9.499907000 |
| H | 14.467217000 | 6.882868000 | 10.086742000 |
| H | 13.753755000 | 6.213645000 | 8.596624000 |
| H | 12.804395000 | 6.243744000 | 10.088178000 |
| C | 9.519038000 | 8.390338000 | 12.729267000 |
| C | 9.246628000 | 9.056964000 | 11.372564000 |
| H | 9.914213000 | 9.914255000 | 11.205709000 |
| H | 8.210027000 | 9.418864000 | 11.318844000 |
| H | 9.402560000 | 8.337194000 | 10.557278000 |
| C | 9.185275000 | 9.348461000 | 13.886388000 |
| H | 9.478606000 | 8.891249000 | 14.841937000 |
| H | 8.104770000 | 9.550240000 | 13.916568000 |
| H | 9.703958000 | 10.308416000 | 13.791315000 |
| C | 8.596926000 | 7.167117000 | 12.873195000 |
| H | 8.778781000 | 6.423940000 | 12.088666000 |
| H | 7.551436000 | 7.501691000 | 12.805228000 |
| H | 8.734674000 | 6.678038000 | 13.846867000 |

**2a (Singlet Diradical)**

BP86-D3(BJ)/def2-TZVPP

G = -3032.0670824 Hartree

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| Si | 1.659878000 | 0.185473000 | -0.291980000 |
| Si | -0.871866000 | 0.267474000 | 0.004604000 |
| N | 2.966187000 | -1.036427000 | -0.414269000 |

| | | | |
|---|---|---|---|
| N | 3.189915000 | 1.117102000 | -0.655844000 |
| N | 0.316618000 | 0.350665000 | -1.324513000 |
| N | 0.597668000 | 0.176381000 | 1.077412000 |
| N | -2.012842000 | 1.602784000 | 0.221499000 |
| C | 3.879691000 | -0.067952000 | -0.748111000 |
| C | -3.328243000 | 1.091494000 | 0.013860000 |
| C | -3.403472000 | -0.305547000 | -0.130410000 |
| C | -2.162921000 | -1.009395000 | -0.141574000 |
| C | -1.991664000 | -2.438305000 | -0.315847000 |
| C | -2.972212000 | -3.396066000 | 0.059422000 |
| H | -3.915159000 | -3.055887000 | 0.480138000 |
| C | -2.752565000 | -4.763197000 | -0.078011000 |
| H | -3.534403000 | -5.459750000 | 0.231134000 |
| C | -1.544838000 | -5.251809000 | -0.592468000 |
| H | -1.376067000 | -6.323894000 | -0.698169000 |
| C | -0.559940000 | -4.333381000 | -0.967752000 |
| H | 0.388011000 | -4.691021000 | -1.373317000 |
| C | -0.778983000 | -2.963743000 | -0.835949000 |
| H | -0.004634000 | -2.263404000 | -1.154246000 |
| C | -4.682931000 | -0.956392000 | -0.519107000 |
| C | -5.699207000 | -1.176887000 | 0.423374000 |
| H | -5.538964000 | -0.855905000 | 1.453950000 |
| C | -6.886580000 | -1.816196000 | 0.059303000 |
| H | -7.664937000 | -1.982513000 | 0.805997000 |
| C | -7.075890000 | -2.243664000 | -1.257920000 |
| H | -8.002789000 | -2.742215000 | -1.545280000 |
| C | -6.068928000 | -2.030541000 | -2.204744000 |
| H | -6.209654000 | -2.360971000 | -3.235194000 |
| C | -4.881200000 | -1.397386000 | -1.835704000 |
| H | -4.089510000 | -1.240936000 | -2.568904000 |
| C | -4.369968000 | 1.955040000 | -0.580361000 |
| C | -5.693651000 | 2.001126000 | -0.106754000 |
| H | -5.956234000 | 1.438015000 | 0.787088000 |
| C | -6.662278000 | 2.769694000 | -0.754926000 |
| H | -7.681673000 | 2.788698000 | -0.365667000 |
| C | -6.332669000 | 3.518056000 | -1.888400000 |
| H | -7.090303000 | 4.119779000 | -2.392092000 |
| C | -5.018239000 | 3.485543000 | -2.370934000 |
| H | -4.748812000 | 4.055706000 | -3.262150000 |
| C | -4.053408000 | 2.716019000 | -1.725720000 |
| H | -3.031402000 | 2.680509000 | -2.106997000 |
| C | -1.805368000 | 2.796129000 | 1.110920000 |
| C | -2.791533000 | 3.949318000 | 0.862732000 |
| H | -2.755847000 | 4.304767000 | -0.173761000 |

| | | | |
|---|---|---|---|
| H | -2.504660000 | 4.780717000 | 1.523269000 |
| H | -3.826955000 | 3.677494000 | 1.093404000 |
| C | -0.403533000 | 3.343133000 | 0.844853000 |
| H | 0.364771000 | 2.587953000 | 1.040248000 |
| H | -0.205044000 | 4.205559000 | 1.495778000 |
| H | -0.320318000 | 3.671377000 | -0.199095000 |
| C | -1.949811000 | 2.354801000 | 2.579113000 |
| H | -2.943434000 | 1.910809000 | 2.733794000 |
| H | -1.846674000 | 3.214491000 | 3.257749000 |
| H | -1.192011000 | 1.611448000 | 2.855221000 |
| C | 0.758912000 | 0.113343000 | 2.497224000 |
| C | -0.012533000 | -0.791720000 | 3.283249000 |
| C | 0.084530000 | -0.748901000 | 4.680071000 |
| H | -0.531848000 | -1.435961000 | 5.261548000 |
| C | 0.941493000 | 0.124588000 | 5.336304000 |
| H | 0.997413000 | 0.142817000 | 6.425386000 |
| C | 1.743367000 | 0.959617000 | 4.568424000 |
| H | 2.449575000 | 1.626939000 | 5.064552000 |
| C | 1.674389000 | 0.973313000 | 3.169484000 |
| C | 2.670296000 | 1.867717000 | 2.456228000 |
| H | 2.391558000 | 1.925999000 | 1.398312000 |
| C | 2.691236000 | 3.308724000 | 2.987321000 |
| H | 1.684519000 | 3.745952000 | 2.980633000 |
| H | 3.343910000 | 3.937390000 | 2.362791000 |
| H | 3.076052000 | 3.361658000 | 4.015539000 |
| C | 4.067622000 | 1.226389000 | 2.538606000 |
| H | 4.369734000 | 1.103156000 | 3.588563000 |
| H | 4.825987000 | 1.844128000 | 2.037808000 |
| H | 4.072852000 | 0.230978000 | 2.073514000 |
| C | -0.953790000 | -1.827922000 | 2.704444000 |
| H | -0.823038000 | -1.836150000 | 1.620500000 |
| C | -0.643916000 | -3.252133000 | 3.195976000 |
| H | 0.415410000 | -3.505311000 | 3.060542000 |
| H | -1.244758000 | -3.972052000 | 2.622056000 |
| H | -0.886974000 | -3.380286000 | 4.261460000 |
| C | -2.419597000 | -1.472264000 | 2.999122000 |
| H | -2.605099000 | -1.467101000 | 4.084175000 |
| H | -3.087973000 | -2.212773000 | 2.539316000 |
| H | -2.684629000 | -0.486544000 | 2.598833000 |
| C | 3.542677000 | 2.422807000 | -1.282351000 |
| C | 2.345280000 | 3.351369000 | -1.058741000 |
| H | 1.407995000 | 2.886724000 | -1.378682000 |
| H | 2.483187000 | 4.281070000 | -1.626095000 |
| H | 2.251375000 | 3.613323000 | 0.002455000 |

| | | | |
|---|---|---|---|
| C | 4.763168000 | 3.076122000 | -0.611039000 |
| H | 4.627267000 | 3.137115000 | 0.475208000 |
| H | 4.870713000 | 4.099746000 | -0.996612000 |
| H | 5.691361000 | 2.537941000 | -0.828653000 |
| C | 3.836903000 | 2.252860000 | -2.782875000 |
| H | 4.716213000 | 1.616760000 | -2.944674000 |
| H | 4.041137000 | 3.234846000 | -3.231990000 |
| H | 2.986653000 | 1.807347000 | -3.311369000 |
| C | 5.237342000 | -0.294101000 | -1.227680000 |
| C | 5.437633000 | -1.093117000 | -2.375027000 |
| H | 4.570722000 | -1.477118000 | -2.912054000 |
| C | 6.724574000 | -1.354290000 | -2.837107000 |
| H | 6.861994000 | -1.960028000 | -3.733783000 |
| C | 7.837352000 | -0.835601000 | -2.162249000 |
| H | 8.844608000 | -1.046262000 | -2.521926000 |
| C | 7.647084000 | -0.049211000 | -1.018656000 |
| H | 8.508522000 | 0.341223000 | -0.475263000 |
| C | 6.362700000 | 0.223661000 | -0.554277000 |
| H | 6.220924000 | 0.791220000 | 0.363772000 |
| C | 3.210102000 | -2.428371000 | 0.052875000 |
| C | 3.040228000 | -3.393190000 | -1.131776000 |
| H | 2.069633000 | -3.236806000 | -1.618389000 |
| H | 3.086534000 | -4.433752000 | -0.781965000 |
| H | 3.832667000 | -3.247253000 | -1.876458000 |
| C | 4.605543000 | -2.591211000 | 0.675534000 |
| H | 5.413096000 | -2.513011000 | -0.059824000 |
| H | 4.662867000 | -3.586246000 | 1.137486000 |
| H | 4.774078000 | -1.843882000 | 1.463188000 |
| C | 2.166349000 | -2.733959000 | 1.132860000 |
| H | 2.293358000 | -2.074045000 | 2.001371000 |
| H | 2.279919000 | -3.773934000 | 1.465476000 |
| H | 1.144012000 | -2.619535000 | 0.755058000 |
| C | 0.074267000 | 0.332781000 | -2.786368000 |
| C | 1.173375000 | -0.499410000 | -3.463620000 |
| H | 2.174229000 | -0.112366000 | -3.225722000 |
| H | 1.054453000 | -0.483163000 | -4.556305000 |
| H | 1.121535000 | -1.544023000 | -3.127203000 |
| C | 0.056483000 | 1.769437000 | -3.337699000 |
| H | -0.668009000 | 2.372791000 | -2.772595000 |
| H | -0.242368000 | 1.770312000 | -4.395896000 |
| H | 1.036689000 | 2.252387000 | -3.264435000 |
| C | -1.292364000 | -0.294457000 | -3.112231000 |
| H | -1.368704000 | -1.322881000 | -2.741616000 |
| H | -1.427423000 | -0.303393000 | -4.203629000 |

| | | | |
|---|---|---|---|
| H | -2.112414000 | 0.289855000 | -2.673509000 |

**2a (Triplet)**

BP86-D3(BJ)/def2-TZVPP

G = -3032.0575023 Hartree

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| Si | 12.387082000 | 8.645516000 | 12.010432000 |
| Si | 11.534816000 | 6.707988000 | 13.435675000 |
| N | 12.596919000 | 8.891760000 | 10.280785000 |
| N | 12.932275000 | 10.344809000 | 11.912336000 |
| N | 10.895324000 | 8.209760000 | 12.798115000 |
| N | 13.104917000 | 7.232847000 | 12.794324000 |
| N | 11.520452000 | 6.270600000 | 15.181407000 |
| C | 12.953381000 | 10.243599000 | 10.496765000 |
| C | 10.766296000 | 5.114902000 | 15.351546000 |
| C | 10.221965000 | 4.548952000 | 14.165726000 |
| C | 10.580377000 | 5.190027000 | 12.966799000 |
| C | 10.293784000 | 4.688035000 | 11.628668000 |
| C | 10.156899000 | 3.302912000 | 11.359241000 |
| H | 10.259156000 | 2.587835000 | 12.172189000 |
| C | 9.908863000 | 2.833884000 | 10.073117000 |
| H | 9.817591000 | 1.759581000 | 9.904491000 |
| C | 9.780363000 | 3.725634000 | 9.001780000 |
| H | 9.577048000 | 3.357838000 | 7.995495000 |
| C | 9.929920000 | 5.094227000 | 9.238870000 |
| H | 9.847920000 | 5.801123000 | 8.412797000 |
| C | 10.195101000 | 5.564697000 | 10.523940000 |
| H | 10.322408000 | 6.634827000 | 10.688291000 |
| C | 9.266085000 | 3.414502000 | 14.243037000 |
| C | 9.615349000 | 2.172680000 | 14.798367000 |
| H | 10.621964000 | 2.025979000 | 15.188169000 |
| C | 8.690725000 | 1.128004000 | 14.846413000 |
| H | 8.980883000 | 0.170076000 | 15.280743000 |
| C | 7.400419000 | 1.305487000 | 14.338591000 |
| H | 6.678093000 | 0.488984000 | 14.376808000 |
| C | 7.042849000 | 2.536491000 | 13.779125000 |
| H | 6.038995000 | 2.684326000 | 13.378009000 |
| C | 7.968016000 | 3.579155000 | 13.730706000 |
| H | 7.694840000 | 4.537292000 | 13.286784000 |
| C | 10.483537000 | 4.466875000 | 16.655788000 |
| C | 11.424022000 | 3.633695000 | 17.281943000 |

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|---|---|---|---|
| H | 12.400816000 | 3.487808000 | 16.821002000 |
| C | 11.104882000 | 2.963524000 | 18.463819000 |
| H | 11.846126000 | 2.316962000 | 18.935588000 |
| C | 9.834472000 | 3.105222000 | 19.030223000 |
| H | 9.583647000 | 2.578470000 | 19.951698000 |
| C | 8.881974000 | 3.910807000 | 18.399500000 |
| H | 7.882586000 | 4.011796000 | 18.824736000 |
| C | 9.202805000 | 4.582333000 | 17.219634000 |
| H | 8.457985000 | 5.200903000 | 16.718219000 |
| C | 12.272278000 | 6.960343000 | 16.281416000 |
| C | 11.474676000 | 7.054768000 | 17.596687000 |
| H | 10.451552000 | 7.406782000 | 17.406106000 |
| H | 11.971665000 | 7.790172000 | 18.245174000 |
| H | 11.420192000 | 6.111158000 | 18.144974000 |
| C | 12.533797000 | 8.397321000 | 15.830116000 |
| H | 13.114295000 | 8.428058000 | 14.902847000 |
| H | 13.105552000 | 8.927917000 | 16.602221000 |
| H | 11.588813000 | 8.931102000 | 15.675714000 |
| C | 13.622082000 | 6.256728000 | 16.505333000 |
| H | 13.482004000 | 5.230939000 | 16.863939000 |
| H | 14.207515000 | 6.800327000 | 17.261179000 |
| H | 14.204907000 | 6.226309000 | 15.574999000 |
| C | 14.411117000 | 6.678514000 | 12.958247000 |
| C | 14.639458000 | 5.280402000 | 12.793283000 |
| C | 15.906794000 | 4.747643000 | 13.061800000 |
| H | 16.053274000 | 3.672833000 | 12.944169000 |
| C | 16.974294000 | 5.544019000 | 13.455218000 |
| H | 17.953557000 | 5.108692000 | 13.657827000 |
| C | 16.766793000 | 6.913064000 | 13.564675000 |
| H | 17.600060000 | 7.559239000 | 13.844134000 |
| C | 15.516037000 | 7.498200000 | 13.328407000 |
| C | 15.451945000 | 9.009857000 | 13.424656000 |
| H | 14.403118000 | 9.320907000 | 13.386949000 |
| C | 16.034185000 | 9.559367000 | 14.735643000 |
| H | 15.564529000 | 9.084512000 | 15.607958000 |
| H | 15.863469000 | 10.644397000 | 14.800663000 |
| H | 17.118916000 | 9.395624000 | 14.807291000 |
| C | 16.148608000 | 9.626047000 | 12.198622000 |
| H | 17.194333000 | 9.290722000 | 12.139444000 |
| H | 16.143590000 | 10.723297000 | 12.244071000 |
| H | 15.643270000 | 9.328125000 | 11.270262000 |
| C | 13.581609000 | 4.293916000 | 12.338618000 |
| H | 12.684071000 | 4.855972000 | 12.067678000 |
| C | 13.998722000 | 3.511136000 | 11.082228000 |

| | | | |
|---|---|---|---|
| H | 14.311949000 | 4.185927000 | 10.276297000 |
| H | 13.148484000 | 2.915506000 | 10.719819000 |
| H | 14.831301000 | 2.823141000 | 11.291333000 |
| C | 13.215269000 | 3.322733000 | 13.472375000 |
| H | 14.074273000 | 2.682460000 | 13.723141000 |
| H | 12.381005000 | 2.673178000 | 13.173667000 |
| H | 12.919008000 | 3.861628000 | 14.381007000 |
| C | 12.670224000 | 11.589962000 | 12.684724000 |
| C | 12.419059000 | 11.174964000 | 14.137090000 |
| H | 11.657909000 | 10.394699000 | 14.205542000 |
| H | 12.079870000 | 12.041046000 | 14.720963000 |
| H | 13.341152000 | 10.797784000 | 14.597712000 |
| C | 13.878444000 | 12.546198000 | 12.704141000 |
| H | 14.794223000 | 12.014329000 | 12.989157000 |
| H | 13.696092000 | 13.331917000 | 13.451620000 |
| H | 14.032980000 | 13.035000000 | 11.737972000 |
| C | 11.460861000 | 12.355762000 | 12.116722000 |
| H | 11.648209000 | 12.673199000 | 11.083712000 |
| H | 11.270335000 | 13.253196000 | 12.722780000 |
| H | 10.553859000 | 11.740451000 | 12.124794000 |
| C | 13.098836000 | 11.263489000 | 9.505776000 |
| C | 12.160696000 | 11.364220000 | 8.436324000 |
| H | 11.290448000 | 10.709281000 | 8.441866000 |
| C | 12.305669000 | 12.319454000 | 7.438536000 |
| H | 11.556094000 | 12.382324000 | 6.647020000 |
| C | 13.385119000 | 13.217637000 | 7.452505000 |
| H | 13.496040000 | 13.965244000 | 6.667313000 |
| C | 14.325511000 | 13.126645000 | 8.492173000 |
| H | 15.190772000 | 13.792507000 | 8.501366000 |
| C | 14.194090000 | 12.173762000 | 9.494359000 |
| H | 14.979029000 | 12.063678000 | 10.239975000 |
| C | 13.051312000 | 8.056710000 | 9.134242000 |
| C | 11.925396000 | 7.953388000 | 8.088877000 |
| H | 10.983585000 | 7.667730000 | 8.573436000 |
| H | 12.171672000 | 7.193278000 | 7.333778000 |
| H | 11.775338000 | 8.908956000 | 7.573588000 |
| C | 14.320930000 | 8.626138000 | 8.478598000 |
| H | 14.145680000 | 9.586555000 | 7.982967000 |
| H | 14.677470000 | 7.909885000 | 7.724585000 |
| H | 15.117532000 | 8.759940000 | 9.223545000 |
| C | 13.386960000 | 6.655194000 | 9.656520000 |
| H | 14.244336000 | 6.685149000 | 10.341198000 |
| H | 13.642846000 | 6.003742000 | 8.810133000 |
| H | 12.538967000 | 6.197571000 | 10.178248000 |

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|---|---|---|---|
| C | 9.491695000 | 8.683283000 | 12.685125000 |
| C | 9.261879000 | 9.278108000 | 11.286908000 |
| H | 9.989263000 | 10.068934000 | 11.061604000 |
| H | 8.253672000 | 9.710258000 | 11.215393000 |
| H | 9.359986000 | 8.506139000 | 10.512415000 |
| C | 9.194856000 | 9.738666000 | 13.766075000 |
| H | 9.421917000 | 9.333667000 | 14.762826000 |
| H | 8.130686000 | 10.014535000 | 13.743711000 |
| H | 9.779669000 | 10.652094000 | 13.622483000 |
| C | 8.499648000 | 7.528860000 | 12.910368000 |
| H | 8.600330000 | 6.744162000 | 12.153016000 |
| H | 7.474416000 | 7.922566000 | 12.863816000 |
| H | 8.641341000 | 7.073188000 | 13.901323000 |

**6**

BP86-D3(BJ)/def2-TZVPP

G = -3031.9120247 Hartree

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| Si | 3.709028000 | 9.381029000 | 4.948172000 |
| Si | 4.826325000 | 11.495067000 | 4.145750000 |
| N | 3.747646000 | 7.630632000 | 4.500678000 |
| N | 2.695185000 | 8.476651000 | 6.202869000 |
| N | 4.992974000 | 10.357907000 | 5.501235000 |
| N | 3.407137000 | 10.499701000 | 3.669991000 |
| N | 4.502269000 | 13.234142000 | 4.352640000 |
| C | 3.011570000 | 7.313685000 | 5.588454000 |
| C | 5.548137000 | 13.949447000 | 3.771766000 |
| C | 6.576039000 | 13.165227000 | 3.172315000 |
| C | 6.367981000 | 11.775162000 | 3.183330000 |
| C | 7.181053000 | 10.782949000 | 2.487711000 |
| C | 7.893277000 | 11.093181000 | 1.303454000 |
| H | 7.855443000 | 12.104843000 | 0.906273000 |
| C | 8.633457000 | 10.126709000 | 0.629468000 |
| H | 9.164303000 | 10.400285000 | -0.283285000 |
| C | 8.701021000 | 8.814582000 | 1.112150000 |
| H | 9.292118000 | 8.062577000 | 0.589191000 |
| C | 7.997189000 | 8.481413000 | 2.271583000 |
| H | 8.039734000 | 7.462266000 | 2.657443000 |
| C | 7.242229000 | 9.445277000 | 2.938713000 |
| H | 6.697134000 | 9.171802000 | 3.842637000 |
| C | 7.811287000 | 13.809407000 | 2.657406000 |
| C | 7.785236000 | 14.753013000 | 1.618007000 |

| | | | |
|---|---|---|---|
| H | 6.832199000 | 15.033412000 | 1.171082000 |
| C | 8.968898000 | 15.326290000 | 1.150491000 |
| H | 8.932220000 | 16.056194000 | 0.340904000 |
| C | 10.196056000 | 14.967330000 | 1.715667000 |
| H | 11.119866000 | 15.417638000 | 1.351207000 |
| C | 10.232714000 | 14.028114000 | 2.751058000 |
| H | 11.186126000 | 13.743393000 | 3.197805000 |
| C | 9.050098000 | 13.452483000 | 3.215358000 |
| H | 9.077002000 | 12.713025000 | 4.016907000 |
| C | 5.657757000 | 15.427392000 | 3.754116000 |
| C | 4.940393000 | 16.204031000 | 2.830565000 |
| H | 4.261421000 | 15.717690000 | 2.130213000 |
| C | 5.121412000 | 17.586848000 | 2.776161000 |
| H | 4.560510000 | 18.177420000 | 2.050981000 |
| C | 6.030818000 | 18.209554000 | 3.635816000 |
| H | 6.173569000 | 19.289555000 | 3.591741000 |
| C | 6.770210000 | 17.440098000 | 4.538928000 |
| H | 7.495090000 | 17.917372000 | 5.199066000 |
| C | 6.590383000 | 16.058060000 | 4.592978000 |
| H | 7.176692000 | 15.454210000 | 5.286050000 |
| C | 3.271500000 | 13.856089000 | 4.953212000 |
| C | 3.582042000 | 15.096963000 | 5.809969000 |
| H | 2.690261000 | 15.334319000 | 6.406500000 |
| H | 3.830839000 | 15.981195000 | 5.218967000 |
| H | 4.410980000 | 14.896590000 | 6.502486000 |
| C | 2.266553000 | 14.188503000 | 3.837955000 |
| H | 2.027102000 | 13.293434000 | 3.247589000 |
| H | 2.659812000 | 14.957473000 | 3.164725000 |
| H | 1.334365000 | 14.572529000 | 4.276279000 |
| C | 2.641755000 | 12.823739000 | 5.891167000 |
| H | 3.339754000 | 12.550268000 | 6.691301000 |
| H | 2.340270000 | 11.920071000 | 5.350548000 |
| H | 1.742591000 | 13.250065000 | 6.353233000 |
| C | 2.418916000 | 10.687293000 | 2.649276000 |
| C | 1.036993000 | 10.533675000 | 2.943695000 |
| C | 0.084883000 | 10.818639000 | 1.957059000 |
| H | -0.972381000 | 10.697409000 | 2.195634000 |
| C | 0.451110000 | 11.247513000 | 0.687306000 |
| H | -0.305805000 | 11.479176000 | -0.062098000 |
| C | 1.803403000 | 11.350808000 | 0.388515000 |
| H | 2.109575000 | 11.654662000 | -0.613154000 |
| C | 2.799031000 | 11.064447000 | 1.331868000 |
| C | 4.234999000 | 11.178935000 | 0.860954000 |
| H | 4.889494000 | 10.828263000 | 1.664359000 |

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|---|---|---|---|
| C | 4.595956000 | 12.641075000 | 0.554515000 |
| H | 4.012271000 | 13.011732000 | -0.300594000 |
| H | 5.661285000 | 12.733421000 | 0.304159000 |
| H | 4.388831000 | 13.293618000 | 1.412246000 |
| C | 4.528902000 | 10.286256000 | -0.356622000 |
| H | 4.237514000 | 9.244527000 | -0.171837000 |
| H | 5.605288000 | 10.306787000 | -0.577611000 |
| H | 3.992888000 | 10.631534000 | -1.252229000 |
| C | 0.513431000 | 9.983559000 | 4.255154000 |
| H | 1.338422000 | 9.958093000 | 4.980406000 |
| C | -0.585544000 | 10.851629000 | 4.885199000 |
| H | -0.242623000 | 11.885961000 | 5.020111000 |
| H | -0.879054000 | 10.453168000 | 5.867596000 |
| H | -1.489960000 | 10.876936000 | 4.262501000 |
| C | 0.033993000 | 8.537079000 | 4.037658000 |
| H | -0.769706000 | 8.509313000 | 3.289045000 |
| H | -0.356853000 | 8.096189000 | 4.964745000 |
| H | 0.850412000 | 7.902897000 | 3.662900000 |
| C | 2.106769000 | 8.674806000 | 7.567823000 |
| C | 3.028345000 | 8.068778000 | 8.638425000 |
| H | 4.036037000 | 8.497833000 | 8.596143000 |
| H | 3.106588000 | 6.980394000 | 8.525467000 |
| H | 2.614252000 | 8.273746000 | 9.634682000 |
| C | 0.711502000 | 8.042509000 | 7.684350000 |
| H | 0.744516000 | 6.949139000 | 7.648312000 |
| H | 0.044072000 | 8.409794000 | 6.896366000 |
| H | 0.279866000 | 8.331553000 | 8.652033000 |
| C | 1.960441000 | 10.184210000 | 7.768616000 |
| H | 1.624428000 | 10.386754000 | 8.793166000 |
| H | 1.216000000 | 10.602759000 | 7.080337000 |
| H | 2.908363000 | 10.705668000 | 7.611744000 |
| C | 2.697360000 | 5.945286000 | 6.040750000 |
| C | 1.416772000 | 5.398843000 | 5.875951000 |
| H | 0.630260000 | 5.992382000 | 5.412524000 |
| C | 1.170380000 | 4.085008000 | 6.273530000 |
| H | 0.178220000 | 3.656518000 | 6.131840000 |
| C | 2.190593000 | 3.320235000 | 6.848028000 |
| H | 1.992225000 | 2.295059000 | 7.160899000 |
| C | 3.464971000 | 3.868244000 | 7.019675000 |
| H | 4.261027000 | 3.276241000 | 7.471229000 |
| C | 3.724598000 | 5.176319000 | 6.608631000 |
| H | 4.716809000 | 5.608718000 | 6.738776000 |
| C | 4.177373000 | 6.789033000 | 3.344392000 |
| C | 5.532737000 | 6.150013000 | 3.679275000 |

| | | | |
|---|---|---|---|
| H | 6.260907000 | 6.914397000 | 3.975736000 |
| H | 5.926076000 | 5.623232000 | 2.799828000 |
| H | 5.432781000 | 5.424165000 | 4.496346000 |
| C | 3.144395000 | 5.703650000 | 3.009215000 |
| H | 3.098989000 | 4.911408000 | 3.763389000 |
| H | 3.430503000 | 5.241278000 | 2.055413000 |
| H | 2.141823000 | 6.135274000 | 2.884047000 |
| C | 4.299939000 | 7.730675000 | 2.141494000 |
| H | 3.327839000 | 8.175231000 | 1.889524000 |
| H | 4.658589000 | 7.162955000 | 1.273904000 |
| H | 5.017875000 | 8.538158000 | 2.325089000 |
| C | 6.053950000 | 10.254625000 | 6.540599000 |
| C | 5.573991000 | 10.898950000 | 7.850460000 |
| H | 5.293633000 | 11.947433000 | 7.679136000 |
| H | 6.377727000 | 10.881430000 | 8.599372000 |
| H | 4.711719000 | 10.374238000 | 8.274618000 |
| C | 6.387733000 | 8.772406000 | 6.761525000 |
| H | 5.491519000 | 8.202568000 | 7.046548000 |
| H | 7.126605000 | 8.656782000 | 7.565853000 |
| H | 6.806264000 | 8.326894000 | 5.849083000 |
| C | 7.322565000 | 11.003450000 | 6.101365000 |
| H | 7.755632000 | 10.585177000 | 5.186489000 |
| H | 8.072735000 | 10.933857000 | 6.900865000 |
| H | 7.113223000 | 12.068570000 | 5.928974000 |

**7**

BP86-D3(BJ)/def2-TZVPP

G = -3031.6378571 Hartree

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| Si | 3.688289000 | 9.368672000 | 4.953431000 |
| Si | 4.828765000 | 11.438836000 | 4.142767000 |
| N | 3.720533000 | 7.634971000 | 4.490986000 |
| N | 2.694883000 | 8.480013000 | 6.215273000 |
| N | 5.010945000 | 10.342448000 | 5.488201000 |
| N | 3.410650000 | 10.516002000 | 3.670497000 |
| N | 4.507394000 | 13.243716000 | 4.337193000 |
| C | 2.996203000 | 7.316453000 | 5.590704000 |
| C | 5.516177000 | 13.917518000 | 3.781563000 |
| C | 6.615638000 | 13.125225000 | 3.195908000 |
| C | 6.403128000 | 11.766527000 | 3.170049000 |

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|---|---|---|---|
| C | 7.217994000 | 10.774685000 | 2.474837000 |
| C | 7.971306000 | 11.111983000 | 1.325442000 |
| H | 7.971412000 | 12.135977000 | 0.959787000 |
| C | 8.701728000 | 10.145260000 | 0.643735000 |
| H | 9.263928000 | 10.424864000 | -0.247277000 |
| C | 8.725100000 | 8.822106000 | 1.101152000 |
| H | 9.316920000 | 8.071427000 | 0.577268000 |
| C | 7.981225000 | 8.468032000 | 2.230198000 |
| H | 7.993627000 | 7.438623000 | 2.587096000 |
| C | 7.221181000 | 9.427347000 | 2.894191000 |
| H | 6.639485000 | 9.144032000 | 3.771335000 |
| C | 7.842557000 | 13.805558000 | 2.717161000 |
| C | 7.821192000 | 14.748435000 | 1.675227000 |
| H | 6.877931000 | 15.010795000 | 1.197493000 |
| C | 9.007163000 | 15.339699000 | 1.240423000 |
| H | 8.982446000 | 16.062728000 | 0.424983000 |
| C | 10.222572000 | 15.009389000 | 1.848571000 |
| H | 11.146768000 | 15.479040000 | 1.511686000 |
| C | 10.250311000 | 14.076625000 | 2.890319000 |
| H | 11.195062000 | 13.819545000 | 3.369643000 |
| C | 9.068644000 | 13.472036000 | 3.317516000 |
| H | 9.088860000 | 12.736331000 | 4.122609000 |
| C | 5.611562000 | 15.383946000 | 3.681004000 |
| C | 4.799375000 | 16.106282000 | 2.790320000 |
| H | 4.065483000 | 15.587701000 | 2.175724000 |
| C | 4.976689000 | 17.482336000 | 2.649559000 |
| H | 4.356758000 | 18.035587000 | 1.944175000 |
| C | 5.945839000 | 18.146975000 | 3.406525000 |
| H | 6.073343000 | 19.224457000 | 3.302941000 |
| C | 6.764529000 | 17.427038000 | 4.283544000 |
| H | 7.528200000 | 17.940907000 | 4.866975000 |
| C | 6.621863000 | 16.046859000 | 4.400763000 |
| H | 7.278391000 | 15.482464000 | 5.062376000 |
| C | 3.282365000 | 13.853583000 | 5.005684000 |
| C | 3.610272000 | 15.126922000 | 5.799399000 |
| H | 2.744554000 | 15.352048000 | 6.436043000 |
| H | 3.792255000 | 16.001930000 | 5.171994000 |
| H | 4.477478000 | 14.975556000 | 6.456201000 |
| C | 2.212791000 | 14.103429000 | 3.932099000 |
| H | 2.006851000 | 13.195387000 | 3.349459000 |
| H | 2.507237000 | 14.905258000 | 3.247952000 |
| H | 1.280159000 | 14.410968000 | 4.423984000 |
| C | 2.757466000 | 12.816412000 | 5.999321000 |
| H | 3.513134000 | 12.567992000 | 6.753475000 |

| | | | |
|---|---|---|---|
| H | 2.432132000 | 11.902307000 | 5.491525000 |
| H | 1.885198000 | 13.230329000 | 6.518445000 |
| C | 2.420473000 | 10.718072000 | 2.644873000 |
| C | 1.044314000 | 10.538739000 | 2.935998000 |
| C | 0.095120000 | 10.818008000 | 1.944102000 |
| H | -0.961478000 | 10.675655000 | 2.172165000 |
| C | 0.463315000 | 11.268392000 | 0.682372000 |
| H | -0.292526000 | 11.488472000 | -0.071055000 |
| C | 1.814908000 | 11.413001000 | 0.394942000 |
| H | 2.119179000 | 11.739899000 | -0.599939000 |
| C | 2.807076000 | 11.135700000 | 1.344021000 |
| C | 4.245868000 | 11.300451000 | 0.900586000 |
| H | 4.894657000 | 10.979945000 | 1.725365000 |
| C | 4.572028000 | 12.764341000 | 0.571255000 |
| H | 4.014057000 | 13.096784000 | -0.314736000 |
| H | 5.642634000 | 12.888264000 | 0.357607000 |
| H | 4.299819000 | 13.434760000 | 1.397588000 |
| C | 4.606451000 | 10.389020000 | -0.285171000 |
| H | 4.366160000 | 9.340661000 | -0.072719000 |
| H | 5.681275000 | 10.459296000 | -0.502421000 |
| H | 4.059529000 | 10.683096000 | -1.191582000 |
| C | 0.523989000 | 9.987845000 | 4.247703000 |
| H | 1.354086000 | 9.947704000 | 4.969927000 |
| C | -0.553140000 | 10.875666000 | 4.888948000 |
| H | -0.189393000 | 11.901907000 | 5.032789000 |
| H | -0.855186000 | 10.474978000 | 5.867109000 |
| H | -1.456813000 | 10.926708000 | 4.267383000 |
| C | 0.019471000 | 8.550088000 | 4.034134000 |
| H | -0.796533000 | 8.534738000 | 3.299251000 |
| H | -0.365476000 | 8.116703000 | 4.966433000 |
| H | 0.818643000 | 7.901916000 | 3.646614000 |
| C | 2.106549000 | 8.674893000 | 7.588108000 |
| C | 3.026255000 | 8.051780000 | 8.648954000 |
| H | 4.037015000 | 8.474922000 | 8.614904000 |
| H | 3.097863000 | 6.964527000 | 8.524392000 |
| H | 2.612954000 | 8.246734000 | 9.647148000 |
| C | 0.706965000 | 8.053020000 | 7.697253000 |
| H | 0.732315000 | 6.959931000 | 7.661893000 |
| H | 0.042988000 | 8.425964000 | 6.908953000 |
| H | 0.274950000 | 8.343825000 | 8.663874000 |
| C | 1.971087000 | 10.183648000 | 7.796417000 |
| H | 1.631258000 | 10.381234000 | 8.820309000 |
| H | 1.229548000 | 10.610171000 | 7.109316000 |
| H | 2.923867000 | 10.700848000 | 7.652064000 |

| | | | |
|---|---|---|---|
| C | 2.681377000 | 5.949992000 | 6.038306000 |
| C | 1.392439000 | 5.414474000 | 5.897979000 |
| H | 0.598367000 | 6.014029000 | 5.456214000 |
| C | 1.148545000 | 4.098209000 | 6.288470000 |
| H | 0.151458000 | 3.676038000 | 6.164611000 |
| C | 2.176853000 | 3.323276000 | 6.834529000 |
| H | 1.978901000 | 2.297170000 | 7.144095000 |
| C | 3.458658000 | 3.861484000 | 6.982521000 |
| H | 4.259592000 | 3.261197000 | 7.413743000 |
| C | 3.719016000 | 5.169877000 | 6.573943000 |
| H | 4.717056000 | 5.593344000 | 6.687861000 |
| C | 4.126684000 | 6.790864000 | 3.322263000 |
| C | 5.481835000 | 6.141002000 | 3.633171000 |
| H | 6.222402000 | 6.895624000 | 3.926045000 |
| H | 5.856440000 | 5.614775000 | 2.745480000 |
| H | 5.389685000 | 5.410626000 | 4.446355000 |
| C | 3.080480000 | 5.715036000 | 3.000452000 |
| H | 3.041399000 | 4.921583000 | 3.752925000 |
| H | 3.349655000 | 5.252108000 | 2.042189000 |
| H | 2.078905000 | 6.152181000 | 2.889676000 |
| C | 4.233643000 | 7.738246000 | 2.122366000 |
| H | 3.259762000 | 8.187939000 | 1.886547000 |
| H | 4.573627000 | 7.172392000 | 1.246345000 |
| H | 4.958202000 | 8.542430000 | 2.297181000 |
| C | 6.079568000 | 10.200130000 | 6.526888000 |
| C | 5.619347000 | 10.831699000 | 7.847641000 |
| H | 5.387579000 | 11.896901000 | 7.709023000 |
| H | 6.417508000 | 10.758688000 | 8.598269000 |
| H | 4.734299000 | 10.333656000 | 8.254983000 |
| C | 6.379200000 | 8.707578000 | 6.717248000 |
| H | 5.475565000 | 8.156535000 | 7.013890000 |
| H | 7.127825000 | 8.563241000 | 7.506807000 |
| H | 6.771573000 | 8.262532000 | 5.793170000 |
| C | 7.353153000 | 10.932143000 | 6.082200000 |
| H | 7.780241000 | 10.509828000 | 5.166235000 |
| H | 8.109669000 | 10.856293000 | 6.873827000 |
| H | 7.155650000 | 12.002535000 | 5.921545000 |

**3a**

BP86-D3(BJ)/def2-TZVPP

G = -2520.75104 Hartree

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| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |

| | | | |
|---|---|---|---|
| H | 4.455754000 | 9.458449000 | -0.800681000 |
| Si | 3.009452000 | 5.025187000 | 6.445813000 |
| Si | 3.148975000 | 7.668218000 | 5.541827000 |
| N | 2.244928000 | 4.187261000 | 7.859105000 |
| N | 3.011768000 | 3.228555000 | 6.106740000 |
| N | 2.194149000 | 6.136589000 | 5.526233000 |
| N | 3.157568000 | 8.587380000 | 4.226871000 |
| N | 2.157609000 | 7.863069000 | 8.078636000 |
| C | 2.497577000 | 2.993141000 | 7.320524000 |
| C | 4.705023000 | 5.667313000 | 6.690747000 |
| C | 4.773985000 | 6.951280000 | 6.262517000 |
| C | 2.467043000 | 8.593642000 | 7.076846000 |
| C | 1.704938000 | 8.445141000 | 9.331627000 |
| C | 2.363718000 | 10.076903000 | 7.022389000 |
| C | 3.512784000 | 10.850985000 | 6.855660000 |
| H | 4.477795000 | 10.368090000 | 6.793863000 |
| C | 3.421601000 | 12.231825000 | 6.756276000 |
| H | 4.321201000 | 12.819821000 | 6.632862000 |
| C | 2.179185000 | 12.855978000 | 6.787731000 |
| H | 2.108026000 | 13.930827000 | 6.689661000 |
| C | 1.028534000 | 12.090425000 | 6.930672000 |
| H | 0.057414000 | 12.567394000 | 6.942661000 |
| C | 1.121468000 | 10.709810000 | 7.054534000 |
| H | 0.223810000 | 10.114612000 | 7.158098000 |
| C | 3.512746000 | 8.761814000 | 2.935353000 |
| C | 4.266357000 | 7.818367000 | 2.179902000 |
| C | 4.588765000 | 8.090058000 | 0.852489000 |
| H | 5.162267000 | 7.357419000 | 0.295528000 |
| C | 4.194899000 | 9.266664000 | 0.231528000 |
| C | 3.455777000 | 10.193803000 | 0.961076000 |
| H | 3.138118000 | 11.117235000 | 0.490110000 |
| C | 3.112178000 | 9.964745000 | 2.284616000 |
| C | 2.312096000 | 10.966222000 | 3.064652000 |
| C | 4.720538000 | 6.527601000 | 2.802896000 |
| H | 5.454980000 | 6.686154000 | 3.595482000 |
| C | 1.041262000 | 5.959229000 | 3.364253000 |
| H | 1.605629000 | 5.060683000 | 3.110179000 |
| H | 0.072472000 | 5.909285000 | 2.864225000 |
| H | 1.583319000 | 6.822397000 | 2.985501000 |
| C | 0.039392000 | 7.316357000 | 5.216058000 |
| H | 0.540262000 | 8.210906000 | 4.847226000 |
| H | -0.941583000 | 7.256592000 | 4.743015000 |
| H | -0.096421000 | 7.410392000 | 6.292821000 |

| | | | |
|---|---|---|---|
| C | 0.855341000 | 6.061511000 | 4.882175000 |
| C | 0.089947000 | 4.834295000 | 5.384732000 |
| H | -0.081284000 | 4.891349000 | 6.460141000 |
| H | -0.881801000 | 4.776710000 | 4.894592000 |
| H | 0.628243000 | 3.912497000 | 5.159374000 |
| C | 3.821228000 | 2.339397000 | 5.297893000 |
| C | 2.274076000 | 1.686669000 | 7.934476000 |
| C | 1.763030000 | 0.634783000 | 7.170060000 |
| H | 1.518907000 | 0.797517000 | 6.130097000 |
| C | 1.546904000 | -0.604118000 | 7.753725000 |
| H | 1.139511000 | -1.412777000 | 7.163380000 |
| C | 1.855292000 | -0.804921000 | 9.094979000 |
| H | 1.692741000 | -1.773900000 | 9.546401000 |
| C | 2.372295000 | 0.237358000 | 9.857108000 |
| H | 2.617918000 | 0.078679000 | 10.897756000 |
| C | 2.573899000 | 1.483256000 | 9.283435000 |
| H | 2.984409000 | 2.291492000 | 9.870473000 |
| C | 1.462086000 | 4.531076000 | 9.023434000 |
| C | 5.799110000 | 4.816865000 | 7.199937000 |
| C | 5.640172000 | 4.046488000 | 8.356565000 |
| H | 4.723850000 | 4.133315000 | 8.924785000 |
| C | 6.650328000 | 3.201965000 | 8.800058000 |
| H | 6.509792000 | 2.623183000 | 9.703671000 |
| C | 7.840393000 | 3.104962000 | 8.089705000 |
| H | 8.627910000 | 2.447338000 | 8.431525000 |
| C | 8.011109000 | 3.863313000 | 6.935091000 |
| H | 8.934292000 | 3.795314000 | 6.375119000 |
| C | 7.003185000 | 4.707671000 | 6.494521000 |
| H | 7.138369000 | 5.294345000 | 5.596752000 |
| C | 5.935997000 | 7.839564000 | 6.422323000 |
| C | 6.674149000 | 7.852006000 | 7.613781000 |
| H | 6.406835000 | 7.169705000 | 8.407596000 |
| C | 7.721702000 | 8.741790000 | 7.791901000 |
| H | 8.271326000 | 8.743865000 | 8.723912000 |
| C | 8.063413000 | 9.632315000 | 6.778329000 |
| H | 8.883376000 | 10.324345000 | 6.916369000 |
| C | 7.336567000 | 9.635219000 | 5.593868000 |
| H | 7.586141000 | 10.330474000 | 4.803708000 |
| C | 6.273433000 | 8.759303000 | 5.419329000 |
| H | 5.692239000 | 8.793942000 | 4.510522000 |
| H | 2.081363000 | 11.842327000 | 2.457553000 |
| H | 1.375742000 | 10.530646000 | 3.421066000 |
| H | 2.844826000 | 11.285873000 | 3.961196000 |
| H | 5.180407000 | 5.882960000 | 2.053259000 |

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| H | 3.891991000 | 5.982436000 | 3.257645000 |
| H | 0.980925000 | 5.487033000 | 8.833678000 |
| H | 0.710146000 | 3.769902000 | 9.227271000 |
| H | 2.094256000 | 4.649591000 | 9.905241000 |
| H | 4.741382000 | 2.851215000 | 5.019239000 |
| H | 3.293928000 | 2.058559000 | 4.385762000 |
| H | 4.083668000 | 1.438466000 | 5.848824000 |
| H | 1.848742000 | 9.524984000 | 9.409231000 |
| H | 0.641126000 | 8.229753000 | 9.467872000 |
| H | 2.235087000 | 7.954644000 | 10.150663000 |

**4**

BP86-D3(BJ)/def2-TZVPP

G = -2632.7810936 Hartree

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| P | 3.967520000 | 21.379477000 | 7.335942000 |
| Si | 4.746321000 | 21.173857000 | 5.329530000 |
| Si | 5.242157000 | 23.810926000 | 6.050005000 |
| N | 4.724235000 | 23.054165000 | 7.480630000 |
| N | 3.649537000 | 20.115811000 | 4.261242000 |
| N | 4.491149000 | 25.517622000 | 5.882856000 |
| N | 6.483189000 | 25.100961000 | 6.531211000 |
| N | 5.682504000 | 19.637878000 | 4.707663000 |
| C | 5.179993000 | 23.489779000 | 8.751499000 |
| C | 5.584726000 | 26.071761000 | 6.383793000 |
| C | 4.596456000 | 19.199565000 | 4.083594000 |
| C | 5.382297000 | 22.717673000 | 4.698444000 |
| C | 4.426119000 | 24.422586000 | 9.483138000 |
| C | 6.404513000 | 23.015990000 | 9.265806000 |
| C | 6.027218000 | 22.996894000 | 3.352826000 |
| C | 2.390062000 | 20.264048000 | 3.580574000 |
| C | 3.212167000 | 26.120370000 | 5.619626000 |
| C | 5.306017000 | 22.258541000 | 2.203592000 |
| H | 5.316097000 | 21.186158000 | 2.402955000 |
| H | 4.259379000 | 22.572435000 | 2.185686000 |
| C | 5.759120000 | 27.476290000 | 6.776264000 |
| C | 6.866106000 | 23.508300000 | 10.482958000 |
| H | 7.809735000 | 23.146659000 | 10.872593000 |
| C | 7.839943000 | 25.213894000 | 7.004250000 |
| C | 6.827352000 | 18.873363000 | 5.132721000 |
| C | 6.138839000 | 24.454152000 | 11.195720000 |

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|---|---|---|---|
| H | 6.510309000 | 24.827675000 | 12.140964000 |
| C | 3.387196000 | 17.091440000 | 3.548394000 |
| H | 2.650029000 | 17.347444000 | 4.296423000 |
| C | 4.925094000 | 24.899934000 | 10.696443000 |
| H | 4.340786000 | 25.618112000 | 11.259104000 |
| C | 7.206261000 | 22.008544000 | 8.495668000 |
| H | 7.446675000 | 22.367638000 | 7.492742000 |
| C | 7.505956000 | 22.538637000 | 3.346994000 |
| H | 7.543242000 | 21.473397000 | 3.583827000 |
| H | 8.036116000 | 23.058494000 | 4.149145000 |
| C | 3.092638000 | 24.906599000 | 8.982252000 |
| H | 2.647023000 | 24.180001000 | 8.307242000 |
| C | 5.429253000 | 17.610927000 | 2.371783000 |
| H | 6.259864000 | 18.280351000 | 2.196408000 |
| C | 8.179910000 | 22.810676000 | 1.995739000 |
| H | 9.219396000 | 22.473123000 | 2.029494000 |
| C | 6.677488000 | 24.787895000 | 1.660048000 |
| H | 6.645857000 | 25.862202000 | 1.457816000 |
| C | 5.931218000 | 24.034220000 | 0.551606000 |
| H | 6.389667000 | 24.241021000 | -0.419596000 |
| H | 4.894356000 | 24.377423000 | 0.498334000 |
| C | 3.275489000 | 15.910901000 | 2.827527000 |
| H | 2.442620000 | 15.246178000 | 3.011019000 |
| C | 4.231632000 | 15.584048000 | 1.872162000 |
| H | 4.139820000 | 14.666197000 | 1.307647000 |
| C | 6.227365000 | 29.092797000 | 8.497159000 |
| H | 6.469972000 | 29.320652000 | 9.525866000 |
| C | 5.732756000 | 29.826700000 | 6.255172000 |
| H | 5.600766000 | 30.625192000 | 5.538176000 |
| C | 6.055989000 | 30.120182000 | 7.575340000 |
| H | 6.172099000 | 31.149490000 | 7.886143000 |
| C | 4.467449000 | 17.946641000 | 3.326028000 |
| C | 6.008862000 | 24.503208000 | 3.010967000 |
| H | 4.973045000 | 24.852117000 | 3.001972000 |
| H | 6.529872000 | 25.056674000 | 3.797032000 |
| C | 5.969794000 | 22.529653000 | 0.847710000 |
| H | 5.431768000 | 21.988119000 | 0.064871000 |
| C | 8.137443000 | 24.316513000 | 1.702039000 |
| H | 8.684575000 | 24.862414000 | 2.475802000 |
| H | 8.629088000 | 24.530251000 | 0.748759000 |
| C | 7.428650000 | 22.054918000 | 0.891309000 |
| H | 7.464922000 | 20.978832000 | 1.085279000 |
| C | 6.087809000 | 27.770362000 | 8.100947000 |
| H | 6.206238000 | 26.966092000 | 8.814636000 |

| | | | |
|---|---|---|---|
| C | 5.574419000 | 28.506677000 | 5.855457000 |
| H | 5.321515000 | 28.271306000 | 4.830843000 |
| C | 5.306222000 | 16.436400000 | 1.643164000 |
| H | 6.048497000 | 16.185810000 | 0.897871000 |
| H | 7.909242000 | 22.223474000 | -0.076541000 |
| H | 2.412350000 | 25.081632000 | 9.815929000 |
| H | 3.187754000 | 25.850899000 | 8.441078000 |
| H | 8.136537000 | 21.773485000 | 9.011659000 |
| H | 6.625658000 | 21.095852000 | 8.349247000 |
| H | 8.219371000 | 26.224161000 | 6.854722000 |
| H | 8.468662000 | 24.522016000 | 6.445226000 |
| H | 7.912753000 | 24.961464000 | 8.063269000 |
| H | 3.117355000 | 27.084999000 | 6.117796000 |
| H | 3.064018000 | 26.266421000 | 4.547040000 |
| H | 2.423640000 | 25.462768000 | 5.982389000 |
| H | 6.748249000 | 17.829629000 | 4.830002000 |
| H | 7.744866000 | 19.288867000 | 4.711538000 |
| H | 6.906844000 | 18.915780000 | 6.220966000 |
| H | 1.565356000 | 20.202582000 | 4.292275000 |
| H | 2.259226000 | 19.497060000 | 2.818326000 |
| H | 2.344952000 | 21.242356000 | 3.099841000 |

**4-NMe**

BP86-D3(BJ)/def2-TZVPP

G = -2362.2635805 Hartree

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| P | 4.188470000 | 21.054522000 | 7.486009000 |
| Si | 4.738525000 | 21.078303000 | 5.397908000 |
| Si | 5.037837000 | 23.696792000 | 6.283744000 |
| N | 4.361850000 | 22.866895000 | 7.580864000 |
| N | 3.722441000 | 20.056684000 | 4.176638000 |
| N | 4.389701000 | 25.435048000 | 6.220669000 |
| N | 6.387263000 | 24.916184000 | 6.766298000 |
| N | 5.703434000 | 19.589140000 | 4.816921000 |
| C | 3.960872000 | 23.462454000 | 8.837503000 |
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| C | 5.244199000 | 22.702997000 | 4.857180000 |
| C | 5.882877000 | 23.078696000 | 3.529514000 |
| C | 2.510905000 | 20.187657000 | 3.412717000 |
| C | 3.119928000 | 26.100448000 | 6.091679000 |

| | | | |
|---|---|---|---|
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| H | 5.038367000 | 21.413386000 | 2.431868000 |
| H | 4.066735000 | 22.873333000 | 2.379415000 |
| C | 5.922641000 | 27.365936000 | 6.624131000 |
| C | 7.823297000 | 24.922788000 | 6.885105000 |
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| H | 2.696359000 | 17.338181000 | 3.913921000 |
| C | 7.331027000 | 22.537695000 | 3.432418000 |
| H | 7.310048000 | 21.454160000 | 3.565860000 |
| H | 7.913986000 | 22.944362000 | 4.262240000 |
| C | 5.757092000 | 17.590699000 | 2.473973000 |
| H | 6.618516000 | 18.243402000 | 2.456098000 |
| C | 7.986231000 | 22.898949000 | 2.092859000 |
| H | 9.004128000 | 22.500386000 | 2.063737000 |
| C | 6.598195000 | 24.981945000 | 1.987775000 |
| H | 6.626750000 | 26.070992000 | 1.889907000 |
| C | 5.781809000 | 24.382739000 | 0.836139000 |
| H | 6.228607000 | 24.654147000 | -0.124583000 |
| H | 4.766477000 | 24.788849000 | 0.845935000 |
| C | 3.526724000 | 15.929953000 | 2.523549000 |
| H | 2.663236000 | 15.279579000 | 2.550669000 |
| C | 4.618838000 | 15.606070000 | 1.725879000 |
| H | 4.603404000 | 14.705717000 | 1.127039000 |
| C | 6.964541000 | 29.214150000 | 7.770291000 |
| H | 7.503634000 | 29.600896000 | 8.624039000 |
| C | 5.910612000 | 29.564104000 | 5.631979000 |
| H | 5.639238000 | 30.220746000 | 4.816945000 |
| C | 6.607815000 | 30.062843000 | 6.727511000 |
| H | 6.873727000 | 31.110200000 | 6.767961000 |
| C | 4.658629000 | 17.925488000 | 3.270231000 |
| C | 5.948562000 | 24.608597000 | 3.326136000 |
| H | 4.936065000 | 25.017198000 | 3.382823000 |
| H | 6.525207000 | 25.056275000 | 4.138274000 |
| C | 5.736812000 | 22.857572000 | 0.990365000 |
| H | 5.147564000 | 22.424075000 | 0.177668000 |
| C | 8.027953000 | 24.425659000 | 1.942479000 |
| H | 8.624829000 | 24.863342000 | 2.747775000 |
| H | 8.508956000 | 24.700679000 | 0.999517000 |
| C | 7.164717000 | 22.296894000 | 0.945018000 |
| H | 7.139717000 | 21.207102000 | 1.035736000 |
| C | 6.632896000 | 27.868385000 | 7.716904000 |
| H | 6.907447000 | 27.206081000 | 8.525721000 |
| C | 5.560704000 | 28.222959000 | 5.581711000 |

| | | | |
|---|---|---|---|
| H | 5.026474000 | 27.829221000 | 4.728728000 |
| C | 5.731976000 | 16.440376000 | 1.699972000 |
| H | 6.580981000 | 16.192809000 | 1.077677000 |
| H | 7.631277000 | 22.529244000 | -0.016562000 |
| H | 8.253156000 | 25.853471000 | 6.514374000 |
| H | 8.226532000 | 24.095678000 | 6.301088000 |
| H | 8.136670000 | 24.783185000 | 7.921851000 |
| H | 3.140463000 | 27.086172000 | 6.555494000 |
| H | 2.837198000 | 26.215772000 | 5.042404000 |
| H | 2.352061000 | 25.500636000 | 6.580157000 |
| H | 6.678757000 | 17.761224000 | 5.169903000 |
| H | 7.753826000 | 19.147830000 | 4.924559000 |
| H | 6.845020000 | 18.997791000 | 6.433845000 |
| H | 1.644337000 | 19.861922000 | 3.992183000 |
| H | 2.553577000 | 19.608398000 | 2.490230000 |
| H | 2.366569000 | 21.237275000 | 3.157686000 |
| H | 4.570405000 | 23.098871000 | 9.673164000 |
| H | 4.061578000 | 24.550551000 | 8.802932000 |
| H | 2.916234000 | 23.227263000 | 9.069666000 |

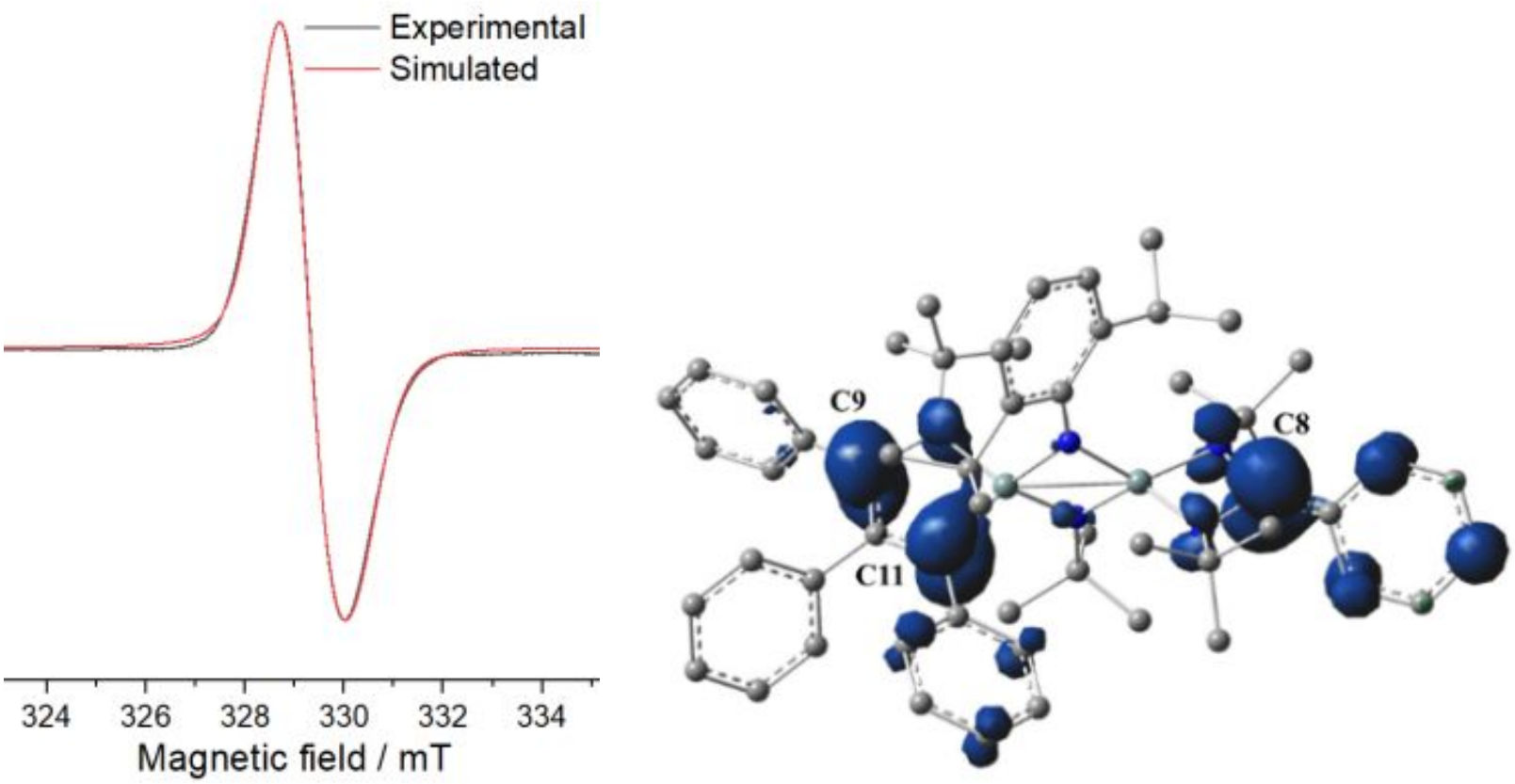


**Fig. S13.** Red and black lines (left) represent the simulated (red) and the experimental (black)) X-band EPR spectra at rt of the **2a** (triplet diradical) using the EasySpin program. **2a:** [$g_{\perp}$ = 2.00487, $g_{\parallel}$ = 1.99749, LWPP (Gaussian broadening) = 0.884889 mT, LWPP (Lorentzian broadening) = 0.255459 mT, A($^{14}$N) = 2.19651 MHz, A($^{29}$Si) = 0.717497 MHz, A($^{13}$C) = 14.8933 MHz, frequency = 9.232014 GHz]. Isodensity values at 0.03.

## Multiconfigurational investigation of $Si_2$-diradical system “230302_ly_wcf0301_1_0m_a_sq”

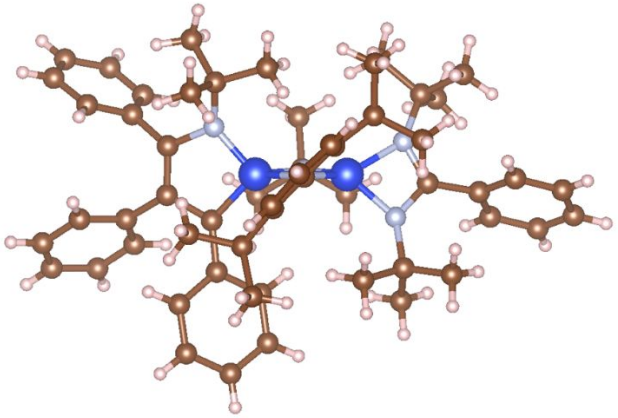

**Figure S14**. Structure of the full molecule **2a**.

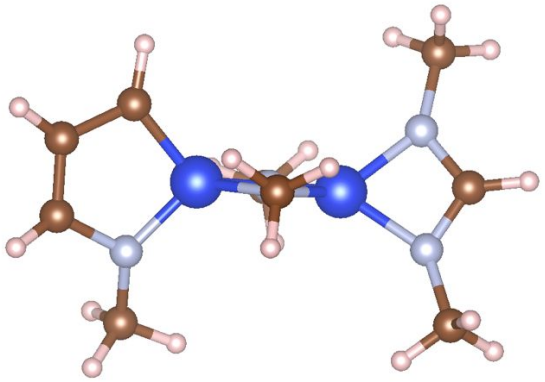

**Figure S15**. Structure of the reduced molecule **2a**.

**Computational details**

Ab initio calculations for the mentioned $Si_2$-diradical system (**2a**) were performed with ORCA 6.0.1 quantum chemistry package.[15] Two structural models were employed: the full molecule (Figure S14) and the reduced one (Figure S15), where *tert*-butyl and *phenyl*- groups were replaced by methyl and hydrogen atoms, respectively.

All atoms were described by the def2-SVP and def2-TZVP basis sets. [16] All calculations were sped up by the resolution of identity (RI) methods, where all auxiliary density fitting basis sets were generated on the fly using the "AutoAux" generation procedure, [17] as implemented in ORCA. [18] An approximate second-order convergence method accelerated all DFT and CASSCF calculations. [19]

Broken-symmetry DFT procedure was employed to find the magnetic exchange between the two radicals. [20] In this case, this method did not provide reasonable results. Similar untrustworthy results were obtained for the correct-spin DFT calculations, which is a true indicator of the multiconfigurational character of the ground state for this di-radical system.

Complete Active Space Self-Consistent Field calculations were performed to accurately estimate the singlet-triplet gap in the investigated system. Various sizes of active space were employed. [21] The n-electron valence second-order perturbation theory (NEVPT2) accounted for the dynamical electron correlation, as implemented in the ORCA package. [22]

## DFT calculations for the ground spin state

**Table S6**: DFT Energy gaps between the ground spin S=0 and the first excited state S=1, in different computational approximations (in $cm^{-1}$).

**Reduced Structure, SVP basis**

| DFT functional | Total energy (a.u.) | | ΔE (a.u.) | ΔE ($cm^{-1}$) |
|---|---|---|---|---|
| | S=0 | S=1 | | |
| **B3LYP** | -1206.256772883 | -1206.235925168 | 0.020847716 | 4575.5 |
| **M062X** | -1206.427552562 | -1206.408896386 | 0.018656176 | 4094.6 |
| **PBE** | -1205.680272978 | -1205.646542319 | 0.033730658 | 7403.0 |
| **TPSS** | -1206.936340233 | -1206.906030695 | 0.030309538 | 6652.2 |

**Reduced Structure, TZVP basis**

| DFT functional | Total energy (a.u.) | | ΔE (a.u.) | ΔE ($cm^{-1}$) |
|---|---|---|---|---|
| | S=0 | S=1 | | |
| **B3LYP** | -1206.973693261 | -1206.952402569 | 0.021290692 | 4672.8 |
| **M062X** | -1207.126386760 | -1207.106824591 | 0.019562169 | 4293.4 |
| **PBE** | -1206.347671062 | -1206.314498087 | 0.033172975 | 7280.6 |
| **TPSS** | -1207.597914962 | -1207.567895267 | 0.030019695 | 6588.6 |

**Full Structure, SVP basis**

| DFT functional | Total energy (a.u.) | | ΔE (a.u.) | ΔE ($cm^{-1}$) [kcal/mol] |
|---|---|---|---|---|
| | S=0 | S=1 | | |
| **B3LYP** | -3026.363217202 | -3026.331742197 | 0.031475005 | 6908.0 [19.75] |
| **M062X** | -3027.021904206 | -3026.986527994 | 0.035376213 | 7764.2 [22.20] |
| **PBE** | -3024.526486448 | -3024.490446881 | 0.036039567 | 7909.8 [22.62] |
| **TPSS** | -3028.616995586 | -3028.582264133 | 0.034731454 | 7622.7 [21.79] |

**Full Structure, TZVP basis**

| DFT functional | Total energy (a.u.) | | ΔE (a.u.) | ΔE ($cm^{-1}$) [kcal/mol] |
|---|---|---|---|---|
| | S=0 | S=1 | | |
| **B3LYP** | -3029.168204372 | -3029.135557695 | 0.032646677 | 7165.1 [20.49] |
| **M062X** | -3029.835511738 | -3029.798669503 | 0.036842235 | 8085.9 [23.12] |
| **PBE** | -3027.228057327 | -3027.191714481 | 0.036342847 | 7976.3 [22.81] |
| **TPSS** | -3031.285514786 | -3031.250395239 | 0.035119547 | 7707.9 [22.04] |

In all calculations, the ground state is a spin singlet S=0.

In all calculations for S=0, the expectation value of $\langle S^2 \rangle$ is exactly zero.

In all calculations for S=1, the expectation value of $\langle S^2 \rangle$ is very close to two, with a deviation from the ideal value (2.0) varying between a maximal value of 0.034530 for the *full-M062X-TZVP* case and a minimum value of 0.010932 for the *reduced-PBE-SVP* case.

## Broken-Symmetry DFT calculations of magnetic exchange

**Table S7**: Broken Symmetry DFT results (in $cm^{-1}$).

**Reduced Structure, SVP basis**

| | Energy HS | $\langle S^2 \rangle$ for HS | Energy BS | $\langle S^2 \rangle$ for BS | J(1) | J(2) | J(3) |
|---|---|---|---|---|---|---|---|
| **B3LYP** | -1206.235925 | 2.0245 | -1206.259520 | 0.3736 | -5178.0 | -2589.0 | -3136.6 |
| **M062X** | -1206.376967 | 2.0271 | -1206.395448 | 0.0491 | -4055.9 | -2027.9 | -2050.6 |
| **PBE** | -1205.611737 | 2.0109 | -1205.646174 | 0.2390 | -7557.4 | -3778.7 | -4265.1 |
| **TPSS** | -1206.874731 | 2.0180 | -1206.906460 | 0.3056 | -6963.0 | -3481.5 | -4066.3 |

**Reduced Structure, TZVP basis**

| | Energy HS | $\langle S^2 \rangle$ for HS | Energy BS | $\langle S^2 \rangle$ for BS | J(1) | J(2) | J(3) |
|---|---|---|---|---|---|---|---|
| **B3LYP** | -1206.928422 | 2.0241 | -1206.951877 | 0.3489 | -5147.4 | -2573.7 | -3072.7 |
| **M062X** | -1207.084949 | 2.0267 | -1207.104385 | 0.0000 | -4265.4 | -2132.7 | -2104.6 |
| **PBE** | -1206.290370 | 2.0112 | -1206.324072 | 0.2188 | -7395.9 | -3698.0 | -4126.4 |
| **TPSS** | -1207.546083 | 2.0184 | -1207.577262 | 0.2865 | -6842.5 | -3421.2 | -3950.9 |

**Full Structure, SVP basis**

| | Energy HS | $\langle S^2 \rangle$ for HS | Energy BS | $\langle S^2 \rangle$ for BS | J(1) | J(2) | J(3) |
|---|---|---|---|---|---|---|---|
| **B3LYP** | -3026.331742 | 2.0303 | -3026.363217 | 0.0000 | -6907.3 | -3453.7 | -3402.1 |
| **M062X** | -3026.952648 | 2.0319 | -3026.988137 | 0.0000 | -7788.2 | -3894.1 | -3832.9 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **PBE** | -3024.454198 | 2.0112 | -3024.490256 | 0.0159 | -7913.0 | -3956.5 | -3965.8 |
| **TPSS** | -3028.549617 | 2.0185 | -3028.584397 | 0.0722 | -7632.8 | -3816.4 | -3921.6 |

**Full Structure, TZVP basis**

| | Energy HS | $\langle S^2 \rangle$ for HS | Energy BS | $\langle S^2 \rangle$ for BS | J(1) | J(2) | J(3) |
|---|---|---|---|---|---|---|---|
| **B3LYP** | -3029.112200 | 2.0299 | -3029.144815 | 0.0000 | -7157.6 | -3578.8 | -3526.1 |
| **M062X** | -3029.777370 | 2.0339 | -3029.814212 | 0.0000 | -8085.2 | -4042.6 | -3975.2 |
| **PBE** | -3027.168173 | 2.0114 | -3027.204502 | 0.0000 | -7972.5 | -3986.3 | -3963.6 |
| **TPSS** | -3031.229131 | 2.0189 | -3031.264234 | 0.0364 | -7703.6 | -3851.8 | -3885.8 |

## CASSCF/NEVPT2 calculations

**Table S8**: CASSCF Energy gaps between the ground spin S=0 and the first excited state S=1, in different computational approximations (in $cm^{-1}$)

| Size of the active space | SVP basis | | TZVP basis | |
|---|---|---|---|---|
| | Reduced structure | Full structure | Reduced structure | Full structure |
| 2 el in 2 orbs | 171.6 | 144.0 | 186.1 | 157.2 |
| 4 el in 4 orbs | 129.8 | 113.1 | 141.2 | 124.1 |
| 6 el in 6 orbs | 131.6 | 114.3 | 143.1 | 124.1 |
| 8 el in 8 orbs | 134.9 | 114.7 | 173.8 | 125.8 |
| 10 el in 10 orbs | 139.8 | 110.4 | 188.9 | 124.0 |
| 12 el in 12 orbs | 161.4 | 110.7 | 227.3 | 125.0 |
| 14 el in 14 orbs | 197.4 | 120.8 | 215.4 | 125.2 |

**Table S9**: NEVPT2 Energy gaps between the ground spin S=0 and the first excited state S=1, in different computational approximations (in $cm^{-1}$)

| Size of the active space | SVP basis | | TZVP basis | |
|---|---|---|---|---|
| | Reduced structure | Full structure | Reduced structure | Full structure |
| 2 el in 2 orbs | 364.5 | 359.9 | 394.6 | |
| 4 el in 4 orbs | 279.2 | 283.2 | 301.2 | |
| 6 el in 6 orbs | 273.7 | 284.7 | 291.3 | |
| 8 el in 8 orbs | 281.8 | 285.7 | 360.4 | |
| 10 el in 10 orbs | 293.5 | 277.8 | 380.2 | |
| 12 el in 12 orbs | 307.3 | 277.6 | 504.5 | |

| | | | |
|---|---|---|---|
| 14 el in 14 orbs | 403.8 | 295.2 | 479.1 |

NEVPT2 calculations on the full molecular structure using a large basis set is not possible, the calculation requires too much memory.

These data can be used in a simple Heisenberg Hamiltonian, $\hat{H}_{exch} = -J\hat{s}_1\hat{s}_2$, with

$\hat{s}_1 = \hat{s}_2 = \frac{1}{2}$. This model provides the parameter of the magnetic exchange parameter as a function of the energy gap between S=0 and S=1 states.

$$E(S=1) = -\frac{J}{4}$$

$$E(S=0) = +\frac{3J}{4}$$

Considering that the state $S = 0$ is ground state, the energy of the state $S = 1$ is:

$$\Delta E_{ST} = -\frac{J}{4} - \frac{3J}{4} = -J$$

Or:

$$J = -\Delta E_{ST}$$

As we can infer from the above tables, the magnetic exchange parameter is predicted to be antiferro, ranging in the domain (-110.4 -215.4) $cm^{-1}$ for the CASSCF-only results, and (-273.7 -504.5) $cm^{-1}$ for NEVPT2 results. [1 kcal/mol = 349.7600 $cm^{-1}$].

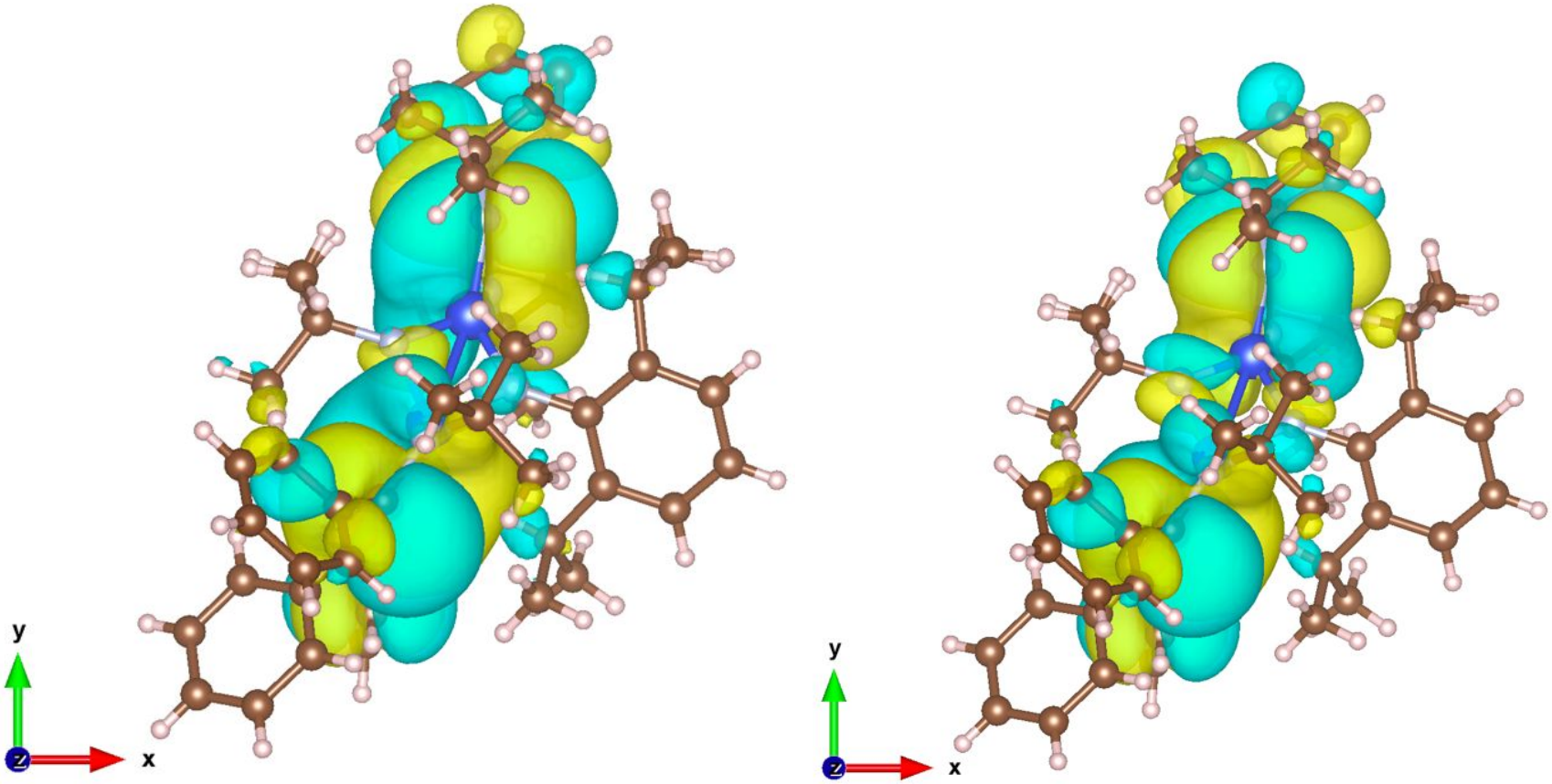


**Figure S16**. Singly occupied molecular orbitals, using the outcome of the TZVP basis, S=1, full structure, CAS (14 el in 14 orbs). Orbitals #235 and #236.

**Table S10**: Calculation of the diradicaloid character following the formula proposed by Neese et. al. [18] using formula:

$$d = 200\sqrt{\frac{c_0^2 c_d^2}{c_0^2 + c_d^2}}$$

***Full structure results, CASSCF SVP basis***

| Size of the active space | As extracted from ORCA output | | Re-normalized coefficients | | $d$ computed with original coeffs | $d$ computed with re-normalized coeffs |
|---|---|---|---|---|---|---|
| | $c_0^2$ | $c_d^2$ | $c_0^2$ | $c_d^2$ | in % | in % |
| 2 el in 2 orbs | 0.55759 | 0.44241 | 0.557590 | 0.442410 | 99.33 | 99.33 |
| 4 el in 4 orbs | 0.51119 | 0.41776 | 0.550288 | 0.449712 | 95.89 | 99.49 |
| 6 el in 6 orbs | 0.50121 | 0.40876 | 0.550798 | 0.449202 | 94.90 | 99.48 |
| 8 el in 8 orbs | 0.47836 | 0.38988 | 0.550954 | 0.449046 | 92.69 | 99.48 |
| 10 el in 10 orbs | 0.46525 | 0.37744 | 0.552101 | 0.447899 | 91.30 | 99.46 |
| 12 el in 12 orbs | 0.44412 | 0.36009 | 0.552244 | 0.447756 | 89.19 | 99.45 |
| 14 el in 14 orbs | 0.44365 | 0.35846 | 0.553104 | 0.446896 | 89.05 | 99.43 |

***Full structure results, CASSCF TZVP basis***

| Size of the active space | As extracted from ORCA output | | Re-normalized coefficients | | $d$ computed with original coeffs | $d$ computed with re-normalized coeffs |
|---|---|---|---|---|---|---|
| | $c_0^2$ | $c_d^2$ | $c_0^2$ | $c_d^2$ | | |
| 2 el in 2 orbs | 0.56023 | 0.43977 | 0.560230 | 0.439770 | 99.27 | 99.27 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 4 el in 4 orbs | 0.51402 | 0.41607 | 0.552656 | 0.447344 | 95.90 | 99.44 |
| 6 el in 6 orbs | 0.50338 | 0.40739 | 0.552697 | 0.447303 | 94.90 | 99.44 |
| 8 el in 8 orbs | 0.48157 | 0.38872 | 0.553344 | 0.446656 | 92.76 | 99.43 |
| 10 el in 10 orbs | 0.47033 | 0.37665 | 0.555302 | 0.444698 | 91.47 | 99.39 |
| 12 el in 12 orbs | 0.46114 | 0.36863 | 0.555744 | 0.444256 | 90.52 | 99.38 |
| 14 el in 14 orbs | 0.45164 | 0.36090 | 0.555837 | 0.444163 | 89.58 | 99.37 |

**IV. ORTEP Pictures**

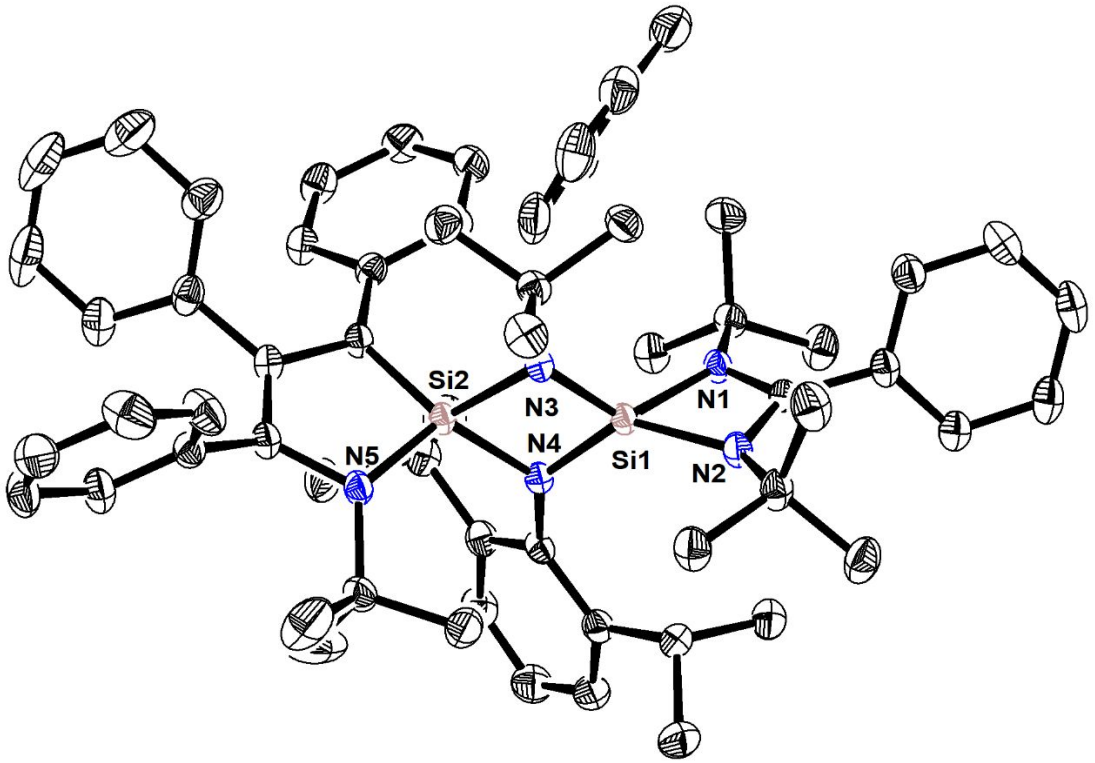


**Figure S17**. ORTEP drawing of complex (**2a**) with thermal ellipsoid shown at 50% probability level. Important bond lengths include, N1-Si1: 1.803, N2-Si1: 1.849, N3-Si1: 1.677, N4-Si1: 1.711, N3-Si2: 1.749, N4-Si2: 1.841, Si2-N5: 1.750, and important bond angles include, C1-N1-Si1: 91.07, N1-Si1-N2: 72.46, Si1-N2-C1: 89.47, Si1-N3-Si2: 94.76, N3-Si2-N4: 82.81, Si2-N4-Si1: 91.91, N4-Si1-N3: 90.42, N5-Si2-C4: 95.72 (Bond lengths are in Å and bond angles are in °).

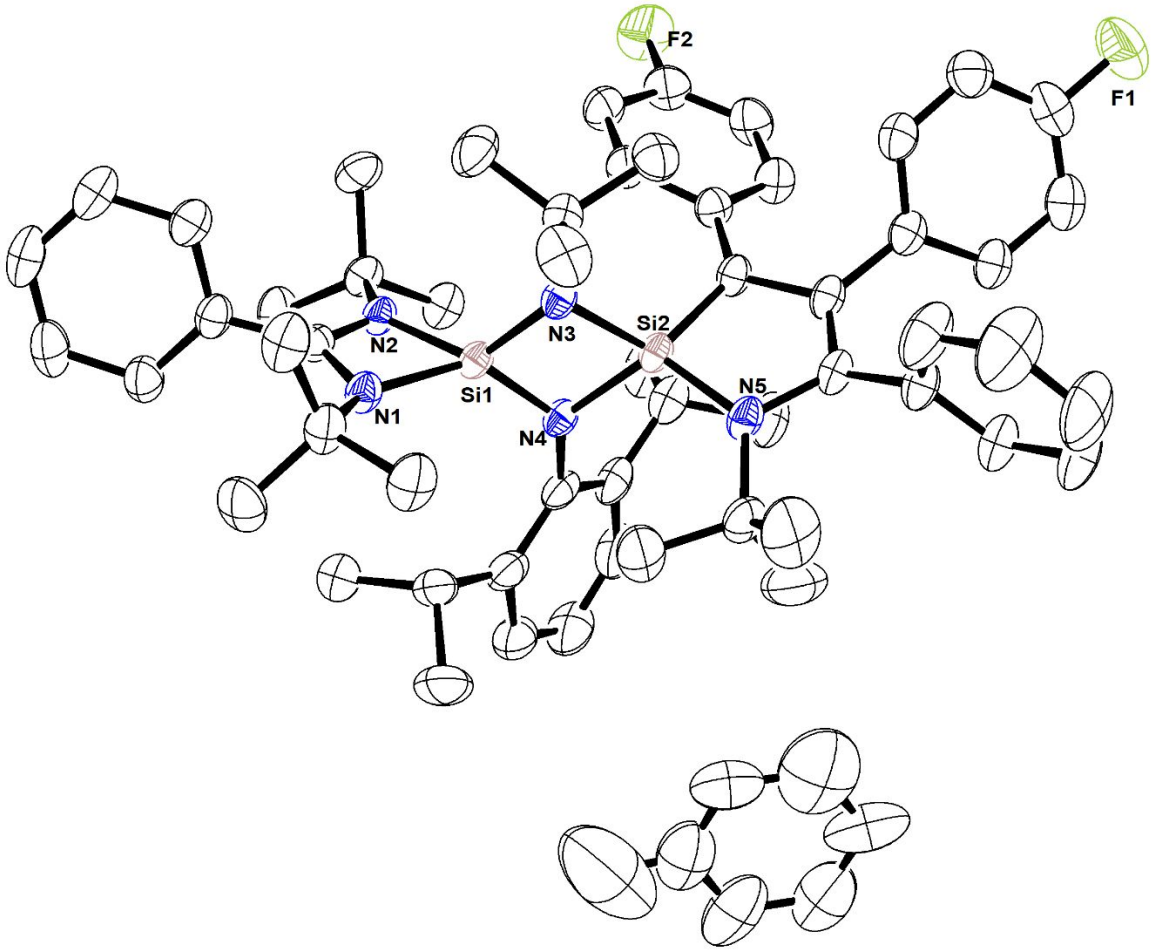


**Figure S18**. ORTEP drawing of complex (**2b**) with thermal ellipsoid shown at 50% probability level. Important bond lengths include, N1-Si1: 1.853, N2-Si1: 1.799, N3-Si1: 1.674, N4-Si1: 1.704, N3-Si2: 1.796, N4-Si2: 1.840, Si2-N5: 1.745, and important bond angles include, C1-N1-

Si1: 89.11, N1-Si1-N2: 72.30, Si1-N2-C1: 91.37, Si1-N3-Si2: 94.69, N3-Si2-N4: 82.62, Si2-N4-Si1: 92.08, N4-Si1-N3: 90.53, N5-Si2-C4: 95.18 (Bond lengths are in Å and bond angles are in °).

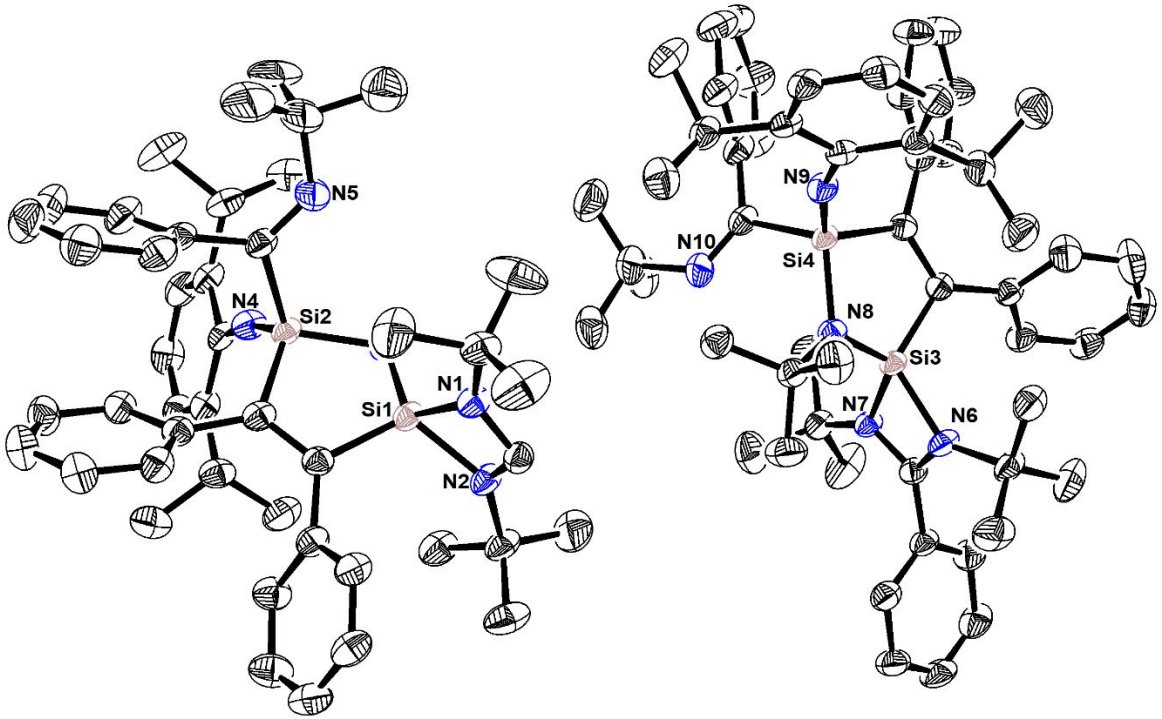


**Figure S19**. ORTEP drawing of complex (**3a**) with thermal ellipsoid shown at 50% probability level. Important bond lengths include, N1-C1: 1.343, C1-N2: 1.346, N2-Si1: 1.812, Si1-N1: 1.817: Si1-C2: 1.836, C2-C3: 1.368, C3-Si2: 1.927, Si2-N3: 1.815, N3-Si1: 1.672, C109-N6: 1.348, N6-Si3: 1.810, Si3-N7: 1.827, N7-C109: 1.338, Si3-C110: 1.832, C110-C111: 1.374, C111-Si4: 1.926, Si4-N8: 1.802, N8-Si3: 1.681 and important bond angles include, N1-C1-N2: 105.42, C1-N2-Si1: 91.15, N2-Si1-N1: 72.22, Si1-N1-C1: 91.05, Si1-N3-Si2: 109.59, N3-Si2-C3: 97.20, Si2-C3-C2: 115.32, C3-C2-Si1: 110.52, C2-Si1-N3: 105.68, C109-N7-Si3: 90.55, N7-Si3-N6: 72.35, Si3-N6-C109: 90.94, N6-C109-N7: 106.13,

C111-C110-Si3: 109.84, C110-Si3-N8: 105.87, Si3-N8-Si4: 109.29, N8-Si4-C111: 97.41, Si4-C111-C110: 115.52 (Bond lengths are in Å and bond angles are in °).

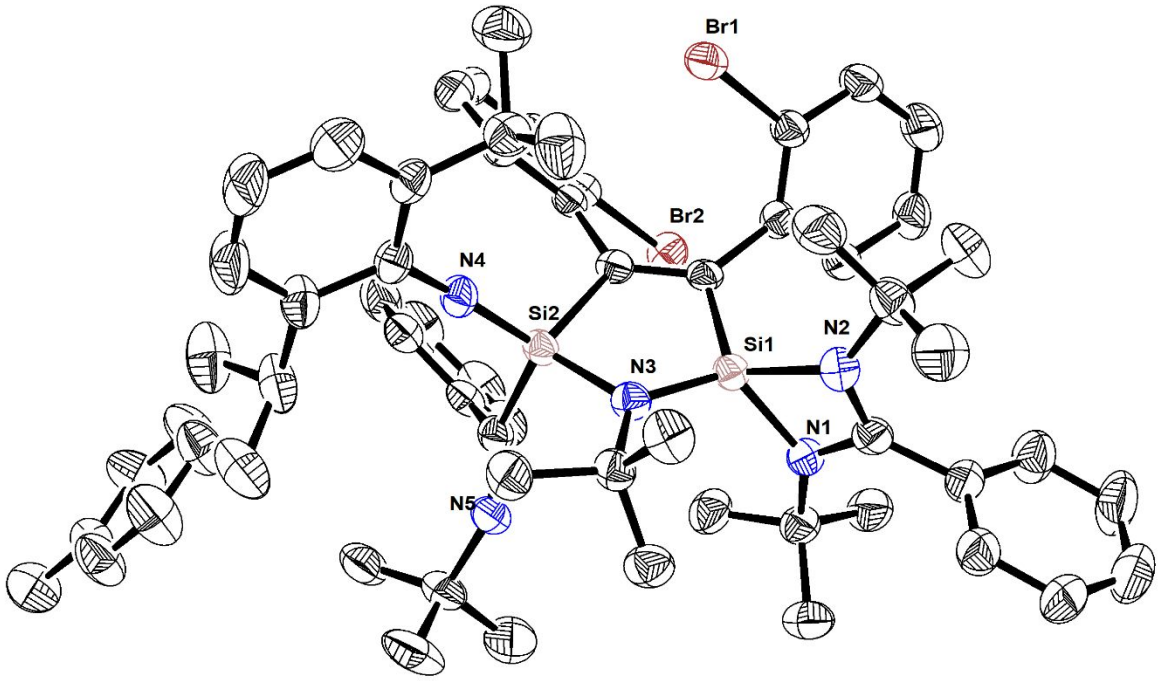


**Figure S20**. ORTEP drawing of complex (**3c**) with thermal ellipsoid shown at 50% probability level. Important bond lengths include N1-Si1: 1.831, N2-Si1: 1.808, N3-Si1: 1.674, N3-Si2: 1.796, N4-Si2: 1.594, and important bond angles include N1-Si1-N2: 72.74, C2-Si1-N3: 105.11, Si1-N3-Si2: 109.52, N3-Si2-C3: 97.49, N3-Si2-N4: 119.33 (Bond lengths are in Å and bond angles are in °).

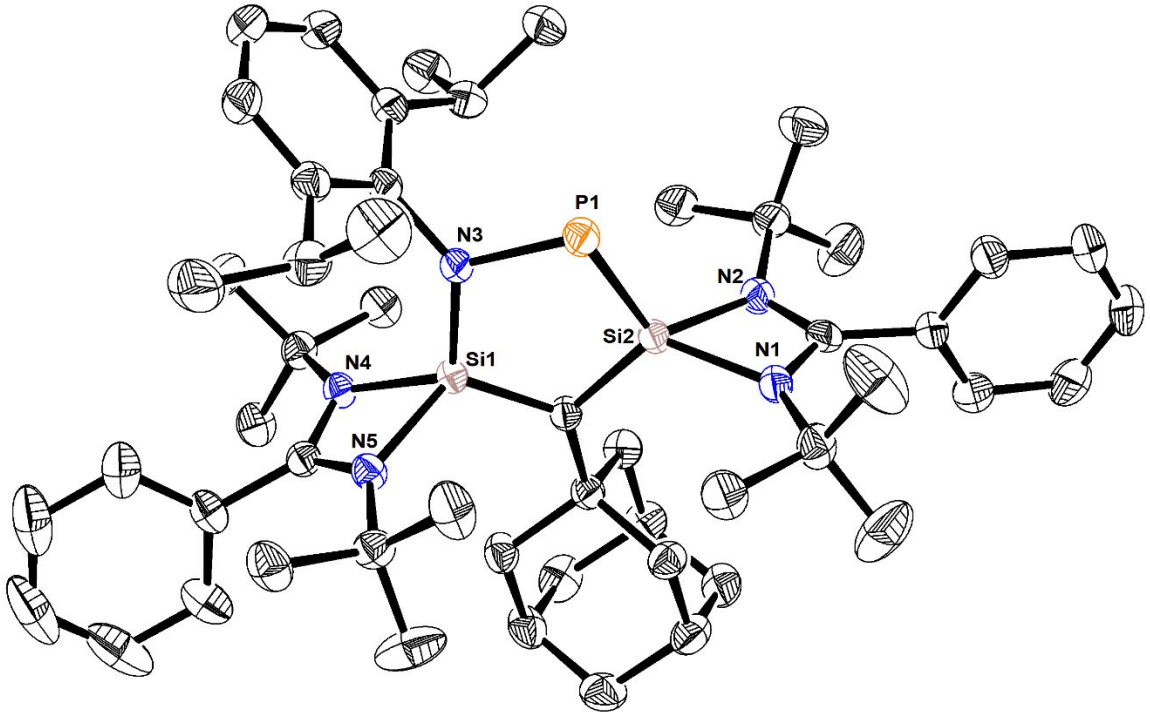


**Figure S21**. ORTEP drawing of complex (**4**) with thermal ellipsoid shown at 50 % probability level. Important bond lengths include N1-C7: 1.334, N2-C7: 1.329, N2-Si2: 1.885, N1-Si2: 1.873, Si2-C26: 1.791, Si2-P1: 2.163, P1-N3: 1.848, N3-Si1: 1.702, Si1-C26: 1.769, N5-Si1: 1.899, N4-Si1: 1.841, N5-C49: 1.327, N4-C49: 1.345, and important bond angles include N1-C7-N2: 106.89, C7-N2-Si2: 91.55, N2-Si2-N1: 69.40, Si2-N1-C7: 91.90, Si1-C26-Si2: 104.40, C26-Si2-P1: 109.48, Si2-P1-N3: 93.14, P1-N3-Si1: 113.52, N3-Si1-C26: 113.33, Si1-N4-C49: 92.42, N4-C49-N5:107.00, C49-N5-Si1: 90.48, N5-Si1-N4: 70.08 (Bond lengths are in Å and bond angles are in °).

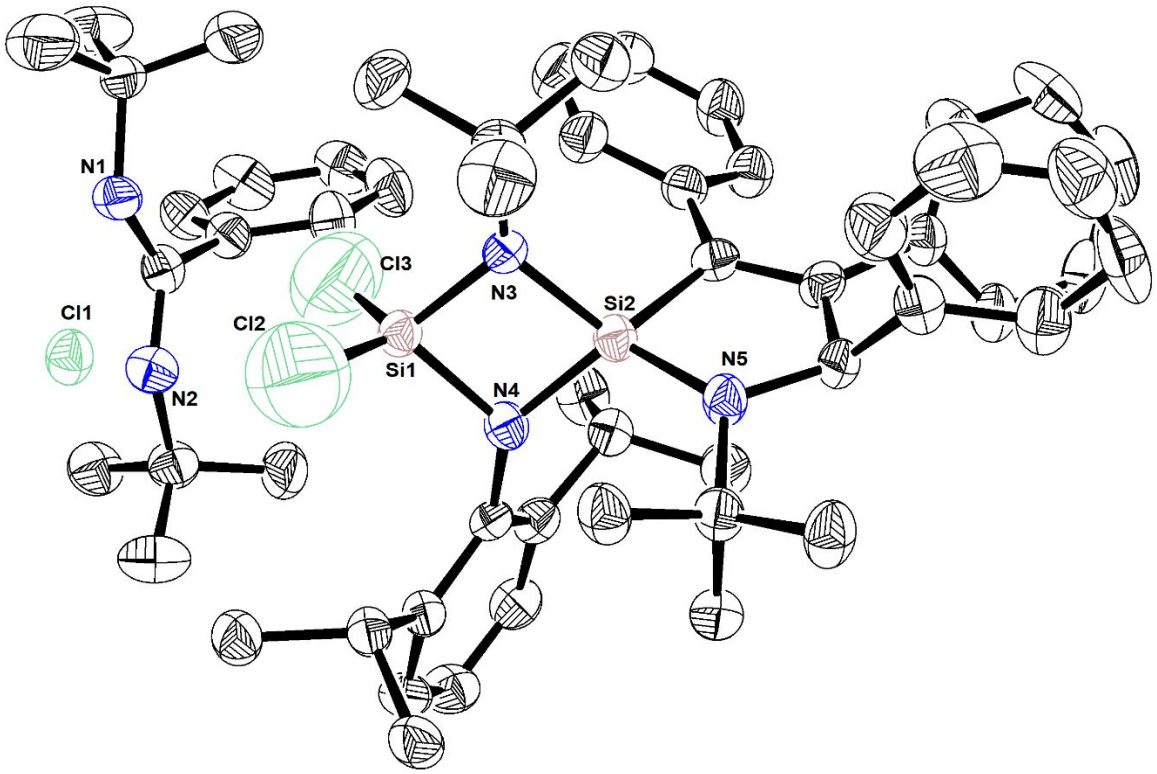


**Figure S22**. ORTEP drawing of complex (**5**) with thermal ellipsoid shown at 50 % probability level. Important bond lengths include Si1-Cl3: 1.737, Si1-Cl2: 1.621, Si1-N3: 1.705, Si1-N4: 1.743, N4-Si2: 1.761, Si2-N3: 1.741, Si2-C4: 1.881, Si2-N5: 1.728, and important bond angles include Cl3-Si1-Cl2: 107.77, N3-Si1-N4: 87.34, Si1-N4-Si2: 92.33, N4-Si2-N3: 85.68, Si2-N3-Si1: 94.39, C4-Si2-N5: 93.49 (Bond lengths are in Å and bond angles are in °).

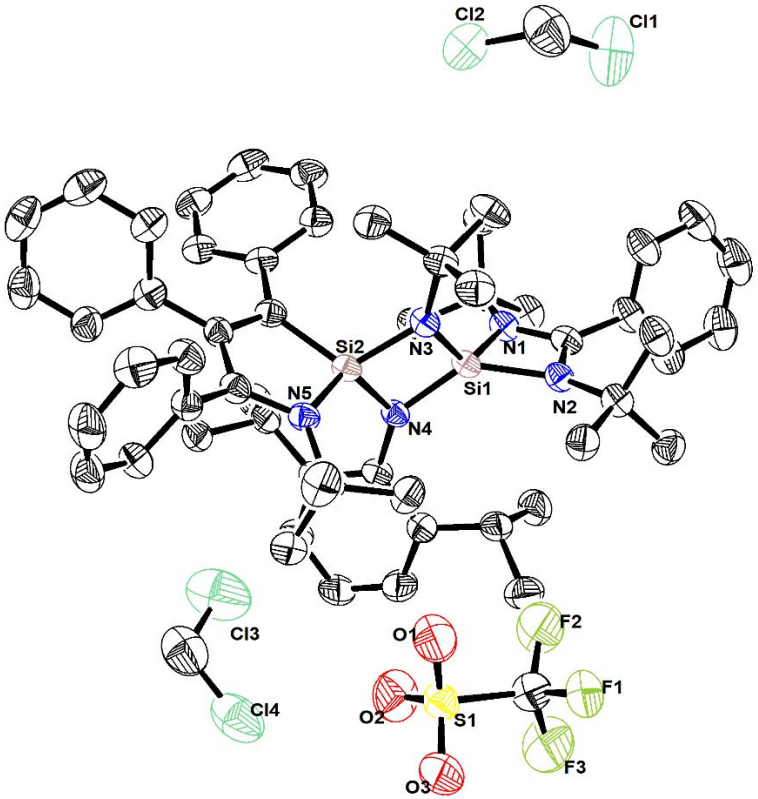


**Figure S23**. ORTEP drawing of complex (**6**) with thermal ellipsoid shown at 50 % probability level. Important bond lengths include C1-N2: 1.351, N2-Si1: 1.829, Si1-N1: 1.792, N1-C1: 1.339, Si1-N3: 1.691, N3-Si2: 1.757, Si2-N4: 1.786, N4-Si1: 1.715, Si2-N5: 1.743, N5-C2: 1.414, C2-C3: 1.412, C3-C4: 1.402, C4-Si2: 1.844, and important bond angles include Si1-N1-C1: 91.11, N1-C1-N2: 106.45, C1-N2-Si1: 89.14, N2-Si1-N1: 73.01, N4-Si1-N3: 89.33, Si1-N3-Si2: 93.62, N3-Si2-N4: 85.02, Si2-N4-Si1: 91.81, Si2-N5-C2: 109.09, N5-C2-C3: 115.06, C2-C3-C4: 115.67, C3-C4-Si2: 106.22, C4-Si2-N5: 93.76 (Bond lengths are in Å and bond angles are in °).

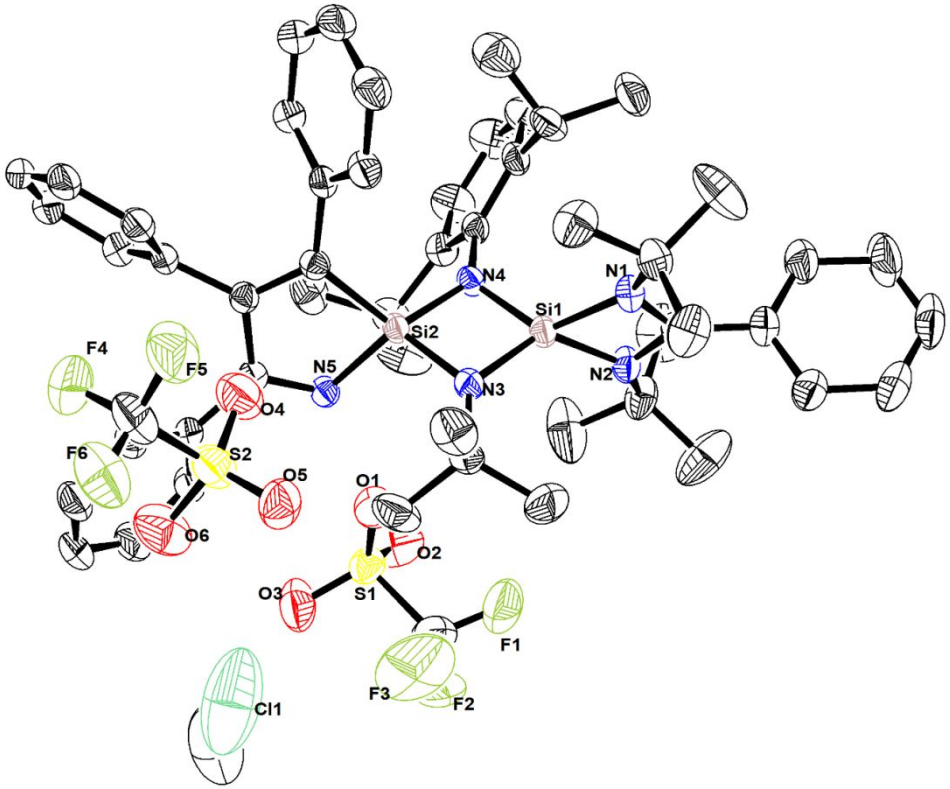


**Figure S24**. ORTEP drawing of complex (**7**) with thermal ellipsoid shown at 50 % probability level. Important bond lengths include N1-C1: 1.345, C1-N2: 1.344, N2-Si1: 1.768, Si1-N1: 1.806, N3-Si1: 1.704, Si1-N4: 1.726, N4-Si2: 1.734, Si2-N3: 1.726, Si2-C4: 1.857, Si2-N5: 1.782, N5-C2: 1.307, C2-C3: 1.498, C3-C4: 1.350, and important bond angles include N1-C1-N2: 106.12, C1-N2-Si1: 90.78, N2-Si1-N1: 73.95, Si1-N1-C1: 89.15, N3-Si1-N4: 88.63, Si1-N4-Si2: 91.20, N4-Si2-N3: 87.67, Si2-N3-Si1: 92.25, N5-Si2-C4: 90.42, Si2-C4-C3: 108.47, C4-C3-C2: 113.60, C3-C2-N5: 113.74, C2-N5-Si2: 111.85 (Bond lengths are in Å and bond angles are in °).

**V. Coordinates:** Theoretical Investigations on the Formation Mechanisms of Compounds **2a**, **3a** and **3c**

Table S1
B3LYP-D3(BJ)/def2-SVP
**1**
G = -2489.104431 Hartree

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| Si | 0.78789800 | 0.82284500 | -0.04283100 |
| Si | -0.45640000 | 2.48234800 | 1.13878200 |
| N | 2.37615700 | 1.05003900 | -0.13999000 |
| N | -2.04747000 | 1.54698400 | 1.72662000 |
| N | 0.03729800 | 0.50539800 | -1.73972600 |
| N | 0.12483000 | -0.97415800 | -0.16972400 |
| N | -0.29074700 | 1.78869600 | 2.93266400 |
| C | 3.65358700 | 1.16662300 | 0.29210600 |
| C | -0.24279400 | -0.76390400 | -1.43508900 |
| C | -3.42490300 | 1.61206500 | 1.21604600 |
| C | -1.57369100 | 1.41246900 | 2.97899300 |
| C | -0.80988200 | -1.77769600 | -2.36340600 |
| C | 4.45859400 | 0.00308500 | 0.52240400 |
| C | 4.23983500 | 2.45387700 | 0.51829700 |
| C | 0.18345800 | 1.20397500 | -3.02656900 |
| C | 0.07081700 | -2.63763200 | -3.03469700 |
| H | 1.14306200 | -2.56182400 | -2.84385500 |
| C | 3.85044200 | -1.35857400 | 0.23389200 |

| | | | |
|---|---|---|---|
| H | 2.79890900 | -1.29244900 | 0.54823700 |
| C | 3.41433200 | 3.69188100 | 0.21954600 |
| H | 2.36446800 | 3.42615200 | 0.42505500 |
| C | -0.18128800 | -2.07658200 | 0.75301500 |
| C | -3.99906600 | 3.01869000 | 1.47032900 |
| H | -4.06724300 | 3.21559600 | 2.55109100 |
| H | -5.00958800 | 3.11288200 | 1.04185800 |
| H | -3.35141800 | 3.78577900 | 1.02065600 |
| C | 0.72976600 | 1.94012200 | 3.98481100 |
| C | 0.43136200 | -1.68326200 | 2.10513300 |
| H | 1.52531300 | -1.60560500 | 2.03879600 |
| H | 0.18655400 | -2.43678000 | 2.86849800 |
| H | 0.04294500 | -0.71016100 | 2.43385500 |
| C | 5.77565200 | 0.14573900 | 0.96443400 |
| H | 6.38457400 | -0.74434100 | 1.13920100 |
| C | -2.34443300 | 0.99579300 | 4.17938900 |
| C | -4.36179200 | 0.56262200 | 1.83516500 |
| H | -3.93961600 | -0.44894400 | 1.76181800 |
| H | -5.31856800 | 0.57205000 | 1.29070600 |
| H | -4.57651100 | 0.76945800 | 2.89082300 |
| C | -0.42605000 | -3.57977400 | -3.93724700 |
| H | 0.26443200 | -4.24440500 | -4.46116400 |
| C | -3.31434400 | 1.35959100 | -0.29554700 |
| H | -2.62141100 | 2.07709500 | -0.76182200 |
| H | -4.29478000 | 1.46141500 | -0.78440200 |
| H | -2.92531900 | 0.34927400 | -0.48437700 |

| | | | |
|---|---|---|---|
| C | -2.51140700 | -0.36469000 | 4.47345800 |
| H | -2.06438500 | -1.11292400 | 3.81783600 |
| C | -2.18756500 | -1.86957400 | -2.59807700 |
| H | -2.86996900 | -1.18942100 | -2.08634700 |
| C | -1.80185800 | -3.67279500 | -4.16748600 |
| H | -2.18971600 | -4.41148700 | -4.87260100 |
| C | 3.76116000 | 4.90896200 | 1.08086600 |
| H | 3.72780200 | 4.66455100 | 2.15459400 |
| H | 3.04665600 | 5.72710300 | 0.89400600 |
| H | 4.76764300 | 5.29987800 | 0.85883500 |
| C | 3.49343800 | 4.03652500 | -1.27711300 |
| H | 4.51538600 | 4.35034100 | -1.54734500 |
| H | 2.80129100 | 4.85471200 | -1.53991800 |
| H | 3.23976900 | 3.15893400 | -1.88840100 |
| C | -2.68093000 | -2.81849700 | -3.49504700 |
| H | -3.75627400 | -2.88704700 | -3.67406300 |
| C | 6.33753800 | 1.40537300 | 1.18736000 |
| H | 7.36953900 | 1.49751200 | 1.53480900 |
| C | -0.95145600 | 0.87904900 | -4.00836700 |
| H | -0.90244600 | -0.15195600 | -4.38058400 |
| H | -0.87818900 | 1.55174900 | -4.87649600 |
| H | -1.93440900 | 1.03392600 | -3.53784500 |
| C | 1.54845800 | 0.83988100 | -3.63654100 |
| H | 2.34978700 | 1.06270100 | -2.91794100 |
| H | 1.72409700 | 1.41049700 | -4.56188800 |
| H | 1.59018200 | -0.23216400 | -3.88208900 |

| | | | |
|---|---|---|---|
| C | 5.56317300 | 2.54426600 | 0.95852300 |
| H | 6.00444500 | 3.52906700 | 1.12971000 |
| C | 4.49508300 | -2.51789300 | 0.99668100 |
| H | 5.52683800 | -2.71074600 | 0.65968300 |
| H | 3.92558700 | -3.44878800 | 0.83726600 |
| H | 4.52948100 | -2.31989700 | 2.07995000 |
| C | -1.70126100 | -2.22578200 | 0.92362300 |
| H | -2.13003800 | -1.26642100 | 1.24210000 |
| H | -1.93151600 | -2.98513000 | 1.68743500 |
| H | -2.18512500 | -2.53481500 | -0.01310900 |
| C | -3.23954800 | -0.75490400 | 5.59753900 |
| H | -3.36287800 | -1.81670000 | 5.82271700 |
| C | 0.14591400 | 2.70466100 | -2.69868700 |
| H | -0.82306900 | 2.98545000 | -2.25852900 |
| H | 0.29810300 | 3.29777300 | -3.61253600 |
| H | 0.93735400 | 2.96816000 | -1.98416900 |
| C | 0.44156100 | -3.39856500 | 0.27625900 |
| H | -0.03470300 | -3.76551100 | -0.64235300 |
| H | 0.31749900 | -4.16996700 | 1.05206500 |
| H | 1.51640700 | -3.27042000 | 0.08623800 |
| C | 0.56067400 | 3.31956200 | 4.64707000 |
| H | 0.61262300 | 4.11558800 | 3.88925900 |
| H | 1.35587300 | 3.49191800 | 5.38908600 |
| H | -0.40893100 | 3.39139300 | 5.16240900 |
| C | -3.80922700 | 0.20988300 | 6.43459700 |
| H | -4.37927600 | -0.09696000 | 7.31454600 |

| | | | |
|---|---|---|---|
| C | -2.91631400 | 1.96031200 | 5.02054600 |
| H | -2.78835900 | 3.01981400 | 4.79006200 |
| C | 3.82603100 | -1.63977900 | -1.27827700 |
| H | 3.29352500 | -0.83617100 | -1.80489200 |
| H | 3.32089900 | -2.59749600 | -1.49787800 |
| H | 4.85088100 | -1.69953100 | -1.67998600 |
| C | -3.64743800 | 1.56746600 | 6.14409600 |
| H | -4.09142500 | 2.32418200 | 6.79494500 |
| C | 0.65306600 | 0.83524800 | 5.04988600 |
| H | -0.24684800 | 0.91361100 | 5.67289800 |
| H | 1.52817300 | 0.91805700 | 5.71193500 |
| H | 0.67228400 | -0.16239600 | 4.58868100 |
| C | 2.09357400 | 1.87085100 | 3.28449800 |
| H | 2.26319000 | 0.88785300 | 2.82505400 |
| H | 2.90583600 | 2.06171100 | 4.00063400 |
| H | 2.16818300 | 2.62305400 | 2.48739600 |

Table S2
B3LYP-D3(BJ)/def2-SVP
**1,2-diphenylethyne**
G = -538.9741600 Hartree

| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |

| | | | |
|---|---|---|---|
| C | -0.14027000 | -0.32058300 | 0.69109300 |
| C | -0.32308900 | -1.37668600 | 1.27199600 |
| C | -0.53707500 | -2.61238000 | 1.95151300 |
| C | -0.95936600 | -5.05060300 | 3.29212600 |
| C | -0.65027500 | -3.81944500 | 1.22928400 |
| C | -0.63954000 | -2.65060800 | 3.35844600 |
| C | -0.84861900 | -3.86025300 | 4.01806200 |
| C | -0.85940700 | -5.02444600 | 1.89732000 |
| H | -0.57180900 | -3.79552500 | 0.14092100 |
| H | -0.55265400 | -1.71991500 | 3.92194200 |
| H | -0.92597600 | -3.87538300 | 5.10777700 |
| H | -0.94523500 | -5.95156800 | 1.32567700 |
| H | -1.12328700 | -5.99706900 | 3.81254100 |
| C | 0.07370500 | 0.91501700 | 0.01140200 |
| C | 0.49595300 | 3.35297400 | -1.32970700 |
| C | 0.18036300 | 2.12309900 | 0.73291700 |
| C | 0.18269400 | 0.95208900 | -1.39507700 |
| C | 0.39182700 | 2.16159600 | -2.05492300 |
| C | 0.38939700 | 3.32798400 | 0.06463800 |
| H | 0.09674600 | 2.10009100 | 1.82091900 |
| H | 0.10097500 | 0.02059100 | -1.95801000 |
| H | 0.47437400 | 2.17580500 | -3.14427400 |
| H | 0.47001900 | 4.25591800 | 0.63571300 |
| H | 0.65985700 | 4.29934500 | -1.85030100 |

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Table S3
B3LYP-D3(BJ)/def2-SVP
**TS1A**
G = -3028.052383 Hartree

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| Si | 0.00000000 | 0.00000000 | 0.00000000 |
| C | 0.00000000 | 0.00000000 | 2.36047000 |
| C | 1.15164700 | 0.00000000 | 2.86394300 |
| C | 2.22135100 | -0.55506500 | -0.44512200 |
| H | 4.95066300 | -2.07036600 | 4.46868900 |
| C | 4.45884700 | -1.13605700 | 4.18494000 |
| H | 2.61784400 | -2.12454600 | 3.66165800 |
| C | 3.14540700 | -1.17300500 | 3.72733600 |
| C | 5.15231500 | 0.07696200 | 4.28614100 |
| H | 6.18419300 | 0.09906200 | 4.64249600 |
| C | 2.46989400 | 0.01921600 | 3.34029800 |
| C | 4.49233700 | 1.26412000 | 3.94237400 |
| C | 3.17867400 | 1.24536100 | 3.48590800 |
| H | 5.01275200 | 2.22147300 | 4.03063900 |
| H | 2.67350600 | 2.17757300 | 3.22810200 |
| H | -2.02845400 | -1.68867900 | 1.69090400 |
| H | -4.33190800 | -1.70802400 | 2.63047200 |
| C | -2.32706000 | -0.93512300 | 2.42148900 |

| | | | |
|---|---|---|---|
| C | -3.62220200 | -0.93785700 | 2.94212500 |
| C | -1.38711300 | 0.02517400 | 2.83282100 |
| C | -4.01838900 | 0.04719600 | 3.85071600 |
| H | -5.03697200 | 0.05513000 | 4.24547200 |
| C | -1.79432300 | 1.00743600 | 3.75357000 |
| C | -3.10013500 | 1.02445900 | 4.24717700 |
| H | -1.06891800 | 1.75667400 | 4.07644800 |
| H | -3.40120500 | 1.80341000 | 4.95221700 |
| C | -0.43172800 | 0.77384500 | -4.82882300 |
| Si | -1.11316700 | 0.29197400 | -2.13307200 |
| N | 1.71381700 | 0.67823700 | -0.34951900 |
| N | 1.18948100 | -1.40656400 | -0.35227000 |
| C | 3.65122100 | -0.90823100 | -0.64414900 |
| C | 4.51778500 | -1.03375000 | 0.44899300 |
| C | 4.13714500 | -1.08610200 | -1.94566000 |
| C | 5.86314100 | -1.33795600 | 0.23673200 |
| H | 4.14424900 | -0.88493400 | 1.46095800 |
| C | 5.48474200 | -1.38532200 | -2.15392000 |
| H | 3.45648200 | -0.98589400 | -2.78892400 |
| C | 6.34968000 | -1.51212000 | -1.06268200 |
| H | 6.53212700 | -1.42998300 | 1.09508400 |
| H | 5.85734800 | -1.51798200 | -3.17218200 |
| H | 7.40465700 | -1.74498200 | -1.22579400 |
| C | 2.34386900 | 1.99257300 | -0.59249600 |
| C | 1.17050700 | -2.87209900 | -0.22621500 |
| C | -0.30590600 | -3.26917100 | -0.08167100 |

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|---|---|---|---|
| H | -0.92337100 | -2.79520200 | -0.85605200 |
| H | -0.42220600 | -4.35969500 | -0.16080100 |
| H | -0.68845500 | -2.95968700 | 0.90094900 |
| C | 1.77770600 | -3.52387700 | -1.48044500 |
| H | 1.33310800 | -3.10637600 | -2.39400500 |
| H | 2.86236900 | -3.36275900 | -1.52756500 |
| H | 1.59848300 | -4.60990600 | -1.46691300 |
| C | 1.92077900 | -3.33431500 | 1.03243100 |
| H | 1.81764100 | -4.42421300 | 1.15269100 |
| H | 2.99143300 | -3.09865800 | 0.97709400 |
| H | 1.49936200 | -2.84258900 | 1.91967700 |
| C | 2.45230600 | 2.23173700 | -2.10630100 |
| H | 2.81202900 | 3.25404600 | -2.30381000 |
| H | 3.17343400 | 1.53195500 | -2.55081000 |
| H | 1.48302500 | 2.07603300 | -2.60336400 |
| C | 3.73318500 | 2.11275800 | 0.05451200 |
| H | 4.48932700 | 1.52353800 | -0.47758200 |
| H | 4.04946600 | 3.16648300 | 0.01611000 |
| H | 3.71840300 | 1.79395700 | 1.10422300 |
| C | 1.41053100 | 3.03179000 | 0.03621200 |
| H | 0.43178000 | 3.01560400 | -0.45793300 |
| H | 1.26711000 | 2.83496000 | 1.10945400 |
| H | 1.82801300 | 4.04170200 | -0.08547900 |
| N | -2.84924000 | 0.97379000 | -1.55247500 |
| N | -2.46232200 | -1.00598100 | -2.35168600 |
| C | -3.40371800 | -0.20005100 | -1.82476400 |

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|---|---|---|---|
| C | -4.80847600 | -0.59823200 | -1.54817500 |
| C | -5.86328300 | -0.15022400 | -2.35336500 |
| C | -5.07229400 | -1.44175700 | -0.46019100 |
| C | -7.17344000 | -0.54278700 | -2.06822500 |
| H | -5.65567300 | 0.49651700 | -3.20733300 |
| C | -6.38231400 | -1.82079700 | -0.17035000 |
| H | -4.24418900 | -1.78521300 | 0.16003900 |
| C | -7.43524900 | -1.37305800 | -0.97513200 |
| H | -7.99219700 | -0.19678700 | -2.70287000 |
| H | -6.58303400 | -2.46981200 | 0.68505200 |
| H | -8.46112200 | -1.67395200 | -0.75083200 |
| C | -2.65895400 | -2.12225500 | -3.31020900 |
| C | -3.40729500 | -3.30116300 | -2.66792800 |
| H | -2.92372500 | -3.60805800 | -1.72860800 |
| H | -4.45645000 | -3.06086000 | -2.45529800 |
| H | -3.39366300 | -4.16031400 | -3.35590900 |
| C | -1.26696600 | -2.58552100 | -3.75201000 |
| H | -0.71171600 | -1.76263000 | -4.21772600 |
| H | -0.68679000 | -2.96901500 | -2.90419000 |
| H | -1.36216300 | -3.39411000 | -4.49109800 |
| C | -3.41634100 | -1.61462000 | -4.54960400 |
| H | -2.87578400 | -0.77941200 | -5.01799900 |
| H | -3.50513000 | -2.42156700 | -5.29304600 |
| H | -4.43249700 | -1.28525200 | -4.29229200 |
| C | -3.37794000 | 2.12046500 | -0.78085900 |
| C | -4.42563600 | 2.88588800 | -1.60575900 |

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|---|---|---|---|
| H | -4.01791600 | 3.18956100 | -2.57783100 |
| H | -5.32514100 | 2.28001600 | -1.77346400 |
| H | -4.73101200 | 3.79241500 | -1.06121700 |
| C | -3.97763400 | 1.69223200 | 0.56479300 |
| H | -4.90332000 | 1.11592400 | 0.44263500 |
| H | -3.26138700 | 1.08663000 | 1.13202400 |
| H | -4.21607000 | 2.58516800 | 1.16191900 |
| C | -2.17863300 | 3.03522100 | -0.51577400 |
| H | -2.50664800 | 3.96841900 | -0.03543000 |
| H | -1.47039400 | 2.54072800 | 0.16410600 |
| H | -1.66113100 | 3.28835700 | -1.45271900 |
| C | -1.50885700 | 1.38379300 | -5.55123800 |
| C | 0.58151200 | 0.10164200 | -5.58324700 |
| C | -1.57780000 | 1.25623600 | -6.94142400 |
| C | 0.46471300 | -0.00381200 | -6.97314600 |
| C | -0.61091600 | 0.55281500 | -7.66184500 |
| H | -0.68876400 | 0.45548400 | -8.74724700 |
| H | 1.24265700 | -0.53047100 | -7.53313700 |
| C | -2.51887700 | 2.22737500 | -4.79402100 |
| H | -2.40686300 | 1.71781500 | -7.48139600 |
| C | 1.82629100 | -0.43626400 | -4.89404000 |
| H | -2.70465200 | 1.72480300 | -3.83511000 |
| C | -3.87374100 | 2.38154000 | -5.48958300 |
| C | -1.90173700 | 3.59820100 | -4.46673700 |
| H | -0.96162000 | 3.46950100 | -3.91073400 |
| H | -2.58275900 | 4.21911900 | -3.86061500 |

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|---|---|---|---|
| H | -1.67805400 | 4.14937500 | -5.39439600 |
| H | -4.30497000 | 1.40266400 | -5.75411000 |
| H | -3.80250000 | 2.97615300 | -6.41446800 |
| H | -4.58671600 | 2.90191400 | -4.82937300 |
| H | 1.63111900 | -0.35558400 | -3.81365300 |
| C | 3.03463600 | 0.45313000 | -5.23273300 |
| C | 2.12727900 | -1.90498200 | -5.22458000 |
| H | 2.83138400 | 1.50387900 | -4.98119200 |
| H | 3.26324400 | 0.40629600 | -6.31001700 |
| H | 3.94018000 | 0.13850000 | -4.68677300 |
| H | 1.27315500 | -2.55661500 | -4.99004200 |
| H | 2.99621500 | -2.26888000 | -4.65083400 |
| H | 2.36502500 | -2.04139700 | -6.29188200 |
| N | -0.34400300 | 0.81841200 | -3.45888000 |

Table S4
B3LYP-D3(BJ)/def2-SVP
**Int1A**
G = -3029.133439 Hartree

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| Si | 0.64736300 | -0.12513800 | 1.14814300 |
| C | 0.08412500 | -0.01123200 | 2.92145400 |

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|---|---|---|---|
| C | 0.89105600 | 0.46311400 | 3.88932900 |
| C | 2.83042000 | -0.57672100 | 0.57210200 |
| H | 5.23506000 | -0.71605100 | 4.86167500 |
| C | 4.52278900 | 0.09951200 | 4.69717900 |
| H | 2.91747800 | -1.25802500 | 4.22986600 |
| C | 3.22012900 | -0.21316200 | 4.32191100 |
| C | 4.93464400 | 1.42950900 | 4.86387600 |
| H | 5.95873200 | 1.66805500 | 5.15776500 |
| C | 2.23366600 | 0.80435800 | 4.11161500 |
| C | 3.98127400 | 2.44280500 | 4.67713200 |
| C | 2.66879800 | 2.15124700 | 4.32368500 |
| H | 4.27099200 | 3.48904100 | 4.81550100 |
| H | 1.94127800 | 2.96023300 | 4.22220200 |
| H | -1.57618100 | -1.75029300 | 1.54091800 |
| H | -3.73198300 | -2.67068900 | 2.27891600 |
| C | -2.00311500 | -1.39594900 | 2.47946200 |
| C | -3.23998500 | -1.90676000 | 2.88655500 |
| C | -1.29734000 | -0.47275400 | 3.26708700 |
| C | -3.82736300 | -1.46722900 | 4.07378200 |
| H | -4.79457700 | -1.86214200 | 4.39405300 |
| C | -1.90460700 | -0.03931300 | 4.46279900 |
| C | -3.15227000 | -0.51768700 | 4.85384500 |
| H | -1.34722500 | 0.67290700 | 5.07516800 |
| H | -3.60398700 | -0.15513200 | 5.78127900 |
| C | -0.19007700 | 0.68136900 | -3.38113200 |
| Si | -0.82098400 | 0.30407000 | -0.67495900 |

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|---|---|---|---|
| N | 2.28879900 | 0.63199500 | 0.77007800 |
| N | 1.86171100 | -1.48766500 | 0.74725600 |
| C | 4.25348600 | -0.85416500 | 0.26615600 |
| C | 5.21477800 | -0.68591600 | 1.27292500 |
| C | 4.63714900 | -1.28866700 | -1.00780000 |
| C | 6.55428000 | -0.96333900 | 1.00021100 |
| H | 4.90560700 | -0.34790900 | 2.26255500 |
| C | 5.98176500 | -1.54895800 | -1.27876700 |
| H | 3.88533100 | -1.40334400 | -1.78540200 |
| C | 6.94078200 | -1.39134100 | -0.27408800 |
| H | 7.29942100 | -0.83610200 | 1.78855800 |
| H | 6.27830100 | -1.87412700 | -2.27838300 |
| H | 7.99229300 | -1.59947300 | -0.48540100 |
| C | 2.81016100 | 1.96677100 | 0.36229300 |
| C | 1.96231100 | -2.95564300 | 0.92351600 |
| C | 0.60941700 | -3.42513900 | 1.46927300 |
| H | -0.20450900 | -3.18511600 | 0.77083100 |
| H | 0.61915500 | -4.51583400 | 1.60584600 |
| H | 0.38674500 | -2.95610500 | 2.43757500 |
| C | 2.24050100 | -3.63520300 | -0.42713400 |
| H | 1.53767100 | -3.28866400 | -1.19550100 |
| H | 3.25959500 | -3.42638100 | -0.77600400 |
| H | 2.13737200 | -4.72638200 | -0.32590100 |
| C | 3.05354000 | -3.33150200 | 1.93794400 |
| H | 3.01516100 | -4.41481100 | 2.12767800 |
| H | 4.05897900 | -3.09047100 | 1.57173500 |

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|---|---|---|---|
| H | 2.89449700 | -2.80743500 | 2.88981600 |
| C | 3.00448600 | 1.99884500 | -1.15924300 |
| H | 3.29289400 | 3.01367000 | -1.47437400 |
| H | 3.80644100 | 1.31492800 | -1.46865100 |
| H | 2.07157300 | 1.71115300 | -1.66466300 |
| C | 4.12173900 | 2.31534000 | 1.07923900 |
| H | 4.96835500 | 1.74475300 | 0.67972400 |
| H | 4.33839500 | 3.38189400 | 0.91453900 |
| H | 4.04613300 | 2.14455900 | 2.15896600 |
| C | 1.72600000 | 2.96995700 | 0.75459800 |
| H | 0.81615100 | 2.77839400 | 0.17228000 |
| H | 1.49536100 | 2.90794600 | 1.82704500 |
| H | 2.05670700 | 3.99314200 | 0.52702600 |
| N | -2.45917700 | 1.10367700 | -0.04263900 |
| N | -2.27022300 | -0.85513300 | -0.94206400 |
| C | -3.14715800 | 0.05003900 | -0.48512000 |
| C | -4.63005200 | -0.04512200 | -0.57724200 |
| C | -5.27365500 | 0.61098200 | -1.63661900 |
| C | -5.38688700 | -0.76575000 | 0.35416300 |
| C | -6.66151100 | 0.53674000 | -1.76626300 |
| H | -4.68549200 | 1.17098400 | -2.36278600 |
| C | -6.77515400 | -0.83162400 | 0.22449900 |
| H | -4.88763600 | -1.24724700 | 1.19244300 |
| C | -7.41514000 | -0.18480200 | -0.83636600 |
| H | -7.15363600 | 1.04628700 | -2.59751200 |
| H | -7.35869900 | -1.38881100 | 0.96070300 |

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|---|---|---|---|
| H | -8.50151500 | -0.24016400 | -0.93663200 |
| C | -2.48983800 | -2.05078600 | -1.78610100 |
| C | -3.27149900 | -3.11841900 | -1.00503900 |
| H | -2.76072500 | -3.36068200 | -0.06037600 |
| H | -4.29304400 | -2.78965300 | -0.77487400 |
| H | -3.34098300 | -4.03981800 | -1.60300100 |
| C | -1.09854100 | -2.59192800 | -2.12704700 |
| H | -0.53954700 | -1.87123600 | -2.73498500 |
| H | -0.52712500 | -2.79684800 | -1.21263000 |
| H | -1.18622000 | -3.53028600 | -2.69310700 |
| C | -3.20878400 | -1.68746000 | -3.09594100 |
| H | -2.68464100 | -0.86728500 | -3.60898100 |
| H | -3.21468700 | -2.55989000 | -3.76692700 |
| H | -4.25185100 | -1.39332900 | -2.92199500 |
| C | -2.94104700 | 2.25711800 | 0.76115000 |
| C | -3.69667000 | 3.26736000 | -0.11781800 |
| H | -3.05880900 | 3.64271700 | -0.92702000 |
| H | -4.60181800 | 2.82753300 | -0.55558300 |
| H | -4.00544900 | 4.12515100 | 0.49884200 |
| C | -3.84510000 | 1.80399800 | 1.91817300 |
| H | -4.82641200 | 1.46576300 | 1.56416300 |
| H | -3.37782000 | 0.99848200 | 2.49527600 |
| H | -4.01351700 | 2.65415200 | 2.59608100 |
| C | -1.69513800 | 2.93752000 | 1.33168000 |
| H | -1.98713400 | 3.80347700 | 1.94293600 |
| H | -1.11967200 | 2.25197600 | 1.97023500 |

| | | | |
|---|---|---|---|
| H | -1.05310100 | 3.30221300 | 0.51902500 |
| C | -1.22038300 | 1.42895600 | -4.03940600 |
| C | 0.67554700 | -0.11554200 | -4.19597700 |
| C | -1.42923000 | 1.26939400 | -5.41273800 |
| C | 0.41951600 | -0.24879900 | -5.56536800 |
| C | -0.63905500 | 0.41320900 | -6.18055300 |
| H | -0.82939400 | 0.29005600 | -7.24915800 |
| H | 1.07801500 | -0.87859000 | -6.16935600 |
| C | -2.01348500 | 2.45517100 | -3.24971200 |
| H | -2.22583400 | 1.83024800 | -5.90368300 |
| C | 1.94279700 | -0.73460500 | -3.62327700 |
| H | -2.29584100 | 1.99008100 | -2.29484400 |
| C | -3.30384300 | 2.92261300 | -3.92779600 |
| C | -1.11258300 | 3.65741300 | -2.91366100 |
| H | -0.22283200 | 3.33007700 | -2.35745600 |
| H | -1.64630800 | 4.40802400 | -2.30720600 |
| H | -0.77713800 | 4.15090400 | -3.83990800 |
| H | -3.93480200 | 2.07430900 | -4.23788500 |
| H | -3.09984900 | 3.52524300 | -4.82698500 |
| H | -3.89003800 | 3.55364700 | -3.24149300 |
| H | 1.87103200 | -0.63541800 | -2.52932100 |
| C | 3.15836100 | 0.07420900 | -4.11235000 |
| C | 2.12233200 | -2.22008900 | -3.96659600 |
| H | 3.04572600 | 1.14059600 | -3.87322100 |
| H | 3.26144800 | -0.01135600 | -5.20611200 |
| H | 4.09879900 | -0.28121400 | -3.66042700 |

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|---|---|---|---|
| H | 1.26125700 | -2.82236000 | -3.64433500 |
| H | 3.02193700 | -2.63099800 | -3.47908100 |
| H | 2.24782300 | -2.37368400 | -5.05007600 |
| N | 0.00183500 | 0.71321000 | -2.01538500 |

Table S5
B3LYP-D3(BJ)/def2-SVP
**TS2A**
G = -3029.121039 Hartree

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| N | 1.37796500 | -0.78325900 | 2.93989300 |
| Si | -0.04328800 | -0.97066000 | 1.76002100 |
| N | 0.45312700 | -2.64134000 | 1.67849900 |
| C | 2.12713900 | -1.47688400 | 1.98694200 |
| C | 2.17699300 | -0.68364800 | 0.67002800 |
| C | 0.95784100 | -0.20694600 | 0.32457800 |
| Si | -2.11527200 | 0.20210900 | 1.97628500 |
| N | -3.24970400 | 0.20203800 | 0.85415700 |
| N | -1.66583400 | 1.79752200 | 2.96017600 |
| C | -2.41731500 | 1.36827500 | 3.97746100 |
| N | -2.87006600 | 0.14878200 | 3.67459500 |
| H | 6.09790300 | 1.70378300 | -0.11253400 |

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|---|---|---|---|
| C | 5.49871600 | 0.82233900 | -0.35412600 |
| H | 3.89507500 | 1.35814000 | 0.99389900 |
| C | 4.26330300 | 0.63105200 | 0.26573500 |
| C | 5.96755900 | -0.11235700 | -1.28208900 |
| H | 6.93511100 | 0.03370900 | -1.76817600 |
| C | 3.47469200 | -0.49366900 | -0.03116600 |
| C | 5.19015900 | -1.23221300 | -1.58610300 |
| C | 3.95283300 | -1.42235400 | -0.96583300 |
| H | 5.54761700 | -1.96557500 | -2.31300300 |
| H | 3.35031100 | -2.29798400 | -1.20500000 |
| H | -1.41338700 | -0.34591700 | -0.90589700 |
| H | -2.19505600 | 0.89567900 | -2.87431400 |
| C | -0.74047700 | 0.36753400 | -1.37958400 |
| C | -1.18955400 | 1.07643200 | -2.49368400 |
| C | 0.55179400 | 0.56522400 | -0.85398900 |
| C | -0.35722700 | 2.02357900 | -3.09614000 |
| H | -0.70848100 | 2.59204900 | -3.96081200 |
| C | 1.37970900 | 1.52031800 | -1.47928600 |
| C | 0.92534900 | 2.24370800 | -2.58152000 |
| H | 2.37800600 | 1.70765500 | -1.08743600 |
| H | 1.57962200 | 2.98744400 | -3.04361100 |
| C | -4.07982500 | 0.35946400 | -0.21020400 |
| C | -4.29977100 | 1.66068000 | -0.77062000 |
| C | -4.78324000 | -0.74268800 | -0.79307300 |
| C | -5.12899000 | 1.81766600 | -1.88239100 |
| C | -5.59076600 | -0.53637500 | -1.91649300 |

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|---|---|---|---|
| C | -5.76417100 | 0.72754500 | -2.47854100 |
| H | -6.39714500 | 0.86375400 | -3.35846800 |
| H | -6.11243000 | -1.38901800 | -2.35707000 |
| H | -5.27798500 | 2.81492100 | -2.30137700 |
| C | -2.76908800 | 2.14270200 | 5.19657400 |
| C | -2.09565800 | 1.96874000 | 6.41164100 |
| C | -3.82962400 | 3.05619600 | 5.10909200 |
| C | -2.47998600 | 2.70875700 | 7.53144800 |
| H | -1.28010900 | 1.24933400 | 6.48171800 |
| C | -4.21603600 | 3.78639900 | 6.23375700 |
| H | -4.34109900 | 3.19441800 | 4.15441200 |
| C | -3.54084000 | 3.61492700 | 7.44599200 |
| H | -1.95060300 | 2.57211400 | 8.47694700 |
| H | -5.04444100 | 4.49441100 | 6.16136200 |
| H | -3.84166100 | 4.18888700 | 8.32533500 |
| C | 3.36525800 | -2.25395600 | 2.30599700 |
| C | 4.51186800 | -1.54703800 | 2.70195000 |
| C | 3.45546800 | -3.63623500 | 2.13065900 |
| C | 5.71531000 | -2.21490400 | 2.93091700 |
| H | 4.46507600 | -0.46482200 | 2.81658100 |
| C | 4.65886300 | -4.30697100 | 2.35724600 |
| H | 2.56239200 | -4.17915600 | 1.84110600 |
| C | 5.79394900 | -3.59943800 | 2.75925500 |
| H | 6.59735200 | -1.64735000 | 3.23657500 |
| H | 4.70595300 | -5.39001600 | 2.22085100 |
| H | 6.73670600 | -4.12286300 | 2.93507200 |

| | | | |
|---|---|---|---|
| C | -3.97420600 | -0.65585200 | 4.22968100 |
| C | -3.80966700 | -2.06102200 | 3.63056100 |
| C | -3.91004900 | -0.75592100 | 5.76054000 |
| C | -5.31107300 | -0.04108600 | 3.78197700 |
| H | -3.85097400 | -2.02271400 | 2.53464200 |
| H | -2.84723600 | -2.50368700 | 3.93041400 |
| H | -4.61717100 | -2.72028100 | 3.97998100 |
| H | -4.13743900 | 0.19822400 | 6.25152800 |
| H | -4.65224700 | -1.49307000 | 6.10238100 |
| H | -2.91612600 | -1.09220600 | 6.09152900 |
| H | -6.15403600 | -0.67820900 | 4.09092100 |
| H | -5.45182400 | 0.95196000 | 4.23343600 |
| H | -5.32563500 | 0.06672800 | 2.68890000 |
| C | -0.72206900 | 2.94097500 | 2.89764000 |
| C | 0.41401300 | 2.76623500 | 3.91962800 |
| C | -0.10473000 | 2.93496100 | 1.49695200 |
| C | -1.43556400 | 4.28023200 | 3.13952000 |
| H | 0.03543100 | 2.73534700 | 4.95054400 |
| H | 0.97541000 | 1.84523900 | 3.71216000 |
| H | 1.11058400 | 3.61536600 | 3.84547900 |
| H | -0.86819500 | 3.00797700 | 0.71275500 |
| H | 0.58087000 | 3.78724800 | 1.38565300 |
| H | 0.47377200 | 2.01817000 | 1.33093400 |
| H | -1.80084000 | 4.37395200 | 4.16961400 |
| H | -0.72909100 | 5.10457900 | 2.95968000 |
| H | -2.28420100 | 4.40029600 | 2.45502500 |

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|---|---|---|---|
| C | 0.03735600 | -3.63198300 | 0.68399000 |
| C | -1.41009800 | -3.33590200 | 0.26642000 |
| C | 0.92417100 | -3.60054300 | -0.57532900 |
| C | 0.05998900 | -5.04516700 | 1.30261300 |
| H | -2.06901900 | -3.31612900 | 1.14692800 |
| H | -1.47943400 | -2.36246400 | -0.24048600 |
| H | -1.79380700 | -4.09720500 | -0.42827500 |
| H | 1.97429800 | -3.79815200 | -0.31602500 |
| H | 0.60039600 | -4.36949200 | -1.29491600 |
| H | 0.87232600 | -2.62169000 | -1.07230900 |
| H | -0.31888700 | -5.79700900 | 0.59117300 |
| H | 1.07333200 | -5.35262900 | 1.59721800 |
| H | -0.57022800 | -5.06791500 | 2.20470000 |
| C | 1.33845400 | -1.19365600 | 4.38440700 |
| C | -0.02316600 | -0.75980500 | 4.92946900 |
| C | 1.48609900 | -2.70392700 | 4.65480500 |
| C | 2.43159300 | -0.42204600 | 5.14359600 |
| H | -0.20206100 | 0.29889200 | 4.72081300 |
| H | -0.83645100 | -1.34473300 | 4.47935000 |
| H | -0.06390000 | -0.91290500 | 6.01822100 |
| H | 2.52151800 | -3.04644500 | 4.54884500 |
| H | 1.17465600 | -2.91170600 | 5.69081600 |
| H | 0.85601600 | -3.27172100 | 3.95863800 |
| H | 2.36312700 | -0.63702100 | 6.22205500 |
| H | 3.43352200 | -0.71836500 | 4.81035700 |
| H | 2.32231700 | 0.66251800 | 4.99735200 |

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|---|---|---|---|
| C | -4.73931300 | -2.10693100 | -0.13181200 |
| C | -4.72875000 | -3.27878500 | -1.11856000 |
| C | -5.90122900 | -2.25529700 | 0.86497300 |
| H | -3.80631200 | -2.13833900 | 0.44351800 |
| H | -3.91859000 | -3.17598600 | -1.85636900 |
| H | -4.58877600 | -4.23227700 | -0.58432700 |
| H | -5.67828700 | -3.35631200 | -1.67199300 |
| H | -5.90695700 | -1.43258900 | 1.59261200 |
| H | -6.86825300 | -2.23753800 | 0.33613100 |
| H | -5.83279200 | -3.20565400 | 1.42145600 |
| C | -3.66485200 | 2.85745900 | -0.09550600 |
| C | -4.51450900 | 3.27627300 | 1.11635100 |
| C | -3.39375300 | 4.04364100 | -1.02265200 |
| H | -2.69677200 | 2.50913700 | 0.28860600 |
| H | -4.61113100 | 2.44063500 | 1.82591500 |
| H | -4.07162200 | 4.13626900 | 1.64522300 |
| H | -5.52600300 | 3.56942800 | 0.79211300 |
| H | -2.81238500 | 3.73175600 | -1.90377400 |
| H | -4.32475800 | 4.51663400 | -1.37509100 |
| H | -2.82023400 | 4.82165500 | -0.49242100 |

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Table S6
B3LYP-D3(BJ)/def2-SVP
**Int2A**
G = -3028.118259 Hartree

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| Si | 1.07144000 | 1.31486400 | 0.24193700 |
| Si | -0.41142100 | 1.63767600 | 2.01078200 |
| N | 2.34447100 | 0.34666300 | 0.51360600 |
| N | -1.21397700 | 0.25701200 | 2.31750100 |
| N | 1.13169800 | 2.90680500 | -0.81880500 |
| N | 0.08101300 | 1.09070600 | -1.32026500 |
| N | 0.60441500 | 2.55650800 | 3.40743800 |
| C | 2.98966100 | -0.64019500 | -0.20200800 |
| C | 0.34493800 | 2.33236800 | -1.73490600 |
| C | -2.29375300 | -0.18568000 | 3.16545700 |
| C | 0.13664700 | 3.76768500 | 3.58127400 |
| C | -0.15856200 | 2.95746400 | -2.98387100 |
| C | 2.83360300 | -2.00845600 | 0.18857800 |
| C | 3.80694500 | -0.35138800 | -1.33946800 |
| C | 1.64658300 | 4.28180500 | -0.70742300 |
| C | 0.60942100 | 2.91806400 | -4.15508000 |
| H | 1.59110600 | 2.44128600 | -4.14336300 |
| C | 2.03523700 | -2.35277000 | 1.43637000 |
| H | 1.33892100 | -1.52107000 | 1.61402000 |
| C | 4.02783500 | 1.09597400 | -1.74286300 |
| H | 3.08779100 | 1.62776300 | -1.54261600 |
| C | -0.47527300 | -0.08795400 | -2.01803800 |

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|---|---|---|---|
| C | -3.11580900 | 0.97770100 | 3.76777200 |
| H | -2.45950000 | 1.63149700 | 4.36642800 |
| H | -3.92390000 | 0.61378300 | 4.42480000 |
| H | -3.57184300 | 1.58939400 | 2.97496300 |
| C | 1.74363100 | 1.91623700 | 4.15664200 |
| C | -0.62294400 | -1.17711200 | -0.94662600 |
| H | 0.36557500 | -1.48918200 | -0.58609600 |
| H | -1.12099900 | -2.05962200 | -1.37427800 |
| H | -1.19812400 | -0.81902900 | -0.07942800 |
| C | 3.46525600 | -3.01585900 | -0.54692700 |
| H | 3.33534400 | -4.05723700 | -0.24240900 |
| C | 0.64126800 | 4.76934700 | 4.56506800 |
| C | -1.74341500 | -1.03671800 | 4.33085500 |
| H | -1.08634100 | -1.82762300 | 3.93903200 |
| H | -2.55508000 | -1.50484600 | 4.91284600 |
| H | -1.15352500 | -0.41293400 | 5.02077000 |
| C | 0.11473100 | 3.49141300 | -5.32866400 |
| H | 0.71325300 | 3.45667000 | -6.24163000 |
| C | -3.23525100 | -1.07843800 | 2.32741100 |
| H | -3.67063400 | -0.50620200 | 1.49330900 |
| H | -4.06231900 | -1.48525400 | 2.93309300 |
| H | -2.66717400 | -1.91803500 | 1.89909600 |
| C | -0.10450600 | 5.01941100 | 5.72587000 |
| H | -1.00661800 | 4.43716400 | 5.92212900 |
| C | -1.41737200 | 3.57174500 | -2.98932600 |
| H | -2.01496800 | 3.58906000 | -2.07940300 |

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|---|---|---|---|
| C | -1.14052700 | 4.10719700 | -5.33428800 |
| H | -1.52456900 | 4.55488300 | -6.25386000 |
| C | 5.09718800 | 1.73961700 | -0.84518600 |
| H | 4.81933100 | 1.62991000 | 0.21329200 |
| H | 5.22176700 | 2.81385100 | -1.06582800 |
| H | 6.07236700 | 1.24811000 | -0.99399200 |
| C | 4.35082200 | 1.29896800 | -3.22579000 |
| H | 5.33990400 | 0.89611300 | -3.49654500 |
| H | 4.36495000 | 2.37312800 | -3.47443000 |
| H | 3.60415000 | 0.80661400 | -3.86949900 |
| C | -1.90373200 | 4.14769600 | -4.16332700 |
| H | -2.88651600 | 4.62431800 | -4.16036700 |
| C | 4.25814000 | -2.72563900 | -1.65718400 |
| H | 4.74245500 | -3.52779600 | -2.21931700 |
| C | 0.50689000 | 5.30161800 | -0.56392400 |
| H | -0.13733100 | 5.31748000 | -1.45283800 |
| H | 0.92220900 | 6.31260900 | -0.42890700 |
| H | -0.11136300 | 5.06273000 | 0.30909700 |
| C | 2.52852300 | 4.64686300 | -1.91306200 |
| H | 3.31276900 | 3.89346300 | -2.06435900 |
| H | 3.01367800 | 5.61894500 | -1.73537800 |
| H | 1.93927200 | 4.73065000 | -2.83525300 |
| C | 4.42564900 | -1.39410400 | -2.03734000 |
| H | 5.05034000 | -1.16506600 | -2.90328300 |
| C | 2.98246400 | -2.43764100 | 2.64457500 |
| H | 3.68071900 | -3.28348200 | 2.52807700 |

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|---|---|---|---|
| H | 2.42201700 | -2.58216200 | 3.58346300 |
| H | 3.58154600 | -1.52042200 | 2.73635700 |
| C | -1.84278400 | 0.21529600 | -2.64390300 |
| H | -2.53053400 | 0.62475300 | -1.89299100 |
| H | -2.27445600 | -0.71701000 | -3.03816000 |
| H | -1.77154000 | 0.92913700 | -3.47495200 |
| C | 0.30545600 | 6.00238500 | 6.62500700 |
| H | -0.27567400 | 6.18227700 | 7.53211200 |
| C | 2.50159800 | 4.29830800 | 0.56579500 |
| H | 1.89142400 | 4.02657600 | 1.43700300 |
| H | 2.91930600 | 5.30217500 | 0.73354300 |
| H | 3.33032600 | 3.58144600 | 0.49290000 |
| C | 0.51817100 | -0.55855000 | -3.09396500 |
| H | 0.62000700 | 0.18772600 | -3.89582000 |
| H | 0.16137800 | -1.49538800 | -3.54896900 |
| H | 1.50815900 | -0.74676500 | -2.65353500 |
| C | 1.66810600 | 2.19662800 | 5.66665600 |
| H | 2.35562600 | 1.50688800 | 6.17753800 |
| H | 0.65420900 | 2.00517300 | 6.04951500 |
| H | 1.95992200 | 3.21691000 | 5.93741200 |
| C | 1.45025900 | 6.76155300 | 6.36200400 |
| H | 1.76826700 | 7.53477100 | 7.06499200 |
| C | 1.77325500 | 5.54702200 | 4.29248700 |
| H | 2.32715400 | 5.39191200 | 3.36645700 |
| C | 1.19771100 | -3.63125500 | 1.31877600 |
| H | 0.54476000 | -3.60659200 | 0.43307400 |

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|---|---|---|---|
| H | 0.55624800 | -3.74583200 | 2.20779700 |
| H | 1.82334100 | -4.53653300 | 1.24990300 |
| C | 2.17787400 | 6.53691700 | 5.19138600 |
| H | 3.06333100 | 7.13743300 | 4.97115400 |
| C | 1.66519500 | 0.40142000 | 3.94297900 |
| H | 0.72948000 | -0.01985900 | 4.32155700 |
| H | 2.50459000 | -0.06514300 | 4.47618800 |
| H | 1.76585400 | 0.14377900 | 2.88105300 |
| C | 3.08048900 | 2.39731900 | 3.56837900 |
| H | 3.16057800 | 2.09944300 | 2.51362600 |
| H | 3.90163300 | 1.90892000 | 4.11439800 |
| H | 3.21207500 | 3.48193900 | 3.66253900 |
| C | -1.39932600 | 3.26038400 | 1.80683700 |
| C | -1.00620600 | 4.17997800 | 2.74511500 |
| C | -2.47460700 | 3.43309200 | 0.81974300 |
| C | -1.69255100 | 5.46927500 | 3.03989300 |
| C | -3.93413200 | 4.79837600 | -0.58609200 |
| C | -4.58034900 | 3.65102200 | -1.06039600 |
| C | -4.15962000 | 2.39484000 | -0.61594300 |
| C | -3.11010700 | 2.28592400 | 0.29585500 |
| C | -2.90161200 | 4.69428300 | 0.34385400 |
| H | -2.76925700 | 1.30692900 | 0.63628100 |
| H | -4.64760400 | 1.49061700 | -0.98651500 |
| H | -5.39966900 | 3.73664700 | -1.77812000 |
| H | -2.41731100 | 5.60190200 | 0.69604000 |
| H | -4.23948600 | 5.78561800 | -0.94090800 |

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|---|---|---|---|
| C | -2.99985100 | 5.44479200 | 3.55113500 |
| C | -1.07802400 | 6.71005000 | 2.81127300 |
| C | -1.75524700 | 7.89921400 | 3.08704500 |
| C | -3.05668300 | 7.86462300 | 3.59636600 |
| C | -3.67718100 | 6.63325200 | 3.82743600 |
| H | -3.48239400 | 4.48014300 | 3.72412400 |
| H | -4.69415800 | 6.59823300 | 4.22548100 |
| H | -0.06398900 | 6.74195500 | 2.41003100 |
| H | -1.26398500 | 8.85779100 | 2.90346600 |
| H | -3.58581400 | 8.79553300 | 3.81345500 |

Table S7
B3LYP-D3(BJ)/def2-SVP
**TS3A**
G = -3028.113637 Hartree

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| Si | 1.07743000 | 0.02578200 | -0.28315900 |
| N | -1.03626500 | 1.30385500 | 0.76052100 |
| C | 3.60042500 | 0.47294900 | -0.75987600 |
| N | 2.37024600 | 1.05178900 | -1.03149300 |
| C | 2.22806200 | -1.34665500 | -0.04115400 |
| C | 3.53702900 | -0.83332800 | -0.24557500 |

| | | | |
|---|---|---|---|
| N | -0.36728900 | -0.31110400 | -1.26296900 |
| Si | -1.69027600 | 0.21472000 | -0.27414700 |
| N | -3.35143200 | 0.58015700 | -1.06154800 |
| N | -2.91443400 | -1.21945300 | 0.07269000 |
| C | -1.31560600 | 2.04327100 | 1.91022500 |
| C | -3.86847900 | -0.56664500 | -0.59400200 |
| C | -1.69320700 | 1.41701200 | 3.15175400 |
| C | -1.20188900 | 3.47757500 | 1.93949200 |
| C | -2.01335600 | 2.18475200 | 4.27578800 |
| H | -2.29459800 | 1.68518700 | 5.20192700 |
| C | -1.97144500 | 3.57534100 | 4.25948800 |
| C | -1.55455500 | 4.19511300 | 3.09223000 |
| H | -1.47279700 | 5.28417900 | 3.07323700 |
| C | -0.35265600 | -0.98840100 | -2.60546200 |
| C | -1.33375600 | -0.28539700 | -3.55284100 |
| H | -1.10546100 | 0.78501600 | -3.64030900 |
| H | -1.27763400 | -0.72958900 | -4.55840200 |
| H | -2.36708600 | -0.38436600 | -3.19815500 |
| C | 1.04776700 | -0.94438700 | -3.23587100 |
| H | 1.37379600 | 0.08101400 | -3.43369600 |
| H | 1.79551100 | -1.41432400 | -2.58386200 |
| H | 1.02706800 | -1.48473600 | -4.19435100 |
| C | -0.76620300 | -2.45998800 | -2.50639200 |
| H | -0.07062100 | -3.02184300 | -1.87189600 |
| H | -1.77536900 | -2.55231000 | -2.09272100 |
| H | -0.76779800 | -2.92164000 | -3.50623000 |

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|---|---|---|---|
| C | -0.61433400 | 4.32606600 | 0.81919100 |
| H | -0.37332700 | 3.65894100 | -0.01426400 |
| C | 0.68342200 | 5.00142800 | 1.30268700 |
| H | 1.39675900 | 4.27180100 | 1.71057200 |
| H | 1.17317900 | 5.55298900 | 0.48544100 |
| H | 0.46403500 | 5.72544600 | 2.10272900 |
| C | -1.56209800 | 5.43100200 | 0.31517700 |
| H | -2.57170100 | 5.06062000 | 0.10880200 |
| H | -1.66068500 | 6.23507900 | 1.06188300 |
| H | -1.16776100 | 5.89141900 | -0.60620800 |
| C | -1.67067200 | -0.09306900 | 3.29847100 |
| H | -2.09469200 | -0.51075300 | 2.37451600 |
| C | -0.22759800 | -0.60289400 | 3.41639900 |
| H | -0.20328700 | -1.70220500 | 3.48526000 |
| H | 0.37284100 | -0.29856300 | 2.54774800 |
| H | 0.24837700 | -0.19382400 | 4.32220100 |
| C | -2.50273000 | -0.61799500 | 4.47495800 |
| H | -2.08496000 | -0.29766100 | 5.44129700 |
| H | -3.54887400 | -0.27418400 | 4.42756600 |
| H | -2.50226600 | -1.71885000 | 4.49225300 |
| C | -5.26227800 | -1.02790400 | -0.80061100 |
| C | -5.67468800 | -1.42846500 | -2.07867500 |
| C | -6.17564700 | -1.03511900 | 0.26124100 |
| C | -6.98897300 | -1.84881200 | -2.28726700 |
| H | -4.96045600 | -1.41878800 | -2.90414200 |
| C | -7.49119300 | -1.44698300 | 0.04731800 |

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|---|---|---|---|
| H | -5.86220400 | -0.68817600 | 1.24650300 |
| C | -7.89885900 | -1.85815200 | -1.22523300 |
| H | -7.30608300 | -2.16649500 | -3.28295100 |
| H | -8.20127400 | -1.44217700 | 0.87718700 |
| H | -8.92898100 | -2.18176100 | -1.39026700 |
| C | 4.90427600 | 1.19561400 | -0.74518400 |
| C | 5.89870000 | 0.88141600 | -1.68513800 |
| C | 5.21401100 | 2.11907600 | 0.26717900 |
| C | 7.14702400 | 1.50601800 | -1.64544500 |
| H | 5.67839000 | 0.14036900 | -2.45609800 |
| C | 6.45989200 | 2.74724400 | 0.30899200 |
| H | 4.46748000 | 2.33791300 | 1.03264700 |
| C | 7.42846700 | 2.45038700 | -0.65464700 |
| H | 7.90296800 | 1.25535800 | -2.39373500 |
| H | 6.67797800 | 3.46794500 | 1.10129000 |
| H | 8.40175800 | 2.94669300 | -0.62732300 |
| C | 4.76193900 | -1.57584800 | 0.16785600 |
| C | 5.23059200 | -2.65592900 | -0.59572800 |
| C | 5.46618200 | -1.22552600 | 1.33051100 |
| C | 6.37472100 | -3.36105600 | -0.21518900 |
| H | 4.69110300 | -2.93582600 | -1.50280700 |
| C | 6.61246700 | -1.92500500 | 1.71197700 |
| H | 5.11016600 | -0.38862300 | 1.93440400 |
| C | 7.07163700 | -2.99569200 | 0.93934400 |
| H | 6.72528800 | -4.19766200 | -0.82509400 |
| H | 7.15125200 | -1.63196800 | 2.61674300 |

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|---|---|---|---|
| H | 7.96970900 | -3.54314800 | 1.23630700 |
| C | -4.04203700 | 1.79133600 | -1.57578700 |
| C | -2.93386700 | -2.62111100 | 0.58766100 |
| C | 2.22740000 | 2.34427400 | -1.77140300 |
| C | 2.00654500 | -2.70428500 | 0.50216900 |
| C | 1.94839100 | -3.81196200 | -0.36473300 |
| C | 1.88105300 | -2.94737500 | 1.88038600 |
| C | 1.73538900 | -5.10351400 | 0.12114900 |
| H | 2.07816600 | -3.64884100 | -1.43639500 |
| C | 1.66065700 | -4.23647100 | 2.37066300 |
| H | 1.96853300 | -2.10717300 | 2.56879000 |
| C | 1.57883400 | -5.32117200 | 1.49309900 |
| H | 1.69162000 | -5.94448900 | -0.57600100 |
| H | 1.56212800 | -4.39518400 | 3.44784200 |
| H | 1.40927100 | -6.33053500 | 1.87599800 |
| C | 0.75547900 | 2.53669600 | -2.16323100 |
| H | 0.44431300 | 1.81305800 | -2.92232500 |
| H | 0.09238800 | 2.42970500 | -1.29714500 |
| H | 0.62035800 | 3.54465700 | -2.58062900 |
| C | 2.65404300 | 3.54063300 | -0.90691300 |
| H | 2.25406100 | 4.47456700 | -1.32799800 |
| H | 2.26100900 | 3.42407200 | 0.10699900 |
| H | 3.74249200 | 3.64043400 | -0.85053500 |
| C | 3.06189400 | 2.33135700 | -3.06506600 |
| H | 4.13824700 | 2.32522600 | -2.86083200 |
| H | 2.82439400 | 1.45819600 | -3.68881500 |

| | | | |
|---|---|---|---|
| H | 2.83592700 | 3.24006300 | -3.64477300 |
| C | -3.26672600 | 2.99387600 | -1.03689700 |
| H | -3.29559600 | 3.01749700 | 0.06113300 |
| H | -2.21232400 | 2.96498200 | -1.34229100 |
| H | -3.71148600 | 3.92146000 | -1.42362900 |
| C | -4.01633500 | 1.81745900 | -3.11296000 |
| H | -4.49117000 | 0.92163600 | -3.54099400 |
| H | -4.56472600 | 2.70043700 | -3.47483500 |
| H | -2.98744100 | 1.88199400 | -3.48952200 |
| C | -5.49828500 | 1.91268400 | -1.09201100 |
| H | -6.17283200 | 1.19705600 | -1.57784800 |
| H | -5.57282100 | 1.78524800 | -0.00206300 |
| H | -5.85690600 | 2.92322700 | -1.33711000 |
| C | -3.66434400 | -2.71102300 | 1.93813500 |
| H | -3.10258700 | -2.19639300 | 2.72406700 |
| H | -4.67798600 | -2.28552300 | 1.89642200 |
| H | -3.75379800 | -3.77141500 | 2.22489900 |
| C | -1.47719300 | -3.04581300 | 0.80645300 |
| H | -0.95589000 | -3.22782000 | -0.13078600 |
| H | -0.91714200 | -2.28509400 | 1.35711100 |
| H | -1.43806600 | -3.97279100 | 1.39308300 |
| C | -3.62756300 | -3.59393600 | -0.38707300 |
| H | -4.72073900 | -3.50429000 | -0.34979100 |
| H | -3.30669200 | -3.44813100 | -1.42652200 |
| H | -3.36909000 | -4.62327200 | -0.09716200 |
| H | -2.22966200 | 4.15721300 | 5.14775200 |

Table S8
uB3LYP-D3(BJ)/def2-SVP
**2a (Singlet)**
G = -3028.166103 Hartree

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| Si | -0.00717000 | -0.02509500 | -0.00070400 |
| Si | -0.03985900 | 0.00945600 | 2.57435400 |
| N | 1.22360600 | 0.01677400 | 1.20004600 |
| N | -1.21137800 | 0.02183800 | 1.18253100 |
| N | -0.32580400 | 0.90021800 | -1.58922600 |
| N | 0.16611700 | -1.19578800 | -1.38881300 |
| N | -0.04507900 | 1.35575300 | 3.71655600 |
| C | 2.65311600 | 0.02995500 | 1.19696700 |
| C | -0.43236300 | -0.58029000 | 5.05536100 |
| C | -0.60482000 | -3.26509400 | 2.33453300 |
| H | -0.87573300 | -2.57969700 | 1.53118000 |
| C | -0.18939800 | -0.24937600 | -2.27620700 |
| C | -0.25530400 | -1.28212000 | 3.80891000 |
| C | -2.68609800 | -0.04439700 | 1.23829900 |
| C | -0.36009700 | 0.81141500 | 5.01449100 |
| C | -0.46811700 | -0.47689000 | -3.71106100 |

| | | | |
|---|---|---|---|
| C | 3.40066200 | -0.83563000 | 2.04897800 |
| C | -0.29728900 | -2.71771400 | 3.61079200 |
| C | 3.37786300 | 0.93191200 | 0.36378900 |
| C | -0.90784100 | 2.19747500 | -2.03161800 |
| C | -0.59110900 | -4.63649300 | 2.08411000 |
| H | -0.83283800 | -5.00323400 | 1.08287500 |
| C | 0.43900200 | -0.08006800 | -4.70312300 |
| H | 1.36631600 | 0.41673200 | -4.41881900 |
| C | 2.78408200 | -1.92128400 | 2.91005800 |
| H | 1.72588700 | -1.98704400 | 2.66047400 |
| C | 0.00815000 | -3.66949000 | 4.62337600 |
| H | 0.26489000 | -3.32255100 | 5.62142300 |
| C | 2.73823200 | 1.77510500 | -0.72571500 |
| H | 1.65314600 | 1.75460500 | -0.58925800 |
| C | 0.61383800 | -2.59942000 | -1.57778000 |
| C | -3.27534400 | 1.37673100 | 1.26600400 |
| H | -2.82087700 | 1.94704700 | 2.08932100 |
| H | -4.36458600 | 1.34535900 | 1.42395500 |
| H | -3.08746600 | 1.91900000 | 0.33164100 |
| C | 0.78915100 | 2.59231400 | 3.61810800 |
| C | 1.60388200 | -2.90104200 | -0.44686800 |
| H | 2.49065200 | -2.25522500 | -0.51844300 |
| H | 1.92791700 | -3.94925600 | -0.50886700 |
| H | 1.15117300 | -2.75779300 | 0.54035500 |
| C | 4.79436300 | -0.70725100 | 2.11507900 |
| H | 5.34298500 | -1.36448100 | 2.79220000 |

| | | | |
|---|---|---|---|
| C | -1.14711700 | 1.62840700 | 5.97009200 |
| C | -0.94312300 | -1.27787900 | 6.26826000 |
| C | -3.16420800 | -0.76349200 | 2.51210600 |
| H | -2.75334200 | -1.77726200 | 2.58817600 |
| H | -4.26351700 | -0.82884300 | 2.49359600 |
| H | -2.87170200 | -0.21305700 | 3.41623700 |
| C | 0.16603500 | -0.35284600 | -6.04375600 |
| H | 0.88112700 | -0.05245100 | -6.81250000 |
| C | 0.01147200 | -5.03833400 | 4.37242800 |
| H | 0.26058100 | -5.72458100 | 5.18694800 |
| C | -3.19702000 | -0.82418500 | 0.01735600 |
| H | -2.85505800 | -0.36740900 | -0.92339800 |
| H | -4.29737700 | -0.84501400 | -0.00201500 |
| H | -2.83595400 | -1.86252500 | 0.04886400 |
| C | -0.83279100 | 1.72672500 | 7.33726200 |
| H | 0.06992900 | 1.24232500 | 7.70814100 |
| C | -1.64904900 | -1.14414400 | -4.07043100 |
| H | -2.35415500 | -1.44886200 | -3.29512500 |
| C | -1.01374900 | -1.01265100 | -6.40189100 |
| H | -1.22469300 | -1.22325400 | -7.45260500 |
| C | 3.14821400 | 3.25324000 | -0.68233700 |
| H | 2.95125700 | 3.68691500 | 0.30815700 |
| H | 2.58388400 | 3.83457100 | -1.42968900 |
| H | 4.21714700 | 3.39147600 | -0.90499700 |
| C | -0.28311900 | -5.54509300 | 3.09991100 |
| H | -0.27610900 | -6.62034200 | 2.90789400 |

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|---|---|---|---|
| C | 3.04832500 | 1.14886800 | -2.09655300 |
| H | 4.13480000 | 1.11631400 | -2.26941600 |
| H | 2.59706600 | 1.72438600 | -2.91885100 |
| H | 2.67893600 | 0.11380000 | -2.14970300 |
| C | -0.14303900 | -1.43116500 | 7.41073800 |
| H | 0.87013700 | -1.02365300 | 7.40002300 |
| C | -1.92204100 | -1.40455800 | -5.41400500 |
| H | -2.84599600 | -1.91750400 | -5.68926100 |
| C | 5.49155700 | 0.21400300 | 1.34542300 |
| H | 6.57803100 | 0.29961100 | 1.41881300 |
| C | -2.37148500 | 2.01810700 | -2.46827000 |
| H | -2.45199600 | 1.34762000 | -3.33461300 |
| H | -2.79090500 | 2.99289300 | -2.75867600 |
| H | -2.98749400 | 1.61374100 | -1.65619000 |
| C | -0.11362400 | 2.81685300 | -3.19266400 |
| H | 0.95206100 | 2.89559200 | -2.94509600 |
| H | -0.49258200 | 3.83304700 | -3.37703300 |
| H | -0.22390000 | 2.24874800 | -4.12376600 |
| C | 4.77333600 | 1.00665500 | 0.45979000 |
| H | 5.30939800 | 1.70722900 | -0.18348000 |
| C | 2.88607700 | -1.57834200 | 4.40316100 |
| H | 3.94044200 | -1.52912600 | 4.72281900 |
| H | 2.38137300 | -2.34811500 | 5.00357900 |
| H | 2.41014300 | -0.61660700 | 4.63102300 |
| C | -0.60748400 | -3.52624300 | -1.48812600 |
| H | -1.13914700 | -3.38114800 | -0.53872500 |

| | | | |
|---|---|---|---|
| H | -0.29003800 | -4.57802800 | -1.54384700 |
| H | -1.30768800 | -3.33623300 | -2.31429100 |
| C | -1.64349500 | 2.44937800 | 8.21577400 |
| H | -1.37316100 | 2.50665400 | 9.27362400 |
| C | -0.82129700 | 3.14936900 | -0.83514700 |
| H | -1.26451100 | 2.70691100 | 0.06214200 |
| H | -1.35810300 | 4.08159200 | -1.06110400 |
| H | 0.22152700 | 3.40582500 | -0.60972600 |
| C | 1.33470900 | -2.80215300 | -2.91877400 |
| H | 0.65946400 | -2.75584000 | -3.78124600 |
| H | 1.79989000 | -3.79860300 | -2.91252500 |
| H | 2.13472200 | -2.05961400 | -3.05593800 |
| C | 0.66386600 | 3.14371300 | 2.19675000 |
| H | 1.00737600 | 2.41881200 | 1.45291800 |
| H | 1.26960800 | 4.05525500 | 2.08402100 |
| H | -0.38403300 | 3.39826700 | 1.98581300 |
| C | -2.23209500 | -1.83241800 | 6.27690000 |
| H | -2.85465000 | -1.73228000 | 5.38615100 |
| C | -2.78572000 | 3.10533200 | 7.75041500 |
| H | -3.41666300 | 3.67431300 | 8.43770700 |
| C | -2.30557100 | 2.29515800 | 5.51871200 |
| H | -2.56629500 | 2.22543700 | 4.46060800 |
| C | 3.38449400 | -3.30905200 | 2.63551400 |
| H | 3.39148700 | -3.54470700 | 1.56133100 |
| H | 2.78169400 | -4.07438800 | 3.14829500 |
| H | 4.42071900 | -3.39284600 | 3.00200500 |

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|---|---|---|---|
| C | -3.11152400 | 3.02334200 | 6.39114900 |
| H | -4.00779600 | 3.52294800 | 6.01251000 |
| C | -0.61824700 | -2.11187800 | 8.53445200 |
| H | 0.02142800 | -2.22329600 | 9.41394600 |
| C | -2.71280700 | -2.50817300 | 7.39903500 |
| H | -3.72203300 | -2.92804200 | 7.38901900 |
| C | -1.90697600 | -2.65169600 | 8.53300300 |
| H | -2.28170400 | -3.18445400 | 9.41067300 |
| C | 0.35162300 | 3.72166600 | 4.56665900 |
| H | -0.69725900 | 4.00409900 | 4.41173500 |
| H | 0.98046500 | 4.60234100 | 4.36142800 |
| H | 0.47729600 | 3.45879300 | 5.62282700 |
| C | 2.25537700 | 2.24942700 | 3.93921800 |
| H | 2.31622400 | 1.80263600 | 4.94289300 |
| H | 2.88773400 | 3.15174700 | 3.92325900 |
| H | 2.67070200 | 1.53310700 | 3.21936900 |

Table S9
B3LYP-D3(BJ)/def2-SVP
**TS1B**
G = -3028.051304 Hartree

| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |

| | | | |
|---|---|---|---|
| Si | -0.51973700 | 0.46836100 | -0.80510200 |
| C | -0.90521000 | 1.12001300 | 3.57383800 |
| C | 0.26100000 | 0.70347900 | 3.41771900 |
| Si | 0.84669500 | 0.01340200 | 1.10842500 |
| N | 0.79792100 | -1.84467800 | 1.45368000 |
| N | -1.02700800 | 2.32520900 | -0.61536000 |
| N | -2.37982600 | 0.62817700 | -0.61307500 |
| N | -0.08655200 | -0.12936000 | -2.23049300 |
| N | 2.33956200 | -0.87765800 | 0.30471000 |
| C | -0.11068600 | -2.86351300 | 2.01306500 |
| C | 2.01303400 | -2.02476500 | 0.90372500 |
| C | -0.41427400 | 3.61473600 | -0.21570700 |
| C | -2.30772000 | 1.96772100 | -0.55708200 |
| C | -3.49783300 | -0.22167700 | -1.08091500 |
| C | 0.57846700 | -0.34402700 | -3.38996500 |
| C | 3.57473700 | -0.50220400 | -0.40922300 |
| C | 1.42582000 | 0.18878900 | 4.13302900 |
| C | -1.33837200 | -2.12624500 | 2.55658700 |
| C | -0.53968000 | -3.82061600 | 0.88669900 |
| C | 0.52345800 | -3.66327400 | 3.16601500 |
| C | 2.90160400 | -3.19382800 | 1.15150600 |
| C | 1.10445400 | 3.43261600 | -0.28519000 |
| C | -0.78960200 | 3.96158000 | 1.23246600 |
| C | -0.82436700 | 4.74695000 | -1.17108200 |
| C | -3.47306300 | 2.88623800 | -0.49298900 |
| C | -3.11463200 | -1.66533500 | -0.73993500 |

| | | | |
|---|---|---|---|
| C | -4.82520200 | 0.10526800 | -0.37873400 |
| C | -3.64069200 | -0.06534100 | -2.60475400 |
| C | 0.98459200 | 0.74738700 | -4.22770200 |
| C | 0.90163700 | -1.67455600 | -3.81580700 |
| C | 3.33562600 | 0.89287300 | -0.99442600 |
| C | 3.83403400 | -1.47796100 | -1.56821400 |
| C | 4.78488700 | -0.45413000 | 0.53895200 |
| C | 2.74066700 | 0.46415000 | 3.72272600 |
| C | 1.23255700 | -0.61933700 | 5.27017000 |
| C | -2.22787900 | 1.58567300 | 3.71101600 |
| H | -1.72271600 | -1.40871000 | 1.81909500 |
| H | -2.13760800 | -2.84536500 | 2.78951100 |
| H | -1.09250500 | -1.57133900 | 3.46896900 |
| H | -0.98286200 | -3.26311600 | 0.05229800 |
| H | -1.28210300 | -4.54365000 | 1.25890600 |
| H | 0.31930200 | -4.38701600 | 0.50320800 |
| H | 1.28814000 | -4.36568900 | 2.81309700 |
| H | -0.25906400 | -4.24930000 | 3.67322700 |
| H | 0.98105200 | -2.98766200 | 3.90202700 |
| C | 2.97100500 | -4.28606800 | 0.27984600 |
| C | 3.67189100 | -3.19316200 | 2.32541800 |
| H | 1.42528500 | 2.64579200 | 0.41307500 |
| H | 1.60622600 | 4.36654900 | 0.00691200 |
| H | 1.43503800 | 3.16625000 | -1.29716600 |
| H | -0.49399400 | 3.14475800 | 1.90512800 |
| H | -0.26415800 | 4.87680100 | 1.54693100 |

| | | | |
|---|---|---|---|
| H | -1.86637000 | 4.13706700 | 1.34736500 |
| H | -0.62192900 | 4.46598100 | -2.21397500 |
| H | -0.24140800 | 5.65135400 | -0.93905300 |
| H | -1.88741100 | 5.00050100 | -1.07610900 |
| C | -3.90480200 | 3.52630800 | -1.66320200 |
| C | -4.15678300 | 3.08991700 | 0.71056300 |
| H | -3.12031200 | -1.82251500 | 0.34656500 |
| H | -3.83064700 | -2.36621100 | -1.19289500 |
| H | -2.11638700 | -1.90199500 | -1.12676800 |
| H | -4.68896200 | 0.16000500 | 0.71147000 |
| H | -5.54725300 | -0.69657800 | -0.59734900 |
| H | -5.26407000 | 1.04969000 | -0.72162400 |
| H | -3.92451500 | 0.96479000 | -2.86507700 |
| H | -4.42096300 | -0.73996000 | -2.98991200 |
| H | -2.68847300 | -0.29930800 | -3.10015300 |
| C | 0.55040700 | 2.15273700 | -3.85448900 |
| C | 1.70500900 | 0.49762700 | -5.39749100 |
| C | 0.41129000 | -2.84788800 | -2.98738500 |
| C | 1.61619300 | -1.87102200 | -5.00080400 |
| H | 3.20739700 | 1.63406700 | -0.19378300 |
| H | 4.19624600 | 1.19901300 | -1.60641000 |
| H | 2.44283000 | 0.89123500 | -1.63454300 |
| H | 2.96124400 | -1.52660900 | -2.23367900 |
| H | 4.69166400 | -1.12563300 | -2.16127800 |
| H | 4.07078600 | -2.48648700 | -1.20587400 |
| H | 4.58566200 | 0.21524000 | 1.38848400 |

| | | | |
|---|---|---|---|
| H | 5.66638400 | -0.07371300 | -0.00007200 |
| H | 5.03359200 | -1.44840900 | 0.93280800 |
| C | 3.83090000 | -0.05611900 | 4.42128600 |
| H | 2.88995500 | 1.08857100 | 2.84058100 |
| C | 2.32338600 | -1.15680900 | 5.95539400 |
| H | 0.21324700 | -0.82578300 | 5.60189000 |
| C | -3.34335800 | 0.71880900 | 3.55406800 |
| C | -2.49143400 | 2.93678800 | 4.06601300 |
| C | 3.80101400 | -5.36993600 | 0.57853600 |
| H | 2.38080800 | -4.28619800 | -0.63459300 |
| C | 4.50195400 | -4.27490900 | 2.61845700 |
| H | 3.60630500 | -2.34675300 | 3.01050800 |
| C | -5.02342000 | 4.36088100 | -1.62673000 |
| H | -3.36234200 | 3.36642000 | -2.59655900 |
| C | -5.26588200 | 3.93525700 | 0.74448100 |
| H | -3.82549400 | 2.58290700 | 1.61380600 |
| C | 1.47211600 | 3.26311700 | -4.36315000 |
| C | -0.90340500 | 2.39169000 | -4.29707900 |
| H | 0.55295400 | 2.19967300 | -2.75728700 |
| C | 2.03323100 | -0.80047200 | -5.79260900 |
| H | 2.01435300 | 1.33688500 | -6.02453800 |
| C | 1.25911900 | -4.11567000 | -3.12555500 |
| C | -1.05507800 | -3.16148500 | -3.32886500 |
| H | 0.44632000 | -2.51916300 | -1.93523400 |
| H | 1.86031700 | -2.88770200 | -5.31630100 |
| C | 3.62776100 | -0.87981800 | 5.53349900 |

| | | | |
|---|---|---|---|
| H | 4.84594400 | 0.17666700 | 4.09019700 |
| H | 2.15318000 | -1.79650400 | 6.82490000 |
| C | -4.64133900 | 1.17980500 | 3.75988300 |
| H | -3.17347500 | -0.32054300 | 3.27692300 |
| C | -3.79380900 | 3.38227700 | 4.26768900 |
| H | -1.65132100 | 3.62070500 | 4.19462600 |
| C | 4.56736500 | -5.36681100 | 1.74659000 |
| H | 3.84862500 | -6.21815400 | -0.10806900 |
| H | 5.09601500 | -4.26666300 | 3.53527900 |
| C | -5.70390900 | 4.56802700 | -0.42264300 |
| H | -5.36192100 | 4.85315200 | -2.54113600 |
| H | -5.78826900 | 4.08944200 | 1.69055100 |
| H | 1.43971700 | 3.35950600 | -5.46049000 |
| H | 1.16797500 | 4.23691600 | -3.94522200 |
| H | 2.51885800 | 3.07965500 | -4.07364100 |
| H | -0.98923700 | 2.32234700 | -5.39351900 |
| H | -1.25926300 | 3.39054500 | -3.99186700 |
| H | -1.56802700 | 1.63711500 | -3.85447500 |
| H | 2.59948600 | -0.97566900 | -6.71030500 |
| H | 1.16365800 | -4.56418600 | -4.12728700 |
| H | 0.92810200 | -4.87967300 | -2.40289700 |
| H | 2.32711900 | -3.91239800 | -2.95676000 |
| H | -1.13005000 | -3.54779500 | -4.35856800 |
| H | -1.47804500 | -3.91899900 | -2.64708900 |
| H | -1.67261600 | -2.25719200 | -3.26643400 |
| H | 4.48114300 | -1.29935400 | 6.07156200 |

| | | | |
|---|---|---|---|
| C | -4.88138900 | 2.51092900 | 4.12125000 |
| H | -5.47911600 | 0.48927900 | 3.63373800 |
| H | -3.96469000 | 4.42544800 | 4.54562800 |
| H | 5.21595500 | -6.21493900 | 1.97827700 |
| H | -6.57694000 | 5.22433200 | -0.39516300 |
| H | -5.90130200 | 2.86423400 | 4.28718900 |

Table S10
B3LYP-D3(BJ)/def2-SVP
**Int1B**
G = -3028.102258 Hartree

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| Si | -0.19910800 | 0.42847400 | -0.71874300 |
| C | -0.69446300 | 0.41160600 | 2.61311100 |
| C | 0.62948100 | 0.62315700 | 2.86179600 |
| Si | 0.45636500 | -0.40119500 | 1.36274600 |
| N | 0.51288800 | -2.25888800 | 1.53491300 |
| N | -0.72755000 | 2.26480600 | -0.38772100 |
| N | -2.07063600 | 0.61856200 | -0.78143800 |
| N | 0.51786100 | -0.13123900 | -2.06282500 |
| N | 2.27429600 | -1.21193000 | 0.79917100 |
| C | -0.30819900 | -3.29759600 | 2.20517900 |

| | | | |
|---|---|---|---|
| C | 1.79084900 | -2.39427000 | 1.08312600 |
| C | -0.13717900 | 3.54105600 | 0.06982900 |
| C | -2.00990200 | 1.93106000 | -0.53993800 |
| C | -3.14315600 | -0.21850400 | -1.34949400 |
| C | 0.35245600 | -0.27120800 | -3.41908100 |
| C | 3.55512300 | -0.84116100 | 0.16692500 |
| C | 1.44639400 | 1.22134700 | 3.91828600 |
| C | -1.58632600 | -2.64097200 | 2.72845700 |
| C | -0.71915800 | -4.40520100 | 1.21685900 |
| C | 0.43576900 | -3.89552100 | 3.41372700 |
| C | 2.50473000 | -3.69489800 | 0.92697600 |
| C | 1.37880500 | 3.33677100 | 0.05392000 |
| C | -0.56726700 | 3.87623900 | 1.50593700 |
| C | -0.50288600 | 4.70035400 | -0.87170400 |
| C | -3.16992300 | 2.86018000 | -0.50737100 |
| C | -2.77838800 | -1.66358400 | -0.98480400 |
| C | -4.52772500 | 0.10948500 | -0.76843000 |
| C | -3.16128200 | -0.05630800 | -2.87960400 |
| C | 0.11714000 | 0.83714900 | -4.29941100 |
| C | 0.42110300 | -1.57484400 | -4.01042100 |
| C | 3.46779500 | 0.65088400 | -0.16665400 |
| C | 3.78612100 | -1.59696600 | -1.14980200 |
| C | 4.71947900 | -1.05893300 | 1.14943200 |
| C | 2.65460500 | 1.87684600 | 3.61495100 |
| C | 1.07798000 | 1.10543200 | 5.27463300 |
| C | -1.94194900 | 0.89273500 | 3.21146900 |

| | | | |
|---|---|---|---|
| H | -2.14139700 | -2.17431200 | 1.90832100 |
| H | -2.22988300 | -3.40596200 | 3.18668500 |
| H | -1.37221000 | -1.87260400 | 3.48046300 |
| H | -1.16582400 | -3.96489500 | 0.31290100 |
| H | -1.46526500 | -5.06594900 | 1.68508700 |
| H | 0.13082900 | -5.02784000 | 0.91533900 |
| H | 1.29620400 | -4.50512700 | 3.11363600 |
| H | -0.24537100 | -4.54225200 | 3.98833900 |
| H | 0.78769900 | -3.09074000 | 4.07759300 |
| C | 2.24739300 | -4.50415500 | -0.18653100 |
| C | 3.45590800 | -4.10598600 | 1.87064200 |
| H | 1.65305500 | 2.53506600 | 0.74881300 |
| H | 1.88997300 | 4.25612600 | 0.37441700 |
| H | 1.73573800 | 3.06887400 | -0.94845900 |
| H | -0.28896500 | 3.06285800 | 2.18526000 |
| H | -0.06014500 | 4.79475500 | 1.83941700 |
| H | -1.64903500 | 4.04270200 | 1.58180400 |
| H | -0.25166200 | 4.45483400 | -1.91156600 |
| H | 0.06766400 | 5.59648100 | -0.58376000 |
| H | -1.56937600 | 4.95266800 | -0.81935900 |
| C | -3.57338000 | 3.49187900 | -1.69227100 |
| C | -3.87221000 | 3.08809600 | 0.68160100 |
| H | -2.85525000 | -1.82254700 | 0.09962300 |
| H | -3.45548500 | -2.37072800 | -1.48546600 |
| H | -1.74880200 | -1.89174600 | -1.29382600 |
| H | -4.50096200 | 0.14418500 | 0.32946400 |

| | | | |
|---|---|---|---|
| H | -5.23496200 | -0.67708500 | -1.07333200 |
| H | -4.91841800 | 1.06773800 | -1.13243500 |
| H | -3.38419700 | 0.98518600 | -3.15531600 |
| H | -3.93934400 | -0.69792500 | -3.32179200 |
| H | -2.19338400 | -0.32780800 | -3.32230800 |
| C | 0.13951900 | 2.25371100 | -3.75580000 |
| C | -0.07338100 | 0.62130600 | -5.66777500 |
| C | 0.73990600 | -2.80246100 | -3.17047200 |
| C | 0.21078600 | -1.73897700 | -5.38374300 |
| H | 3.29964000 | 1.24390300 | 0.74039900 |
| H | 4.40746200 | 0.99036000 | -0.62676300 |
| H | 2.64934400 | 0.83051900 | -0.87568200 |
| H | 2.92380700 | -1.43719500 | -1.81036900 |
| H | 4.68477500 | -1.20243200 | -1.64898000 |
| H | 3.93430300 | -2.67314300 | -0.99868600 |
| H | 4.50390200 | -0.57300400 | 2.11388000 |
| H | 5.64225200 | -0.61979300 | 0.73903000 |
| H | 4.90898300 | -2.12534500 | 1.32603200 |
| C | 3.44897900 | 2.42523900 | 4.62289500 |
| H | 2.96367300 | 1.95716500 | 2.57265600 |
| C | 1.87938500 | 1.63982300 | 6.28307200 |
| H | 0.15619800 | 0.57848500 | 5.52956100 |
| C | -3.17548100 | 0.31572100 | 2.84794800 |
| C | -1.97685200 | 1.99355700 | 4.09696400 |
| C | 2.93695400 | -5.70461900 | -0.36015400 |
| H | 1.51504500 | -4.17797700 | -0.92243300 |

| | | | |
|---|---|---|---|
| C | 4.13986000 | -5.31161000 | 1.70059300 |
| H | 3.65129200 | -3.48363000 | 2.74525400 |
| C | -4.68220600 | 4.33970900 | -1.68604300 |
| H | -3.01298500 | 3.32335900 | -2.61302400 |
| C | -4.97865300 | 3.93899700 | 0.68260800 |
| H | -3.56316900 | 2.58929900 | 1.59796100 |
| C | 1.58772500 | 2.76815000 | -3.69406300 |
| C | -0.76124700 | 3.23183400 | -4.51821600 |
| H | -0.22954000 | 2.21288200 | -2.72308100 |
| C | -0.04304800 | -0.65734800 | -6.22360000 |
| H | -0.25170700 | 1.47644900 | -6.32310500 |
| C | 2.02454300 | -3.48929300 | -3.66480500 |
| C | -0.42368300 | -3.80700300 | -3.13576600 |
| H | 0.90531000 | -2.43367600 | -2.14656700 |
| H | 0.25254900 | -2.74579600 | -5.80903700 |
| C | 3.06560800 | 2.30932800 | 5.96221000 |
| H | 4.37713900 | 2.93969300 | 4.36133200 |
| H | 1.57773500 | 1.53366800 | 7.32839300 |
| C | -4.38288600 | 0.78268100 | 3.36843700 |
| H | -3.17628200 | -0.50095000 | 2.13033100 |
| C | -3.18405200 | 2.48025700 | 4.59686200 |
| H | -1.04340300 | 2.47847700 | 4.38237600 |
| C | 3.88434200 | -6.11187600 | 0.58348500 |
| H | 2.73386700 | -6.32140500 | -1.23845200 |
| H | 4.87621800 | -5.62555600 | 2.44385300 |
| C | -5.38769800 | 4.56318100 | -0.49924600 |

| | | | |
|---|---|---|---|
| H | -4.99463600 | 4.82859500 | -2.61148500 |
| H | -5.52309800 | 4.10799700 | 1.61424600 |
| H | 2.02039400 | 2.81734100 | -4.70655000 |
| H | 1.64422000 | 3.77688000 | -3.25127800 |
| H | 2.21246800 | 2.08957200 | -3.09450200 |
| H | -0.38148400 | 3.44737200 | -5.52953100 |
| H | -0.82306800 | 4.19670500 | -3.98967800 |
| H | -1.78254000 | 2.83227900 | -4.62728700 |
| H | -0.20464100 | -0.80454600 | -7.29444100 |
| H | 1.89385000 | -3.88082600 | -4.68639800 |
| H | 2.30401400 | -4.34024700 | -3.02160600 |
| H | 2.87135100 | -2.78696800 | -3.68494300 |
| H | -0.60982700 | -4.23571700 | -4.13394400 |
| H | -0.20920800 | -4.64760500 | -2.45160300 |
| H | -1.35675600 | -3.32990700 | -2.80373900 |
| H | 3.69071300 | 2.73131200 | 6.75277700 |
| C | -4.39467900 | 1.87071300 | 4.24570300 |
| H | -5.32116100 | 0.30897400 | 3.06908600 |
| H | -3.18135800 | 3.34010700 | 5.27159300 |
| H | 4.42367600 | -7.05222500 | 0.44847900 |
| H | -6.25596100 | 5.22629700 | -0.49659600 |
| H | -5.33865200 | 2.24660000 | 4.64755900 |

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Table S11
B3LYP-D3(BJ)/def2-SVP

**TS2B**

G = -3028.078952 Hartree

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| Si | 0.00000000 | 0.00000000 | 0.00000000 |
| C | 0.00000000 | 0.00000000 | 2.73565100 |
| C | 1.31951400 | 0.00000000 | 3.02073400 |
| Si | 1.67548100 | -0.75471700 | 1.39473500 |
| N | 1.79815700 | -2.62563400 | 1.57030200 |
| N | -0.35143400 | 1.86467100 | 0.28853200 |
| N | -1.84656700 | 0.29944400 | 0.20379300 |
| N | 0.12003100 | -0.68633600 | -1.48826300 |
| N | 3.44318900 | -1.36242300 | 0.94947800 |
| C | 1.02967000 | -3.65134000 | 2.31433800 |
| C | 3.09273800 | -2.61632700 | 1.21849400 |
| C | 0.35807100 | 3.14024700 | 0.53177400 |
| C | -1.66282200 | 1.61596800 | 0.32052800 |
| C | -3.03973400 | -0.41392700 | -0.31252200 |
| C | 1.12778400 | -1.15608300 | -2.27805000 |
| C | 4.70143000 | -0.82750900 | 0.39066000 |
| C | 2.11777000 | 0.19454200 | 4.24333100 |
| C | -0.44968500 | -3.40171200 | 2.01008400 |
| C | 1.36588200 | -5.08927300 | 1.88961100 |
| C | 1.29528400 | -3.47553900 | 3.81963400 |

| | | | |
|---|---|---|---|
| C | 3.98293400 | -3.80305200 | 1.13574600 |
| C | 1.83449700 | 2.79939200 | 0.74310400 |
| C | -0.15722600 | 3.86814900 | 1.78307500 |
| C | 0.23072400 | 4.05586000 | -0.69839000 |
| C | -2.74697800 | 2.61842000 | 0.48091300 |
| C | -2.80508900 | -1.90700600 | -0.06377700 |
| C | -4.34084900 | -0.00443700 | 0.39723400 |
| C | -3.15291800 | -0.14818600 | -1.82429300 |
| C | 2.00953000 | -0.26446800 | -2.98011300 |
| C | 1.28233200 | -2.56549600 | -2.51521700 |
| C | 4.43598500 | 0.65003700 | 0.09000200 |
| C | 5.09237000 | -1.52695800 | -0.91984000 |
| C | 5.83253400 | -0.94954800 | 1.42602900 |
| C | 3.45055300 | 0.63369000 | 4.14448800 |
| C | 1.60538600 | -0.08386500 | 5.52562400 |
| C | -1.13219100 | 0.34244200 | 3.58260500 |
| H | -0.66479600 | -3.61144500 | 0.95460200 |
| H | -1.08189900 | -4.05242100 | 2.63203400 |
| H | -0.71491800 | -2.35769700 | 2.21232700 |
| H | 1.31266700 | -5.20226200 | 0.79994100 |
| H | 0.61940700 | -5.76266800 | 2.33740800 |
| H | 2.35450100 | -5.41825400 | 2.22948300 |
| H | 2.36486300 | -3.60245600 | 4.04570900 |
| H | 0.73350200 | -4.22654900 | 4.39646600 |
| H | 0.99056800 | -2.47766700 | 4.15963000 |
| C | 4.04779700 | -4.53785600 | -0.05447200 |

| | | | |
|---|---|---|---|
| C | 4.74539300 | -4.19102100 | 2.24447700 |
| H | 1.96501000 | 2.16867100 | 1.63208400 |
| H | 2.41777800 | 3.72146200 | 0.88044200 |
| H | 2.23860100 | 2.27165800 | -0.12793600 |
| H | -0.18485000 | 3.18621200 | 2.64165300 |
| H | 0.52083500 | 4.70166400 | 2.02249000 |
| H | -1.16093800 | 4.28590900 | 1.64028900 |
| H | 0.57398600 | 3.53948900 | -1.60439000 |
| H | 0.84519700 | 4.95890400 | -0.55918500 |
| H | -0.80752600 | 4.37760200 | -0.85149300 |
| C | -3.18256200 | 3.38166000 | -0.60941700 |
| C | -3.35756800 | 2.77445600 | 1.73291900 |
| H | -2.80918800 | -2.12792400 | 1.01199700 |
| H | -3.60250200 | -2.49691500 | -0.53830400 |
| H | -1.84491500 | -2.21682500 | -0.48755000 |
| H | -4.22229100 | -0.02847200 | 1.48904900 |
| H | -5.12949400 | -0.72034600 | 0.11853800 |
| H | -4.68571000 | 0.99500300 | 0.10718800 |
| H | -3.37407000 | 0.91297900 | -2.01386900 |
| H | -3.96587500 | -0.74751400 | -2.26305900 |
| H | -2.20199600 | -0.40337300 | -2.31170400 |
| C | 1.75190800 | 1.23040600 | -2.89054500 |
| C | 3.01209200 | -0.77711700 | -3.80846700 |
| C | 0.23482200 | -3.51352300 | -1.95713100 |
| C | 2.31144100 | -3.02770100 | -3.34093500 |
| H | 4.14085000 | 1.19708400 | 0.99618400 |

| | | | |
|---|---|---|---|
| H | 5.34116900 | 1.12384300 | -0.31574000 |
| H | 3.63542700 | 0.74370500 | -0.65495700 |
| H | 4.24211800 | -1.56529300 | -1.61297200 |
| H | 5.90126900 | -0.96182100 | -1.40791000 |
| H | 5.45982000 | -2.54579600 | -0.74812000 |
| H | 5.54500600 | -0.48515500 | 2.38065900 |
| H | 6.73750200 | -0.44638100 | 1.05164900 |
| H | 6.08810100 | -2.00074900 | 1.61609900 |
| C | 4.24250100 | 0.80437900 | 5.28124000 |
| H | 3.85966100 | 0.84993400 | 3.15656600 |
| C | 2.39845100 | 0.07744800 | 6.66166100 |
| H | 0.57692300 | -0.43370300 | 5.62372100 |
| C | -2.33490700 | -0.39598300 | 3.55330700 |
| C | -1.09579300 | 1.48654500 | 4.41683200 |
| C | 4.86000100 | -5.67007500 | -0.12592400 |
| H | 3.47142200 | -4.20983800 | -0.92080700 |
| C | 5.55667600 | -5.32514700 | 2.16759800 |
| H | 4.69631300 | -3.60852600 | 3.16667500 |
| C | -4.22510400 | 4.29778100 | -0.44766800 |
| H | -2.71447100 | 3.24752400 | -1.58604200 |
| C | -4.39159500 | 3.69588700 | 1.89086900 |
| H | -3.01916000 | 2.17664300 | 2.57701700 |
| C | 2.94080400 | 2.11485400 | -3.27132500 |
| C | 0.50982300 | 1.59803000 | -3.72118400 |
| H | 1.50067700 | 1.44679300 | -1.84128700 |
| C | 3.18938000 | -2.15066500 | -3.98222400 |

| | | | |
|---|---|---|---|
| H | 3.67690400 | -0.08853900 | -4.33392800 |
| C | 0.65825800 | -4.98198500 | -1.87792400 |
| C | -1.05708400 | -3.39757800 | -2.78568300 |
| H | 0.01129500 | -3.16476900 | -0.93700900 |
| H | 2.42025800 | -4.10145300 | -3.51055800 |
| C | 3.71956800 | 0.52457600 | 6.54682000 |
| H | 5.27300000 | 1.15391300 | 5.17781400 |
| H | 1.98287900 | -0.14940600 | 7.64684600 |
| C | -3.43426900 | -0.02481800 | 4.32766000 |
| H | -2.39991000 | -1.26821800 | 2.90485300 |
| C | -2.20406000 | 1.87181000 | 5.16897800 |
| H | -0.17460100 | 2.06807700 | 4.47403700 |
| C | 5.61084700 | -6.06817200 | 0.98460700 |
| H | 4.90700200 | -6.24252100 | -1.05491700 |
| H | 6.14707200 | -5.62945500 | 3.03469400 |
| C | -4.82915200 | 4.45788800 | 0.80237000 |
| H | -4.56659000 | 4.88625400 | -1.30221500 |
| H | -4.85931400 | 3.81337600 | 2.87091400 |
| H | 3.17682200 | 2.04381400 | -4.34535600 |
| H | 2.71292300 | 3.17222500 | -3.05981100 |
| H | 3.84959300 | 1.84530800 | -2.71129300 |
| H | 0.68443900 | 1.37658600 | -4.78649100 |
| H | 0.26868900 | 2.67101300 | -3.63310400 |
| H | -0.35820400 | 1.01599700 | -3.38189200 |
| H | 3.98918400 | -2.53190400 | -4.62123300 |
| H | 0.78324800 | -5.42452500 | -2.87935200 |

| | | | |
|---|---|---|---|
| H | -0.11343500 | -5.57266000 | -1.35866800 |
| H | 1.60478300 | -5.11725600 | -1.33603700 |
| H | -0.87821800 | -3.75616900 | -3.81240400 |
| H | -1.87050500 | -4.00064000 | -2.34851100 |
| H | -1.39032200 | -2.35411500 | -2.84006700 |
| H | 4.33754800 | 0.65118200 | 7.43897300 |
| C | -3.38328600 | 1.11761000 | 5.13345400 |
| H | -4.34782000 | -0.62362400 | 4.28625900 |
| H | -2.14544600 | 2.76619900 | 5.79493600 |
| H | 6.24391200 | -6.95658200 | 0.92653600 |
| H | -5.64310500 | 5.17583900 | 0.92772600 |
| H | -4.25069600 | 1.41686100 | 5.72610900 |

Table S12
B3LYP-D3(BJ)/def2-SVP
**Int2B**
G = -3028.121225 Hartree

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| Si | 0.19242800 | 1.30686200 | -0.82800900 |
| Si | -0.56911000 | 1.32088300 | 2.54913000 |
| N | 1.14108700 | 0.43133300 | 0.10843600 |
| N | -1.59309200 | 1.83673100 | 4.10575600 |

| | | | |
|---|---|---|---|
| N | 0.81426500 | 2.29157700 | -2.35126700 |
| N | -0.31531200 | 0.44844600 | -2.39646300 |
| N | 0.29999500 | 2.69583300 | 3.57748100 |
| C | 2.15342000 | -0.06966700 | 0.86259100 |
| C | 0.29429800 | 1.36498600 | -3.15713500 |
| C | -2.75505600 | 1.25773600 | 4.79386900 |
| C | -0.59707700 | 2.59829900 | 4.56805100 |
| C | 0.37742400 | 1.33114000 | -4.63878700 |
| C | 1.91957000 | -1.11826700 | 1.81296100 |
| C | 3.49089300 | 0.43065000 | 0.73510800 |
| C | 1.33290000 | 3.63951600 | -2.68324700 |
| C | 1.53739100 | 0.84506500 | -5.25566500 |
| H | 2.37779900 | 0.51700200 | -4.64097200 |
| C | 0.60572200 | -1.88364300 | 1.80927500 |
| H | -0.14271600 | -1.20928300 | 1.37256800 |
| C | 3.82224700 | 1.33603900 | -0.43660600 |
| H | 2.95148600 | 1.98614000 | -0.59826000 |
| C | -0.69542000 | -0.94977200 | -2.67516800 |
| C | -3.72373300 | 2.35882500 | 5.25542400 |
| H | -3.27961800 | 2.97614500 | 6.04790000 |
| H | -4.64291200 | 1.90533500 | 5.65894400 |
| H | -3.99631600 | 3.01131800 | 4.41514200 |
| C | 1.65795300 | 3.25506100 | 3.53184700 |
| C | -1.52969600 | -1.40758800 | -1.46927400 |
| H | -0.95827800 | -1.29858500 | -0.53859700 |
| H | -1.80875900 | -2.46523800 | -1.58056700 |

| | | | |
|---|---|---|---|
| H | -2.45239600 | -0.81362000 | -1.38232000 |
| C | 2.95631100 | -1.52343600 | 2.66022200 |
| H | 2.76248100 | -2.31193300 | 3.39133500 |
| C | -0.45983900 | 3.16652600 | 5.93707200 |
| C | -2.31941400 | 0.38916000 | 5.98788800 |
| H | -1.58906200 | -0.36746600 | 5.66215900 |
| H | -3.18980200 | -0.13255100 | 6.41638000 |
| H | -1.86561000 | 0.99390000 | 6.78457800 |
| C | 1.60826600 | 0.77801400 | -6.64931600 |
| H | 2.51155100 | 0.39327400 | -7.12783000 |
| C | -3.46196900 | 0.36261200 | 3.76421000 |
| H | -3.79264000 | 0.95495000 | 2.90012100 |
| H | -4.34554300 | -0.11307000 | 4.21529400 |
| H | -2.78442300 | -0.42861600 | 3.40798700 |
| C | 0.31140600 | 2.51561900 | 6.91007000 |
| H | 0.78988300 | 1.56462600 | 6.66910400 |
| C | -0.70681100 | 1.75665000 | -5.41803600 |
| H | -1.60235900 | 2.13970400 | -4.92671400 |
| C | 0.52786300 | 1.20372800 | -7.42671700 |
| H | 0.58558200 | 1.15314700 | -8.51644100 |
| C | 5.03902200 | 2.23964500 | -0.22809100 |
| H | 4.95073700 | 2.82273700 | 0.70177100 |
| H | 5.14241800 | 2.94829700 | -1.06613300 |
| H | 5.97740200 | 1.66458600 | -0.17576500 |
| C | 3.98293200 | 0.47212100 | -1.70216900 |
| H | 4.80760400 | -0.24608200 | -1.56916900 |

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|---|---|---|---|
| H | 4.20575700 | 1.08256800 | -2.59261000 |
| H | 3.06396400 | -0.09997000 | -1.89559500 |
| C | -0.62691400 | 1.69600800 | -6.80922900 |
| H | -1.47093200 | 2.03293700 | -7.41521000 |
| C | 4.23097600 | -0.96209000 | 2.59158000 |
| H | 5.01945800 | -1.28407600 | 3.27594600 |
| C | 0.36937700 | 4.41016500 | -3.60227100 |
| H | 0.37046000 | 4.00421400 | -4.62171500 |
| H | 0.68878800 | 5.46175000 | -3.66483000 |
| H | -0.65537600 | 4.38811700 | -3.21329700 |
| C | 2.71238100 | 3.54545900 | -3.35444900 |
| H | 3.42893700 | 3.02577100 | -2.70742600 |
| H | 3.09629000 | 4.55867400 | -3.54905900 |
| H | 2.65796100 | 3.01720600 | -4.31563200 |
| C | 4.49038900 | -0.00854800 | 1.60652900 |
| H | 5.50066500 | 0.39459400 | 1.51035700 |
| C | 0.10176600 | -2.27741200 | 3.20071500 |
| H | 0.75768700 | -3.01710900 | 3.68832100 |
| H | -0.90103000 | -2.73129100 | 3.13104300 |
| H | 0.03102300 | -1.39234800 | 3.85034000 |
| C | -1.53988900 | -1.08653300 | -3.95081600 |
| H | -2.39640500 | -0.39571700 | -3.93552600 |
| H | -1.93142300 | -2.11333000 | -4.01176000 |
| H | -0.95824000 | -0.89640000 | -4.86119900 |
| C | 0.46143300 | 3.07783900 | 8.17919300 |
| H | 1.06310600 | 2.56425500 | 8.93268400 |

| | | | |
|---|---|---|---|
| C | 1.48037100 | 4.38582000 | -1.35161700 |
| H | 0.51534000 | 4.47321000 | -0.83758100 |
| H | 1.87073500 | 5.39838300 | -1.52911700 |
| H | 2.17961700 | 3.86273300 | -0.68686600 |
| C | 0.58247300 | -1.79840000 | -2.78517700 |
| H | 1.17273200 | -1.49920300 | -3.66405700 |
| H | 0.33314200 | -2.86566200 | -2.88829600 |
| H | 1.19983600 | -1.66496600 | -1.88645000 |
| C | 1.77531600 | 4.57716300 | 4.30636200 |
| H | 2.75223400 | 5.03575100 | 4.08905100 |
| H | 1.70644100 | 4.43670500 | 5.39218300 |
| H | 0.99016500 | 5.28562500 | 3.99985100 |
| C | -0.15584800 | 4.29486100 | 8.48414800 |
| H | -0.03507300 | 4.73595100 | 9.47638900 |
| C | -1.08382200 | 4.38196300 | 6.24953100 |
| H | -1.68382200 | 4.88321300 | 5.48807700 |
| C | 0.72547400 | -3.12527100 | 0.90882600 |
| H | 1.06456400 | -2.85291000 | -0.10044200 |
| H | -0.24275000 | -3.64661200 | 0.81574600 |
| H | 1.45816200 | -3.83825900 | 1.32166800 |
| C | -0.92961600 | 4.94455200 | 7.51805700 |
| H | -1.41503100 | 5.89465700 | 7.75312100 |
| C | 2.66462600 | 2.22238000 | 4.06940100 |
| H | 2.48905100 | 2.02617400 | 5.13748400 |
| H | 3.69596200 | 2.59118300 | 3.95559900 |
| H | 2.58073700 | 1.27507300 | 3.51875200 |

| | | | |
|---|---|---|---|
| C | 1.94684900 | 3.52148600 | 2.04867900 |
| H | 1.83195900 | 2.59996000 | 1.46196700 |
| H | 2.97647500 | 3.88364100 | 1.91303500 |
| H | 1.25290300 | 4.27503500 | 1.64907900 |
| C | -1.23140900 | 2.33561600 | -0.13768900 |
| C | -1.45554900 | 2.46258100 | 1.20421400 |
| C | -2.04402100 | 3.10694200 | -1.13131400 |
| C | -2.51225200 | 3.38476800 | 1.69791800 |
| C | -2.92709800 | 5.21728300 | -1.98711300 |
| C | -3.61628500 | 4.54215600 | -2.99888700 |
| C | -3.52826500 | 3.14941100 | -3.07116200 |
| C | -2.75153600 | 2.44309000 | -2.14889500 |
| C | -2.15229800 | 4.50873300 | -1.06903800 |
| H | -2.70082500 | 1.35694600 | -2.20685800 |
| H | -4.07881000 | 2.60469100 | -3.84307600 |
| H | -4.22365100 | 5.09598100 | -3.71858700 |
| H | -1.62862500 | 5.04815900 | -0.28009900 |
| H | -2.99133500 | 6.30550500 | -1.91217600 |
| C | -3.87388900 | 3.15706800 | 1.43254800 |
| C | -2.16341600 | 4.52391800 | 2.44704300 |
| C | -3.14150200 | 5.41035600 | 2.89960500 |
| C | -4.49338300 | 5.16981300 | 2.63223000 |
| C | -4.85341400 | 4.03584300 | 1.89827100 |
| H | -4.15915800 | 2.28779900 | 0.83665400 |
| H | -5.90558000 | 3.83816100 | 1.67808800 |
| H | -1.11026600 | 4.70916700 | 2.65865700 |

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|---|---|---|---|
| H | -2.84628400 | 6.29889400 | 3.46465200 |
| H | -5.25913800 | 5.86146100 | 2.99096600 |

Table S13
B3LYP-D3(BJ)/def2-SVP
**TS3B**
G = -3028.083114 Hartree

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| N | 0.59738500 | -1.96885300 | -0.01542000 |
| Si | -1.55508300 | -0.17307200 | 0.58162100 |
| N | -3.09854200 | 0.77187400 | 1.24172100 |
| C | -3.86012200 | 0.22324800 | 0.28519500 |
| N | -3.06104100 | -0.49115600 | -0.50806900 |
| C | -0.54822500 | 1.06781300 | -0.46286000 |
| C | 0.80413000 | 0.92691600 | -0.62799700 |
| Si | 1.79516200 | -0.56857800 | 0.07372900 |
| H | 5.62526000 | 0.11289200 | 2.38090700 |
| C | 5.53835400 | 1.20205300 | 2.24616200 |
| H | 5.10800400 | 1.63253900 | 3.16647300 |
| H | 6.55914400 | 1.60216800 | 2.13197900 |
| C | 5.56699200 | -3.41004600 | -2.42643000 |
| C | 4.68340100 | 1.54049900 | 1.01495100 |

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|---|---|---|---|
| C | 4.54878000 | -0.29299900 | -0.77572700 |
| C | 5.22201000 | 0.84531000 | -0.21980000 |
| H | 3.68161300 | 1.12573400 | 1.18240800 |
| C | 5.19760400 | -0.96144000 | -1.86547500 |
| C | 6.41716800 | 1.30183100 | -0.78098700 |
| C | 6.38848600 | -0.46057500 | -2.39875600 |
| C | 7.00552500 | 0.67645600 | -1.87960500 |
| H | 6.90332000 | 2.17840200 | -0.34319900 |
| H | 6.84872400 | -0.98154300 | -3.24376300 |
| H | 7.93432700 | 1.05775900 | -2.31066400 |
| C | 4.53313200 | 3.05682300 | 0.85046000 |
| H | 4.03825600 | 3.49822400 | 1.73272100 |
| H | 5.51212900 | 3.55236700 | 0.74528400 |
| H | 3.93514000 | 3.30200400 | -0.03636000 |
| H | 5.93611600 | -3.58771700 | -1.40437200 |
| H | 5.07129900 | -4.33139300 | -2.77735500 |
| H | 6.44424200 | -3.24056600 | -3.07245000 |
| H | 3.75075000 | -2.48028100 | -1.81006200 |
| C | 4.59513100 | -2.22257700 | -2.45713500 |
| C | 4.05142100 | -1.99070300 | -3.87450300 |
| H | 3.56110100 | -2.89606000 | -4.27047500 |
| H | 4.86137100 | -1.71500700 | -4.56988700 |
| H | 3.31361400 | -1.17298200 | -3.89185200 |
| N | 3.34569200 | -0.73796400 | -0.30842600 |
| N | 1.14270300 | -0.82416300 | 1.77019200 |
| C | 0.17226000 | -1.68781100 | 1.30319500 |

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|---|---|---|---|
| C | -0.45708000 | -2.72828700 | 2.18947600 |
| C | -1.82351800 | -3.02247300 | 2.19197000 |
| C | -2.33303300 | -4.04807000 | 2.98951500 |
| C | -1.47739500 | -4.79412000 | 3.80498200 |
| C | -0.11028200 | -4.50258800 | 3.81631500 |
| C | 0.39447600 | -3.47733700 | 3.01523000 |
| H | 1.45965100 | -3.24511100 | 3.02380100 |
| H | 0.56774200 | -5.07466000 | 4.45399200 |
| H | -1.87469900 | -5.59458000 | 4.43345100 |
| H | -3.40406500 | -4.26373200 | 2.97588000 |
| H | -2.48933100 | -2.43658200 | 1.55616400 |
| C | -2.18152300 | 3.01748200 | -0.60026600 |
| H | -2.21832800 | 3.05593700 | 0.48524600 |
| C | 1.59083200 | 1.92989900 | -1.39192100 |
| H | 0.72373400 | 3.63965100 | -0.39273700 |
| C | 1.43460900 | 3.30861100 | -1.15058300 |
| C | 2.53790600 | 1.52819100 | -2.35039900 |
| H | 2.69399600 | 0.46750600 | -2.53562500 |
| H | 4.03626700 | 2.12282600 | -3.77490900 |
| C | 3.29289700 | 2.46698900 | -3.05275100 |
| C | 3.11827400 | 3.83157300 | -2.81012300 |
| H | 3.71784700 | 4.56774700 | -3.35087200 |
| C | 2.18568900 | 4.24852200 | -1.85437000 |
| H | 2.05406100 | 5.31292900 | -1.64470800 |
| C | -1.33805300 | 2.08289300 | -1.22370300 |
| C | -1.28639500 | 2.09191200 | -2.63201900 |

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|---|---|---|---|
| H | -0.60889300 | 1.40320400 | -3.13858200 |
| H | -2.00344900 | 2.95251800 | -4.47242100 |
| C | -2.06460300 | 2.97283200 | -3.38151100 |
| C | -2.91212700 | 3.88486100 | -2.74321200 |
| H | -3.51967200 | 4.57865600 | -3.32901100 |
| C | -2.95531900 | 3.91015600 | -1.34706700 |
| H | -3.58971600 | 4.63591000 | -0.83086700 |
| C | -6.20981200 | -0.59494000 | 0.62414400 |
| C | -5.33005800 | 0.37401500 | 0.12653800 |
| C | -5.83404500 | 1.50323700 | -0.53445900 |
| C | -7.21052100 | 1.65967200 | -0.69108000 |
| C | -8.09020000 | 0.69521800 | -0.18739200 |
| C | -7.58904100 | -0.43129800 | 0.46993700 |
| H | -8.27273300 | -1.18665500 | 0.86362400 |
| H | -5.81552800 | -1.47381000 | 1.13780400 |
| H | -9.16837000 | 0.82160100 | -0.30930300 |
| H | -7.59996800 | 2.53873300 | -1.20931600 |
| H | -5.13873400 | 2.24758500 | -0.92638800 |
| C | 1.24174700 | -0.05731600 | 3.02476200 |
| C | 0.85660600 | -3.30774600 | -0.61357700 |
| C | 1.22347900 | 1.44821200 | 2.69287900 |
| H | 2.05998200 | 1.71332400 | 2.03298600 |
| H | 1.31656400 | 2.04581600 | 3.61244100 |
| H | 0.30328400 | 1.74149900 | 2.17530500 |
| C | 2.59963400 | -0.40931500 | 3.65684200 |
| H | 2.62230600 | -1.46704600 | 3.95761800 |

| | | | |
|---|---|---|---|
| H | 2.78642700 | 0.20877400 | 4.54942900 |
| H | 3.41264800 | -0.24521100 | 2.94029400 |
| C | 0.12598100 | -0.38797000 | 4.02944600 |
| H | 0.13510900 | 0.35797200 | 4.83809400 |
| H | 0.26175700 | -1.37697400 | 4.48229700 |
| H | -0.86517800 | -0.37600400 | 3.56211200 |
| C | -3.52921200 | 1.33560200 | 2.53943500 |
| C | -0.33454500 | -4.27308000 | -0.50039400 |
| C | 1.13667300 | -3.05778400 | -2.10561000 |
| C | 2.09780400 | -3.96062400 | 0.03062600 |
| C | -3.35251400 | -1.22118100 | -1.75654900 |
| C | -4.25495600 | -0.42082600 | -2.70911000 |
| C | -2.00026600 | -1.44725600 | -2.43530700 |
| C | -3.99980900 | -2.57422400 | -1.41401000 |
| C | -2.34927400 | 2.12759800 | 3.11316800 |
| C | -4.72207100 | 2.29918600 | 2.40931600 |
| C | -3.89189200 | 0.17967400 | 3.48992500 |
| H | -2.59095300 | 2.48215600 | 4.12554000 |
| H | -1.45094200 | 1.50941100 | 3.18184500 |
| H | -2.11504600 | 3.00524700 | 2.49403300 |
| H | -4.16377500 | 0.56341300 | 4.48557300 |
| H | -4.74983300 | -0.38744400 | 3.09936400 |
| H | -3.04685700 | -0.51494500 | 3.60500400 |
| H | -4.84551200 | 2.83526100 | 3.36244100 |
| H | -4.54343600 | 3.04323900 | 1.61990500 |
| H | -5.66508700 | 1.78444300 | 2.19405800 |

| | | | |
|---|---|---|---|
| H | 0.22337300 | -2.78975300 | -2.64896100 |
| H | 1.86166500 | -2.24704100 | -2.23253700 |
| H | 1.55649600 | -3.96197900 | -2.57025200 |
| H | -0.15246700 | -5.13593800 | -1.15966800 |
| H | -0.47246400 | -4.65864800 | 0.51623600 |
| H | -1.27126700 | -3.79803000 | -0.82100500 |
| H | 2.36638400 | -4.88399800 | -0.50692200 |
| H | 2.95251300 | -3.27100300 | 0.00296800 |
| H | 1.90084100 | -4.23044900 | 1.07632400 |
| H | -1.60091700 | -0.50596200 | -2.83124800 |
| H | -2.10082000 | -2.16082100 | -3.26577300 |
| H | -1.27144000 | -1.84073600 | -1.71844300 |
| H | -3.87393000 | 0.60311800 | -2.83440800 |
| H | -5.29573000 | -0.37495200 | -2.36641700 |
| H | -4.25008800 | -0.91024100 | -3.69510800 |
| H | -4.97862200 | -2.43328600 | -0.93423600 |
| H | -3.35691700 | -3.15256900 | -0.73410600 |
| H | -4.15275300 | -3.16738900 | -2.32862400 |

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Table S14
B3LYP-D3(BJ)/def2-SVP
**3a**
G = -3028.094826 Hartree

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Atomic Coordinates (Angstroms)

| Number | X | Y | Z |
|---|---|---|---|
| H | 3.28394700 | 3.07960200 | 5.83695300 |
| H | -1.62628500 | 1.67453300 | 4.74159500 |
| Si | 0.34049800 | 1.00053400 | -0.16884500 |
| Si | 0.14563500 | 2.52806600 | 2.22394000 |
| N | 0.09789500 | 1.59600900 | -1.66396400 |
| N | -0.21243100 | 4.86129600 | 5.27121900 |
| N | 1.14393600 | 2.26921400 | 0.90749200 |
| N | 1.22021600 | -1.35793000 | -1.03263600 |
| N | 0.55251500 | 3.26407100 | 3.74960900 |
| C | -0.51885300 | 1.32513000 | -2.85021500 |
| C | 1.23766100 | -0.69244400 | 0.05494600 |
| C | -0.88512300 | 6.05073500 | 5.80032600 |
| C | -0.21235800 | 4.40372000 | 4.08834700 |
| C | 1.70474200 | -1.15358700 | 1.40127700 |
| C | 0.21674800 | 0.80567800 | -3.96697900 |
| C | -1.91789400 | 1.59061600 | -3.02913700 |
| C | 2.32061500 | 3.03091600 | 0.36669600 |
| C | 0.78453400 | -1.58507100 | 2.37156200 |
| H | -0.27863600 | -1.59774100 | 2.13376700 |
| C | 1.71809700 | 0.62258100 | -3.82881700 |
| H | 1.87795600 | 0.23590400 | -2.81143800 |
| C | -2.69139500 | 2.25490700 | -1.90301800 |
| H | -2.28831900 | 1.86143400 | -0.95971800 |
| C | 1.62260700 | -2.75307100 | -1.27055200 |

| | | | |
|---|---|---|---|
| C | -2.28741100 | 5.63947900 | 6.28508300 |
| H | -2.93409100 | 5.35523100 | 5.44339200 |
| H | -2.76784800 | 6.47311200 | 6.82079600 |
| H | -2.22010900 | 4.78029100 | 6.96976200 |
| C | 1.48045700 | 2.60135500 | 4.73794400 |
| C | 0.69772300 | -3.23449200 | -2.40384400 |
| H | -0.34410500 | -3.26918300 | -2.05048400 |
| H | 0.98373500 | -4.24182900 | -2.74539400 |
| H | 0.73900800 | -2.53721400 | -3.25134600 |
| C | -0.44387600 | 0.53545400 | -5.16728100 |
| H | 0.12143900 | 0.13669400 | -6.01234300 |
| C | -0.94590600 | 4.95115900 | 2.88785300 |
| C | -0.98213100 | 7.24967300 | 4.83716100 |
| H | -0.00085600 | 7.46933900 | 4.38906900 |
| H | -1.30317000 | 8.14085300 | 5.39821200 |
| H | -1.70336800 | 7.09303500 | 4.02605500 |
| C | 1.22458700 | -2.04744500 | 3.61337600 |
| H | 0.49532800 | -2.40212400 | 4.34610200 |
| C | -0.04215400 | 6.47831800 | 7.01718000 |
| H | 0.05697000 | 5.64143000 | 7.72413600 |
| H | -0.50288700 | 7.33143500 | 7.53905800 |
| H | 0.96943500 | 6.77391700 | 6.69750400 |
| C | -0.22994400 | 5.67077400 | 1.91217600 |
| H | 0.85092400 | 5.77724900 | 2.01116800 |
| C | 3.07142600 | -1.15837200 | 1.72293900 |
| H | 3.79717600 | -0.82748700 | 0.97763800 |

| | | | |
|---|---|---|---|
| C | 2.58905600 | -2.06600600 | 3.91723100 |
| H | 2.93269200 | -2.43003700 | 4.88832100 |
| C | -2.41486900 | 3.76568900 | -1.88395700 |
| H | -1.33671100 | 3.95486900 | -1.78090800 |
| H | -2.93035000 | 4.24731900 | -1.03794100 |
| H | -2.76472000 | 4.23821500 | -2.81673200 |
| C | -4.19463400 | 1.96946900 | -1.90710000 |
| H | -4.69979200 | 2.40921700 | -2.78230800 |
| H | -4.67016400 | 2.40827200 | -1.01363400 |
| H | -4.39792200 | 0.88733200 | -1.90579300 |
| C | 3.51035700 | -1.61158800 | 2.96910700 |
| H | 4.57920800 | -1.61849500 | 3.19706700 |
| C | -1.81408400 | 0.76255600 | -5.31903700 |
| H | -2.31222400 | 0.53523500 | -6.26480300 |
| C | 1.80936400 | 4.05249900 | -0.66276400 |
| H | 1.19699700 | 3.53742800 | -1.41476900 |
| H | 2.65775400 | 4.55547500 | -1.15217900 |
| H | 1.18725200 | 4.81331400 | -0.17439800 |
| C | 3.27743800 | 2.03991500 | -0.31158200 |
| H | 2.78546900 | 1.52170800 | -1.14527200 |
| H | 3.63692300 | 1.29583000 | 0.41254400 |
| H | 4.14656900 | 2.57832700 | -0.71763200 |
| C | -2.53359800 | 1.29490600 | -4.25009600 |
| H | -3.60079600 | 1.49090100 | -4.37496200 |
| C | 2.43500300 | 1.97831700 | -3.94711500 |
| H | 2.31503900 | 2.39047400 | -4.96289500 |

| | | | |
|---|---|---|---|
| H | 3.51580900 | 1.87881600 | -3.74567100 |
| H | 2.01855900 | 2.70335400 | -3.23646600 |
| C | 3.07874800 | -2.71655600 | -1.76609800 |
| H | 3.18128000 | -2.02595600 | -2.61452000 |
| H | 3.39438800 | -3.72009200 | -2.09232900 |
| H | 3.75534500 | -2.38695500 | -0.96290200 |
| C | -0.89650400 | 6.28369200 | 0.85114000 |
| H | -0.33142000 | 6.84355600 | 0.10355900 |
| C | 3.08665600 | 3.76448400 | 1.47253100 |
| H | 2.43219100 | 4.40799400 | 2.07479300 |
| H | 3.85603400 | 4.40312500 | 1.01443900 |
| H | 3.59628500 | 3.06722400 | 2.15020400 |
| C | 1.48690500 | -3.72494200 | -0.08441200 |
| H | 2.22527100 | -3.54463700 | 0.70603800 |
| H | 1.63054800 | -4.75457100 | -0.44890000 |
| H | 0.48258500 | -3.66236100 | 0.35997100 |
| C | 2.55644800 | 3.59731500 | 5.19302400 |
| H | 2.11039900 | 4.42340000 | 5.75814400 |
| H | 3.09742600 | 4.00761500 | 4.32909400 |
| C | -2.28491200 | 6.17693600 | 0.74712100 |
| H | -2.80596500 | 6.64963200 | -0.08758500 |
| C | -2.34523000 | 4.85507800 | 2.77453200 |
| H | -2.91191800 | 4.31300100 | 3.52750700 |
| C | 2.32966900 | -0.37994700 | -4.81066000 |
| H | 1.82015800 | -1.35457700 | -4.77094400 |
| H | 3.39447800 | -0.54327600 | -4.57576100 |

| | | | |
|---|---|---|---|
| H | 2.28377500 | -0.02085300 | -5.85204400 |
| C | -3.00502000 | 5.45573300 | 1.70468900 |
| H | -4.08869000 | 5.35610800 | 1.61881000 |
| C | 0.69782800 | 2.05785600 | 5.94675300 |
| H | 0.07576900 | 2.83784100 | 6.39748900 |
| H | 1.41064800 | 1.69082500 | 6.70076200 |
| H | 0.06993500 | 1.20400900 | 5.65121700 |
| C | 2.14241200 | 1.40602600 | 4.04689300 |
| H | 1.39758700 | 0.69940800 | 3.64568300 |
| H | 2.73245700 | 0.84077100 | 4.77993300 |
| H | 2.81156400 | 1.69605300 | 3.23106800 |
| C | -1.21078800 | 0.69291800 | 0.93298700 |
| C | -1.37507900 | 1.53938700 | 2.00528700 |
| C | -2.09863200 | -0.43190200 | 0.58812600 |
| C | -2.59872500 | 1.72799400 | 2.81395500 |
| C | -2.92288000 | -2.02233300 | -1.07018600 |
| C | -3.67117500 | -2.67897300 | -0.09059000 |
| C | -3.62340400 | -2.22617600 | 1.23359000 |
| C | -2.85451800 | -1.11461600 | 1.56801000 |
| C | -2.13240500 | -0.92323500 | -0.73463200 |
| H | -2.82063000 | -0.78031400 | 2.60456900 |
| H | -4.19057600 | -2.74434500 | 2.01067900 |
| H | -4.28250700 | -3.54588500 | -0.35264500 |
| H | -1.54736100 | -0.44025800 | -1.51540500 |
| H | -2.94388500 | -2.36485900 | -2.10696500 |
| C | -2.56813000 | 1.81189800 | 4.21517300 |

| | | | |
|---|---|---|---|
| C | -3.82926200 | 1.92518200 | 2.15735400 |
| C | -4.98577000 | 2.20437700 | 2.88193600 |
| C | -4.94125100 | 2.29476300 | 4.27912200 |
| C | -3.72834700 | 2.09207700 | 4.94212900 |
| H | -3.67910500 | 2.15961300 | 6.03142600 |
| H | -3.86240500 | 1.87430200 | 1.06838100 |
| H | -5.92911200 | 2.36077100 | 2.35299900 |
| H | -5.84765200 | 2.52081100 | 4.84538500 |

Table S15
B3LYP-D3(BJ)/def2-SVP
**1,1'-(1,2-Ethynediyl)bis(2-bromobenzene)**
G = -5685.543585 Hartree

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| C | -0.14028300 | -0.33459900 | 0.66864300 |
| C | -0.32263400 | -1.36307600 | 1.29388200 |
| C | -0.53582500 | -2.58839500 | 1.98138500 |
| C | -0.95905200 | -5.04921300 | 3.29267100 |
| C | -0.64505300 | -3.79377400 | 1.25245700 |
| C | -0.64566900 | -2.65644100 | 3.38949300 |
| C | -0.85500300 | -3.87321100 | 4.03889200 |
| C | -0.85385800 | -5.00831800 | 1.89843300 |

| | | | |
|---|---|---|---|
| H | -0.56089900 | -3.74590800 | 0.16539500 |
| H | -0.93576800 | -3.89537400 | 5.12645200 |
| H | -0.93507100 | -5.92717400 | 1.31392800 |
| H | -1.12295000 | -5.99913400 | 3.80637400 |
| C | 0.07283800 | 0.89077700 | -0.01878000 |
| C | 0.49589900 | 3.35173200 | -1.32986700 |
| C | 0.18190500 | 2.09611600 | 0.71024200 |
| C | 0.18274000 | 0.95893600 | -1.42687900 |
| C | 0.39198100 | 2.17577600 | -2.07618000 |
| C | 0.39063200 | 3.31072700 | 0.06436500 |
| H | 0.09768000 | 2.04816200 | 1.79729600 |
| H | 0.47279200 | 2.19802600 | -3.16373600 |
| H | 0.47173400 | 4.22954800 | 0.64894200 |
| H | 0.65974900 | 4.30170500 | -1.84349100 |
| Br | -0.50824600 | -1.07186900 | 4.43218500 |
| Br | 0.04554300 | -0.62558300 | -2.46968800 |

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Table S16
B3LYP-D3(BJ)/def2-SVP
**TS1D**
G = -8174.624798 Hartree

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| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |

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| | | | |
|---|---|---|---|
| Si | -1.39991400 | -0.93114000 | 0.20334300 |
| C | 3.03741100 | 0.08200500 | 0.02288400 |
| C | 2.43143500 | 1.05776600 | 0.52266900 |
| Si | 0.00939000 | 0.94201000 | 0.69054800 |
| N | -0.33055800 | 2.18856300 | -0.68695300 |
| N | -0.47989100 | -2.41500400 | 1.02239900 |
| N | -0.84653000 | -2.18007800 | -1.09728100 |
| N | -2.99524700 | -0.64955000 | 0.34243200 |
| N | -1.23883000 | 2.25243800 | 1.26166500 |
| C | -0.00487300 | 2.39811100 | -2.11155700 |
| C | -1.11095600 | 2.92683600 | 0.11607900 |
| C | 0.16284500 | -2.72407500 | 2.31812900 |
| C | -0.29309400 | -2.97778900 | -0.16906200 |
| C | -1.29400200 | -2.52846800 | -2.46660300 |
| C | -4.18182700 | -1.21045500 | -0.07267000 |
| C | -2.02240700 | 2.56886600 | 2.46924500 |
| C | 2.67223600 | 2.45718700 | 0.86787400 |
| C | 0.88554800 | 1.22513500 | -2.53725000 |
| C | -1.30318400 | 2.39777400 | -2.93569000 |
| C | 0.76475400 | 3.70916400 | -2.34735800 |
| C | -1.61301300 | 4.29773000 | -0.16441000 |
| C | -0.39464100 | -1.71501800 | 3.32453800 |
| C | 1.68111700 | -2.53428400 | 2.21767200 |
| C | -0.17755200 | -4.14452200 | 2.79825100 |
| C | 0.37538100 | -4.28214400 | -0.41884700 |
| C | -1.98514100 | -1.28636200 | -3.03667100 |

| | | | |
|---|---|---|---|
| C | -0.09764600 | -2.89759600 | -3.35749000 |
| C | -2.31980600 | -3.67372700 | -2.42006400 |
| C | -4.59122000 | -2.53233200 | 0.30620300 |
| C | -5.06549300 | -0.45689600 | -0.91022300 |
| C | -1.66920600 | 1.51123500 | 3.51817200 |
| C | -3.51801700 | 2.44135700 | 2.14268600 |
| C | -1.69458100 | 3.96376900 | 3.02656600 |
| C | 2.05741100 | 3.04522100 | 1.98844500 |
| C | 3.52262900 | 3.28517300 | 0.09917100 |
| C | 3.65403000 | -1.00931100 | -0.59731200 |
| H | 0.45361500 | 0.26443000 | -2.22273600 |
| H | 0.99632200 | 1.21092300 | -3.63135900 |
| H | 1.88155700 | 1.31593900 | -2.09164700 |
| H | -1.91154200 | 1.51613400 | -2.70269300 |
| H | -1.07170700 | 2.39034800 | -4.01186500 |
| H | -1.90578300 | 3.29180300 | -2.73040200 |
| H | 0.12372100 | 4.58945200 | -2.21410600 |
| H | 1.15118500 | 3.72722100 | -3.37799900 |
| H | 1.61861700 | 3.78831000 | -1.66277600 |
| C | -2.90318100 | 4.51120100 | -0.66362600 |
| C | -0.77347800 | 5.39290200 | 0.08991500 |
| H | -0.08877900 | -0.69746100 | 3.04719300 |
| H | 0.00445100 | -1.92097700 | 4.32825600 |
| H | -1.49127200 | -1.75947900 | 3.36757600 |
| H | 1.92025900 | -1.52177600 | 1.86517200 |
| H | 2.14903600 | -2.66893400 | 3.20418500 |

| | | | |
|---|---|---|---|
| H | 2.14007400 | -3.25759900 | 1.53106000 |
| H | -1.26367900 | -4.31339100 | 2.78511600 |
| H | 0.17657200 | -4.27070500 | 3.83259600 |
| H | 0.30568500 | -4.91472200 | 2.18563000 |
| C | -0.32966300 | -5.47593600 | -0.20712500 |
| C | 1.70585800 | -4.32491400 | -0.85199600 |
| H | -1.28141400 | -0.45091900 | -3.12591800 |
| H | -2.37894600 | -1.50642900 | -4.03941300 |
| H | -2.82451900 | -0.97991800 | -2.39950400 |
| H | 0.67284000 | -2.11316900 | -3.31652500 |
| H | -0.43257900 | -3.00093500 | -4.40104300 |
| H | 0.36367800 | -3.84665800 | -3.05665900 |
| H | -1.86653300 | -4.60947800 | -2.06818600 |
| H | -2.72035400 | -3.85599200 | -3.42902100 |
| H | -3.16116700 | -3.41110100 | -1.76179600 |
| C | -3.76746100 | -3.30697800 | 1.32024400 |
| C | -5.77909300 | -3.06837800 | -0.19969800 |
| C | -4.78498700 | 1.00491500 | -1.22821600 |
| C | -6.23978100 | -1.04202700 | -1.39617600 |
| H | -0.59408900 | 1.51793400 | 3.75416400 |
| H | -2.22528600 | 1.70271700 | 4.44718900 |
| H | -1.94907700 | 0.51487300 | 3.15465200 |
| H | -3.70553500 | 1.45747500 | 1.68931400 |
| H | -4.11909400 | 2.54264300 | 3.05991700 |
| H | -3.84081900 | 3.22238600 | 1.44239100 |
| H | -0.61118500 | 4.08103500 | 3.17609400 |

| | | | |
|---|---|---|---|
| H | -2.19399200 | 4.09576100 | 3.99861900 |
| H | -2.03954400 | 4.76598700 | 2.36276300 |
| C | 2.25202300 | 4.38305900 | 2.32413100 |
| H | 1.40669100 | 2.41151600 | 2.59276200 |
| C | 3.70782200 | 4.63430800 | 0.41483400 |
| C | 3.43711600 | -1.28427400 | -1.97916200 |
| C | 4.57123900 | -1.86581600 | 0.07796100 |
| C | -3.35413900 | 5.81125400 | -0.90439000 |
| H | -3.54995400 | 3.65795700 | -0.86448900 |
| C | -1.22843000 | 6.68975800 | -0.14945800 |
| H | 0.23156100 | 5.22044200 | 0.47902200 |
| C | 0.29287700 | -6.70340000 | -0.43767600 |
| H | -1.36178200 | -5.43971500 | 0.14278900 |
| C | 2.32744200 | -5.55567800 | -1.07042800 |
| H | 2.25204900 | -3.39893500 | -1.02064000 |
| C | -4.04539200 | -2.77171900 | 2.73514500 |
| C | -3.94854300 | -4.82629000 | 1.26432900 |
| H | -2.71051400 | -3.10224300 | 1.11003800 |
| C | -6.60125900 | -2.34539600 | -1.06493900 |
| H | -6.07630900 | -4.07847700 | 0.08830300 |
| C | -5.80205000 | 1.90199700 | -0.50176800 |
| C | -4.78713200 | 1.31408700 | -2.73215900 |
| H | -3.78160100 | 1.21957200 | -0.82929000 |
| H | -6.89460200 | -0.45604100 | -2.04723600 |
| C | 3.06968500 | 5.18768300 | 1.52621000 |
| H | 1.76379400 | 4.79826300 | 3.20853500 |

| | | | |
|---|---|---|---|
| H | 4.35611500 | 5.24525900 | -0.21462600 |
| C | 4.07400000 | -2.33803500 | -2.62303500 |
| H | 2.75516100 | -0.64063400 | -2.53144200 |
| C | 5.19613400 | -2.92917900 | -0.56708300 |
| C | -2.51898300 | 6.90136700 | -0.64638000 |
| H | -4.36195900 | 5.97000300 | -1.29444300 |
| H | -0.57205800 | 7.53936900 | 0.05224000 |
| C | 1.62297000 | -6.74523900 | -0.86757600 |
| H | -0.26245700 | -7.62988100 | -0.27583300 |
| H | 3.36692200 | -5.57307500 | -1.40237400 |
| H | -5.09887900 | -2.94141300 | 3.01075700 |
| H | -3.41222200 | -3.27101500 | 3.48783800 |
| H | -3.85184700 | -1.69006400 | 2.77862800 |
| H | -4.95339300 | -5.13897900 | 1.59022100 |
| H | -3.22755400 | -5.32237000 | 1.93442700 |
| H | -3.79407800 | -5.21475900 | 0.24502400 |
| H | -7.51909600 | -2.78781100 | -1.45915100 |
| H | -6.82094000 | 1.72299300 | -0.88170900 |
| H | -5.58027600 | 2.97281700 | -0.64911100 |
| H | -5.81101100 | 1.69964700 | 0.57832500 |
| H | -5.78308000 | 1.15424400 | -3.17575100 |
| H | -4.51243900 | 2.36576200 | -2.91831600 |
| H | -4.07671400 | 0.67839500 | -3.27947800 |
| H | 3.22273800 | 6.24160600 | 1.76935700 |
| C | 4.95161200 | -3.17522000 | -1.92274000 |
| H | 3.87657700 | -2.51415300 | -3.68301100 |

| | | | |
|---|---|---|---|
| H | 5.89056800 | -3.55671500 | -0.00615700 |
| H | -2.87304100 | 7.91782600 | -0.83344300 |
| H | 2.11042000 | -7.70715700 | -1.04280700 |
| H | 5.45384500 | -4.00424000 | -2.42532100 |
| Br | 5.02067600 | -1.50435400 | 1.89309900 |
| Br | 4.45919300 | 2.61227000 | -1.42096600 |

Table S17
B3LYP-D3(BJ)/def2-SVP
**Int1D**
G = -8174.676863 Hartree

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| Si | -0.21938400 | 0.44151200 | -0.64901000 |
| C | -0.51154700 | 0.51620900 | 2.79877200 |
| C | 0.81968200 | 0.75751200 | 2.89198200 |
| Si | 0.48697100 | -0.32832000 | 1.45187600 |
| N | 0.38329500 | -2.17993000 | 1.62512400 |
| N | -0.78620100 | 2.28254200 | -0.44184500 |
| N | -2.10265300 | 0.61199000 | -0.82709600 |
| N | 0.52735900 | -0.13896600 | -1.97411500 |
| N | 2.19691300 | -1.23011400 | 0.92997600 |
| C | -0.59640400 | -3.15526300 | 2.14772000 |

| | | | |
|---|---|---|---|
| C | 1.65870800 | -2.39273000 | 1.21099200 |
| C | -0.23836400 | 3.56085500 | 0.05840800 |
| C | -2.05245200 | 1.94133500 | -0.68276100 |
| C | -3.15366600 | -0.23803500 | -1.42989300 |
| C | 0.25584400 | -0.32177100 | -3.31046800 |
| C | 3.51636500 | -0.87324600 | 0.38170400 |
| C | 1.77496800 | 1.46939600 | 3.73864600 |
| C | -1.89629300 | -2.40182200 | 2.46086500 |
| C | -0.89672700 | -4.24884000 | 1.10589100 |
| C | -0.09111300 | -3.78601400 | 3.45792100 |
| C | 2.33067200 | -3.71923300 | 1.11283400 |
| C | 1.26460200 | 3.33226900 | 0.24627100 |
| C | -0.88650000 | 3.92974900 | 1.40333300 |
| C | -0.43812400 | 4.70795000 | -0.94654600 |
| C | -3.18642400 | 2.89120900 | -0.86211800 |
| C | -2.59159200 | -1.66250400 | -1.43630600 |
| C | -4.43842400 | -0.20294700 | -0.58738100 |
| C | -3.44205400 | 0.18398700 | -2.88071600 |
| C | 0.01126200 | 0.76684700 | -4.21316400 |
| C | 0.22750200 | -1.64785500 | -3.85395400 |
| C | 3.57290300 | 0.65949900 | 0.37724300 |
| C | 3.64294800 | -1.37740000 | -1.06277900 |
| C | 4.66655500 | -1.40939500 | 1.24976300 |
| C | 1.80282900 | 2.87527400 | 3.80294900 |
| C | 2.75215900 | 0.78168100 | 4.48368300 |
| C | -1.73516400 | 0.81986800 | 3.54082200 |

| | | | |
|---|---|---|---|
| H | -2.23779900 | -1.80716400 | 1.60309600 |
| H | -2.68517200 | -3.12410700 | 2.71675400 |
| H | -1.76936800 | -1.72194000 | 3.31008700 |
| H | -1.15922500 | -3.80221300 | 0.13600300 |
| H | -1.74386200 | -4.86507900 | 1.44435000 |
| H | -0.04065500 | -4.91700700 | 0.95398800 |
| H | 0.78868300 | -4.42087800 | 3.29109200 |
| H | -0.87895900 | -4.41510900 | 3.90119500 |
| H | 0.17282000 | -2.99871000 | 4.17948100 |
| C | 2.23022600 | -4.47131400 | -0.06333300 |
| C | 3.09059900 | -4.21044900 | 2.18307500 |
| H | 1.45313500 | 2.52886000 | 0.96801800 |
| H | 1.74641300 | 4.24626300 | 0.62202800 |
| H | 1.73524100 | 3.06098600 | -0.70869500 |
| H | -0.82321600 | 3.09073300 | 2.10784200 |
| H | -0.37541500 | 4.80039000 | 1.84251200 |
| H | -1.94407900 | 4.19638300 | 1.27743500 |
| H | -0.03001700 | 4.44258000 | -1.93049600 |
| H | 0.09467900 | 5.60097000 | -0.58566100 |
| H | -1.49518800 | 4.97576000 | -1.06535800 |
| C | -3.34034600 | 3.52146000 | -2.10576100 |
| C | -4.08586700 | 3.17554100 | 0.17294800 |
| H | -2.31475000 | -1.97883500 | -0.42218400 |
| H | -3.34394400 | -2.36489000 | -1.82309000 |
| H | -1.70278900 | -1.71926500 | -2.07448800 |
| H | -4.23823300 | -0.52159800 | 0.44663500 |

| | | | |
|---|---|---|---|
| H | -5.17926900 | -0.89393400 | -1.01773600 |
| H | -4.88775100 | 0.79860900 | -0.56557400 |
| H | -3.94840900 | 1.15723400 | -2.92719900 |
| H | -4.10032400 | -0.55770000 | -3.35832100 |
| H | -2.50998300 | 0.23606300 | -3.46205900 |
| C | 0.21439200 | 2.19341000 | -3.73201800 |
| C | -0.34906100 | 0.50826000 | -5.53943600 |
| C | 0.71070500 | -2.83763600 | -3.03693700 |
| C | -0.14976600 | -1.85338300 | -5.18515500 |
| H | 3.43264800 | 1.06638700 | 1.38907700 |
| H | 4.54693500 | 0.99942200 | -0.00416600 |
| H | 2.79316300 | 1.06236900 | -0.28082600 |
| H | 2.78557600 | -1.01739700 | -1.64887500 |
| H | 4.57547200 | -1.00348800 | -1.51445300 |
| H | 3.66886200 | -2.47467100 | -1.10092200 |
| H | 4.53496900 | -1.11417000 | 2.30040200 |
| H | 5.61896800 | -0.99280100 | 0.88703900 |
| H | 4.74283100 | -2.50289100 | 1.19971300 |
| C | 2.76941900 | 3.55436800 | 4.54388000 |
| H | 1.04466500 | 3.43349600 | 3.25683500 |
| C | 3.72251100 | 1.44532400 | 5.23337700 |
| C | -2.92054400 | 0.91292200 | 2.77862500 |
| C | -1.87354000 | 0.96587500 | 4.93754000 |
| C | 2.87864600 | -5.70265300 | -0.16974400 |
| H | 1.64130200 | -4.08502100 | -0.89161500 |
| C | 3.73470100 | -5.44455000 | 2.07718500 |

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|---|---|---|---|
| H | 3.18599500 | -3.61621800 | 3.09229900 |
| C | -4.39128500 | 4.41563900 | -2.31351000 |
| H | -2.63096200 | 3.31273700 | -2.90638100 |
| C | -5.13183400 | 4.07704400 | -0.03654000 |
| H | -3.96237300 | 2.70104900 | 1.14486100 |
| C | 1.71410600 | 2.48013100 | -3.54127300 |
| C | -0.42684500 | 3.26071100 | -4.62305000 |
| H | -0.25021700 | 2.27304600 | -2.73973200 |
| C | -0.46182200 | -0.79263700 | -6.03116000 |
| H | -0.54733200 | 1.34232300 | -6.21427900 |
| C | 2.08809800 | -3.28348300 | -3.56071700 |
| C | -0.25818800 | -4.02901200 | -3.02494500 |
| H | 0.82911800 | -2.47145100 | -2.00567000 |
| H | -0.18556100 | -2.87470900 | -5.57416900 |
| C | 3.73853500 | 2.84211400 | 5.25445600 |
| H | 2.76220000 | 4.64661300 | 4.56921300 |
| H | 4.45326400 | 0.86958400 | 5.80331600 |
| C | -4.15927600 | 1.18225300 | 3.35178300 |
| H | -2.82772000 | 0.74525200 | 1.70575500 |
| C | -3.11374300 | 1.23414700 | 5.52785300 |
| C | 3.63055000 | -6.19340000 | 0.90122000 |
| H | 2.79451200 | -6.27792300 | -1.09452800 |
| H | 4.32505100 | -5.81957000 | 2.91624600 |
| C | -5.28976800 | 4.69522000 | -1.27963800 |
| H | -4.50478000 | 4.89817300 | -3.28673300 |
| H | -5.82515100 | 4.29636400 | 0.77851600 |

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|---|---|---|---|
| H | 2.24275600 | 2.41108800 | -4.50577000 |
| H | 1.88158200 | 3.49213700 | -3.13530600 |
| H | 2.16013000 | 1.74949000 | -2.85200100 |
| H | 0.07556100 | 3.33645500 | -5.60047200 |
| H | -0.35681500 | 4.25227300 | -4.14798800 |
| H | -1.49069300 | 3.04851200 | -4.81651000 |
| H | -0.76158800 | -0.97206800 | -7.06626800 |
| H | 2.00235400 | -3.66554700 | -4.59086900 |
| H | 2.52218400 | -4.08663300 | -2.94248100 |
| H | 2.79636100 | -2.44378100 | -3.57620800 |
| H | -0.38122300 | -4.46142000 | -4.03082400 |
| H | 0.11820500 | -4.83530200 | -2.37320700 |
| H | -1.25542800 | -3.74398100 | -2.66244600 |
| H | 4.50083500 | 3.36630700 | 5.83508200 |
| C | -4.25627800 | 1.35283100 | 4.73658800 |
| H | -5.05190300 | 1.24068000 | 2.72417900 |
| H | -3.17719700 | 1.33818300 | 6.61203700 |
| H | 4.13781200 | -7.15745100 | 0.81912600 |
| H | -6.11054900 | 5.39753000 | -1.44214200 |
| H | -5.22086300 | 1.55774900 | 5.20664300 |
| Br | -0.39154900 | 0.72505000 | 6.10919400 |
| Br | 2.68781400 | -1.12839000 | 4.58091700 |

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Table S18
B3LYP-D3(BJ)/def2-SVP

**TS2D**

G = -8174.646099 Hartree

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| Si | 0.27796800 | -1.46741200 | -0.07246200 |
| C | 1.27819900 | 1.06528900 | -0.25415300 |
| C | 0.37482400 | 1.79178200 | 0.43370000 |
| Si | -0.90254700 | 0.48007100 | 0.37311900 |
| N | -2.20228100 | 0.91192400 | -0.91468400 |
| N | 1.84842100 | -1.71341700 | 1.01642500 |
| N | 1.75051900 | -1.95162000 | -1.13759600 |
| N | -0.81385300 | -2.66173700 | -0.37362900 |
| N | -2.61724100 | 0.64573700 | 1.19335000 |
| C | -2.21300200 | 1.54915800 | -2.25509800 |
| C | -3.17138700 | 0.91449700 | 0.01255500 |
| C | 2.34139700 | -1.48800900 | 2.39630200 |
| C | 2.54241700 | -2.06265100 | -0.06713600 |
| C | 1.85296600 | -2.70034700 | -2.41506100 |
| C | -2.04935100 | -3.07239800 | 0.02132500 |
| C | -3.24586500 | 0.43280100 | 2.51324300 |
| C | 0.25547900 | 3.18074000 | 0.92044900 |
| C | -0.90087100 | 1.16748100 | -2.94571800 |
| C | -3.37840300 | 1.05610900 | -3.12366400 |
| C | -2.28913300 | 3.07592800 | -2.08724300 |

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|---|---|---|---|
| C | -4.62125500 | 1.11638000 | -0.24233000 |
| C | 1.35819300 | -0.52328300 | 3.06362400 |
| C | 3.75178600 | -0.87714200 | 2.43925600 |
| C | 2.34825900 | -2.81439400 | 3.17417900 |
| C | 3.96306200 | -2.49140200 | -0.09296000 |
| C | 0.79598700 | -2.11460100 | -3.35759300 |
| C | 3.22815700 | -2.56266900 | -3.08990800 |
| C | 1.55650600 | -4.18504400 | -2.13834700 |
| C | -2.28693400 | -3.59201100 | 1.34257100 |
| C | -3.15237600 | -3.10648500 | -0.90425800 |
| C | -2.14776600 | -0.12548000 | 3.42256100 |
| C | -4.39862800 | -0.58107000 | 2.45912900 |
| C | -3.73924300 | 1.78025500 | 3.06798000 |
| C | -0.26705900 | 3.36276000 | 2.21763400 |
| C | 0.59327100 | 4.34986000 | 0.21115900 |
| C | 2.57049200 | 1.38396700 | -0.82076600 |
| H | -0.80521600 | 0.07645400 | -3.00896500 |
| H | -0.88508400 | 1.57702500 | -3.96614800 |
| H | -0.03595500 | 1.56642000 | -2.40561500 |
| H | -3.37694200 | -0.03740400 | -3.19057500 |
| H | -3.25947100 | 1.46256600 | -4.13939200 |
| H | -4.35538000 | 1.38239700 | -2.74833800 |
| H | -3.26351600 | 3.37947000 | -1.67954900 |
| H | -2.16193500 | 3.57303600 | -3.06090100 |
| H | -1.49767200 | 3.43681900 | -1.41869300 |
| C | -5.39149800 | 0.00572400 | -0.61191300 |

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|---|---|---|---|
| C | -5.21870400 | 2.37560800 | -0.11345100 |
| H | 1.36912200 | 0.45420600 | 2.56567300 |
| H | 1.62565500 | -0.38305100 | 4.12125900 |
| H | 0.34249800 | -0.93247400 | 3.02492500 |
| H | 3.85092000 | -0.05057200 | 1.72803200 |
| H | 3.93315400 | -0.47371900 | 3.44675400 |
| H | 4.53325200 | -1.61753200 | 2.23195900 |
| H | 1.34243500 | -3.24427900 | 3.23192700 |
| H | 2.70924500 | -2.64142400 | 4.19992500 |
| H | 3.01480900 | -3.54805400 | 2.70104200 |
| C | 4.32242900 | -3.77955900 | 0.32176900 |
| C | 4.94726900 | -1.59761100 | -0.53594400 |
| H | 1.05721100 | -1.08602600 | -3.64366400 |
| H | 0.73386800 | -2.71722500 | -4.27489600 |
| H | -0.18719200 | -2.11290400 | -2.87578400 |
| H | 3.54297500 | -1.51247000 | -3.14689800 |
| H | 3.15319100 | -2.95770600 | -4.11484300 |
| H | 4.01059600 | -3.13122200 | -2.57403100 |
| H | 2.35519000 | -4.62765400 | -1.52460900 |
| H | 1.49919100 | -4.75240900 | -3.08015800 |
| H | 0.60534300 | -4.27304000 | -1.59739500 |
| C | -1.10199400 | -3.79354500 | 2.27110100 |
| C | -3.56513100 | -4.01718900 | 1.71459800 |
| C | -2.89499300 | -2.80148900 | -2.37110900 |
| C | -4.41330100 | -3.53351600 | -0.47632200 |
| H | -1.29597400 | 0.56568400 | 3.49197300 |

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|---|---|---|---|
| H | -2.53940400 | -0.28524600 | 4.43713800 |
| H | -1.78891600 | -1.08864900 | 3.03726700 |
| H | -4.09376200 | -1.49704600 | 1.93639100 |
| H | -4.68477600 | -0.85689500 | 3.48579000 |
| H | -5.28861500 | -0.16981900 | 1.96838300 |
| H | -2.92704100 | 2.52172300 | 3.08143600 |
| H | -4.11177200 | 1.64946800 | 4.09580500 |
| H | -4.56330300 | 2.17970400 | 2.46103800 |
| C | -0.41795300 | 4.62031600 | 2.79425700 |
| H | -0.53421700 | 2.46962800 | 2.78399100 |
| C | 0.43644600 | 5.62135100 | 0.77265100 |
| C | 2.83247900 | 1.00307300 | -2.15978400 |
| C | 3.64191200 | 2.01398700 | -0.14068900 |
| C | -6.75280600 | 0.16208200 | -0.86949800 |
| H | -4.92152900 | -0.97653500 | -0.67528900 |
| C | -6.58294900 | 2.52654900 | -0.37577900 |
| H | -4.61827500 | 3.23570500 | 0.18780400 |
| C | 5.66303100 | -4.17225400 | 0.29433300 |
| H | 3.55098900 | -4.47553100 | 0.65583700 |
| C | 6.28421300 | -1.99058700 | -0.55160200 |
| H | 4.66258300 | -0.59809600 | -0.85907200 |
| C | -1.46237100 | -3.96125500 | 3.74891600 |
| C | -0.26404200 | -4.98804200 | 1.77894300 |
| H | -0.46640600 | -2.89820100 | 2.18378100 |
| C | -4.64293300 | -3.96825600 | 0.83012400 |
| H | -3.72890400 | -4.40029700 | 2.72353900 |

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|---|---|---|---|
| C | -4.14678700 | -2.49513300 | -3.20014600 |
| C | -2.14861300 | -3.98238700 | -3.01713500 |
| H | -2.23051900 | -1.92143200 | -2.40116700 |
| H | -5.24151100 | -3.54863300 | -1.18795000 |
| C | -0.06438100 | 5.76014500 | 2.06658400 |
| H | -0.81184900 | 4.71099400 | 3.80915900 |
| H | 0.70995400 | 6.49995500 | 0.18674900 |
| C | 4.04684900 | 1.25673400 | -2.78609500 |
| H | 2.03408000 | 0.49660400 | -2.69830000 |
| C | 4.88358000 | 2.22790800 | -0.74491700 |
| C | -7.34964300 | 1.42228500 | -0.75780700 |
| H | -7.34909900 | -0.70704700 | -1.15586900 |
| H | -7.04699100 | 3.51068500 | -0.28031100 |
| C | 6.64559400 | -3.27746100 | -0.13816500 |
| H | 5.93949000 | -5.17991700 | 0.61266500 |
| H | 7.04679400 | -1.28597500 | -0.89078800 |
| H | -1.99600800 | -4.90719800 | 3.93351700 |
| H | -0.54969500 | -3.98147400 | 4.36617000 |
| H | -2.10005200 | -3.14135100 | 4.11369400 |
| H | -0.86859500 | -5.90869200 | 1.80794300 |
| H | 0.62726800 | -5.14668400 | 2.40750700 |
| H | 0.06407400 | -4.82130200 | 0.74381100 |
| H | -5.63827300 | -4.29005600 | 1.14454900 |
| H | -4.78707700 | -3.38557500 | -3.30442000 |
| H | -3.86056600 | -2.18572900 | -4.21794200 |
| H | -4.76053800 | -1.69300600 | -2.76687600 |

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|---|---|---|---|
| H | -2.79905800 | -4.87188500 | -3.03059100 |
| H | -1.85773000 | -3.75433300 | -4.05613800 |
| H | -1.24438800 | -4.23007000 | -2.45104200 |
| H | -0.17965500 | 6.75649900 | 2.49918000 |
| C | 5.09206500 | 1.85645100 | -2.07384600 |
| H | 4.18976300 | 0.96148200 | -3.82826400 |
| H | 5.67855600 | 2.70791100 | -0.17215100 |
| H | -8.41581600 | 1.54308800 | -0.96311300 |
| H | 7.69418100 | -3.58381000 | -0.15457900 |
| H | 6.06048400 | 2.03735100 | -2.54497400 |
| Br | 3.43727700 | 2.67615200 | 1.64409800 |
| Br | 1.27010600 | 4.28301400 | -1.57469900 |

Table S19
B3LYP-D3(BJ)/def2-SVP
**Int2D**
G = -8174.695761 Hartree

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| Si | 0.52243400 | 1.47291100 | -0.96546200 |
| Si | -0.38654800 | 1.30246900 | 2.36041100 |
| N | 1.91686600 | 0.95308400 | -0.38432300 |
| N | -1.74241600 | 1.43039300 | 3.75518900 |

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|---|---|---|---|
| N | 0.59952400 | 1.89255900 | -2.79584000 |
| N | -0.62529900 | 0.31659600 | -1.95986800 |
| N | 0.15754500 | 2.43598600 | 3.82069400 |
| C | 2.86115600 | 0.67720500 | 0.55746300 |
| C | -0.24374100 | 0.90380100 | -3.09725200 |
| C | -2.96676100 | 0.69007800 | 4.10912700 |
| C | -0.92745100 | 2.14072700 | 4.54359800 |
| C | -0.67872500 | 0.52801100 | -4.46683000 |
| C | 2.75215600 | -0.47196700 | 1.40809600 |
| C | 4.02018800 | 1.50581600 | 0.70183100 |
| C | 1.59936800 | 2.58252900 | -3.64064500 |
| C | -0.06698000 | -0.54783000 | -5.12186800 |
| H | 0.71942700 | -1.11141200 | -4.61679400 |
| C | 1.67124800 | -1.49623700 | 1.12245600 |
| H | 0.80314400 | -0.92612200 | 0.77054000 |
| C | 4.29305200 | 2.61371100 | -0.30010000 |
| H | 3.39548800 | 2.67468600 | -0.92327400 |
| C | -1.64276400 | -0.73341200 | -1.73330400 |
| C | -4.13019600 | 1.66061700 | 4.37229000 |
| H | -3.94132600 | 2.27577700 | 5.26271000 |
| H | -5.06218400 | 1.09843200 | 4.54113900 |
| H | -4.27726500 | 2.32964300 | 3.51449800 |
| C | 1.46013500 | 2.99393900 | 4.22315700 |
| C | -1.93492700 | -0.74836200 | -0.23194000 |
| H | -1.03143500 | -0.96467200 | 0.35178400 |
| H | -2.68538000 | -1.51767200 | -0.00062000 |

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|---|---|---|---|
| H | -2.32693700 | 0.22308400 | 0.09092500 |
| C | 3.70313900 | -0.68949900 | 2.40857100 |
| H | 3.59945900 | -1.55981700 | 3.06019500 |
| C | -1.16826500 | 2.53115600 | 5.96045000 |
| C | -2.74896400 | -0.22156300 | 5.33126400 |
| H | -1.85667200 | -0.85040100 | 5.18593300 |
| H | -3.61863200 | -0.88473100 | 5.45989500 |
| H | -2.62773800 | 0.35085900 | 6.25923100 |
| C | -0.45330000 | -0.88356600 | -6.42185300 |
| H | 0.03086000 | -1.71919100 | -6.93203500 |
| C | -3.30236100 | -0.19885600 | 2.90583100 |
| H | -3.45621200 | 0.40781100 | 2.00590800 |
| H | -4.22656700 | -0.76427100 | 3.09735000 |
| H | -2.48938200 | -0.91451700 | 2.71345200 |
| C | -0.62523700 | 1.80022600 | 7.02589400 |
| H | -0.04256300 | 0.90058500 | 6.82171600 |
| C | -1.67676000 | 1.26622600 | -5.11676900 |
| H | -2.13757400 | 2.11191300 | -4.60556800 |
| C | -1.45423100 | -0.15190700 | -7.06620000 |
| H | -1.75700400 | -0.41661700 | -8.08186800 |
| C | 4.51307300 | 3.99712400 | 0.32259700 |
| H | 3.63129900 | 4.32341000 | 0.88952100 |
| H | 4.70192900 | 4.74837600 | -0.46238200 |
| H | 5.37932600 | 4.00765500 | 1.00481700 |
| C | 5.46704200 | 2.23409700 | -1.21682600 |
| H | 6.41166900 | 2.18250900 | -0.65025900 |

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|---|---|---|---|
| H | 5.59715600 | 2.97542000 | -2.02387400 |
| H | 5.30571700 | 1.24804700 | -1.67863700 |
| C | -2.06579200 | 0.92209200 | -6.41070100 |
| H | -2.84599200 | 1.49806800 | -6.91335100 |
| C | 4.78982300 | 0.16886600 | 2.59007400 |
| H | 5.51586700 | -0.01381200 | 3.38589400 |
| C | 1.07410400 | 2.94482000 | -5.03827600 |
| H | 0.93748500 | 2.07125100 | -5.68660400 |
| H | 1.81076400 | 3.60455900 | -5.52170900 |
| H | 0.12187200 | 3.49077800 | -4.97197300 |
| C | 2.82913600 | 1.66498200 | -3.75688400 |
| H | 3.17588900 | 1.36467100 | -2.76000000 |
| H | 3.64850700 | 2.17531500 | -4.28619900 |
| H | 2.57251300 | 0.75378600 | -4.31985600 |
| C | 4.94603500 | 1.24308800 | 1.71555700 |
| H | 5.81824000 | 1.89573100 | 1.81685500 |
| C | 1.21795900 | -2.30638800 | 2.33653700 |
| H | 2.00819200 | -2.97748300 | 2.71161100 |
| H | 0.35523900 | -2.94018700 | 2.07143900 |
| H | 0.91050600 | -1.63997100 | 3.15727300 |
| C | -2.95905800 | -0.44190700 | -2.47423300 |
| H | -3.34053200 | 0.55731500 | -2.21570700 |
| H | -3.71636000 | -1.17810700 | -2.16517200 |
| H | -2.85466600 | -0.50964200 | -3.56365500 |
| C | -0.83645900 | 2.21572500 | 8.34167400 |
| H | -0.41057200 | 1.64052200 | 9.16705600 |

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|---|---|---|---|
| C | 1.95670400 | 3.89354500 | -2.92996500 |
| H | 1.12080800 | 4.60230900 | -2.98834700 |
| H | 2.83629800 | 4.35210600 | -3.40497700 |
| H | 2.19121300 | 3.73392100 | -1.87131300 |
| C | -1.08248400 | -2.09928000 | -2.16195300 |
| H | -0.94660000 | -2.15395600 | -3.25067900 |
| H | -1.77783100 | -2.90118800 | -1.86893400 |
| H | -0.11530800 | -2.28366000 | -1.67581400 |
| C | 1.32426700 | 4.18906400 | 5.18158700 |
| H | 2.30546600 | 4.67759000 | 5.28191000 |
| H | 0.99480100 | 3.89295800 | 6.18505000 |
| H | 0.61205800 | 4.93155600 | 4.79182800 |
| C | -1.59044200 | 3.36437100 | 8.60194200 |
| H | -1.75217200 | 3.69055300 | 9.63206800 |
| C | -1.92977400 | 3.67800000 | 6.22479900 |
| H | -2.34263000 | 4.24719100 | 5.39024000 |
| C | 2.12038300 | -2.41214100 | -0.02820700 |
| H | 2.33345900 | -1.81699500 | -0.92907400 |
| H | 1.34361800 | -3.15595000 | -0.27474600 |
| H | 3.03660900 | -2.96104700 | 0.24433200 |
| C | -2.13762200 | 4.09269700 | 7.54186200 |
| H | -2.72759400 | 4.99058400 | 7.74028000 |
| C | 2.31521100 | 1.88517100 | 4.86206900 |
| H | 1.85520300 | 1.51683900 | 5.79042600 |
| H | 3.31885200 | 2.26659800 | 5.10569500 |
| H | 2.43629500 | 1.04586300 | 4.16247000 |

| | | | |
|---|---|---|---|
| C | 2.14210500 | 3.46278500 | 2.93579200 |
| H | 2.20076900 | 2.64938400 | 2.19998100 |
| H | 3.17118700 | 3.78389200 | 3.14609300 |
| H | 1.60048600 | 4.30128400 | 2.47893100 |
| C | -0.63501000 | 2.75757400 | -0.15655500 |
| C | -1.05068400 | 2.71197700 | 1.13827200 |
| C | -1.11323700 | 3.83788200 | -1.07695100 |
| C | -1.98688900 | 3.74109500 | 1.67025400 |
| C | -1.08786400 | 6.13244700 | -1.94573700 |
| C | -2.07484100 | 5.81096100 | -2.87652600 |
| C | -2.57393100 | 4.50627100 | -2.92809200 |
| C | -2.09184000 | 3.54418700 | -2.04429300 |
| C | -0.61335200 | 5.15169600 | -1.06812400 |
| H | -2.48373900 | 2.52962900 | -2.07975800 |
| H | -3.34861400 | 4.24065800 | -3.65155400 |
| H | -2.44656400 | 6.57775700 | -3.55988300 |
| H | -0.67161300 | 7.13958300 | -1.89988800 |
| C | -3.37261200 | 3.76943100 | 1.42308300 |
| C | -1.49049800 | 4.74969500 | 2.52047800 |
| C | -2.31231800 | 5.72920500 | 3.07351700 |
| C | -3.68289800 | 5.72792700 | 2.80299300 |
| C | -4.21371900 | 4.74093700 | 1.97258300 |
| H | -5.28089700 | 4.71665300 | 1.74838100 |
| H | -0.42548600 | 4.75526900 | 2.73100600 |
| H | -1.87592000 | 6.49844300 | 3.71504500 |
| H | -4.33954100 | 6.48891900 | 3.23050300 |

| | | | |
|---|---|---|---|
| Br | 0.82176700 | 5.64525200 | 0.09045600 |
| Br | -4.21917300 | 2.43691100 | 0.33428900 |

Table S20
B3LYP-D3(BJ)/def2-SVP
**TS3D**
G = -8174.65471 Hartree

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| N | 0.60640800 | -1.92630300 | -0.06055500 |
| Si | -1.55273900 | -0.20191300 | 0.46299900 |
| N | -3.05268300 | 0.80431100 | 1.15455500 |
| C | -3.87335800 | 0.20353500 | 0.28653400 |
| N | -3.12869900 | -0.56260300 | -0.51489000 |
| C | -0.54065200 | 1.00175100 | -0.63299000 |
| C | 0.82565500 | 0.98459200 | -0.58799800 |
| Si | 1.80018800 | -0.53090200 | 0.11000800 |
| H | 5.70208900 | -0.12540800 | 2.45976100 |
| C | 5.62598900 | 0.97242400 | 2.42261600 |
| H | 5.20913000 | 1.32332300 | 3.38206900 |
| H | 6.64956800 | 1.37220500 | 2.33352800 |
| C | 5.45838600 | -3.17115300 | -2.67758700 |
| C | 4.75743500 | 1.42337900 | 1.23877800 |

| | | | |
|---|---|---|---|
| C | 4.55780100 | -0.21337800 | -0.72131800 |
| C | 5.26881000 | 0.84492000 | -0.06511400 |
| H | 3.76020000 | 0.99202700 | 1.38316800 |
| C | 5.16435100 | -0.77769000 | -1.89128800 |
| C | 6.46171800 | 1.33294500 | -0.60329400 |
| C | 6.35417400 | -0.24744700 | -2.39811100 |
| C | 7.00953800 | 0.81481500 | -1.77664400 |
| H | 6.97739700 | 2.14853600 | -0.08799200 |
| H | 6.78342700 | -0.68543300 | -3.30436900 |
| H | 7.93750300 | 1.21926200 | -2.18794700 |
| C | 4.60182000 | 2.94808600 | 1.21178100 |
| H | 4.12576900 | 3.31113300 | 2.13833900 |
| H | 5.57712000 | 3.45426300 | 1.12454800 |
| H | 3.98284200 | 3.26720300 | 0.36316000 |
| H | 5.82684700 | -3.45145900 | -1.67859400 |
| H | 4.93565000 | -4.04261100 | -3.10763000 |
| H | 6.33713600 | -2.96631100 | -3.31128300 |
| H | 3.67370900 | -2.25102400 | -1.96378500 |
| C | 4.52005100 | -1.95952400 | -2.59263800 |
| C | 3.96918600 | -1.59021700 | -3.97785600 |
| H | 3.45842700 | -2.44825400 | -4.44635800 |
| H | 4.77690900 | -1.26870300 | -4.65595700 |
| H | 3.24500600 | -0.76279900 | -3.91605400 |
| N | 3.35226600 | -0.67105900 | -0.27487700 |
| N | 1.11888000 | -0.84923900 | 1.77843500 |
| C | 0.14720600 | -1.68355500 | 1.25846600 |

| | | | |
|---|---|---|---|
| C | -0.49785900 | -2.75053400 | 2.10020100 |
| C | -1.86794300 | -3.02341700 | 2.09670400 |
| C | -2.38978800 | -4.07815100 | 2.84757400 |
| C | -1.54267300 | -4.87353400 | 3.62359000 |
| C | -0.17143300 | -4.60046400 | 3.64493200 |
| C | 0.34513900 | -3.54690900 | 2.89041500 |
| H | 1.41349400 | -3.33171400 | 2.90443700 |
| H | 0.50033300 | -5.21087000 | 4.25300600 |
| H | -1.94911900 | -5.69753300 | 4.21465300 |
| H | -3.46397000 | -4.27734500 | 2.82780500 |
| H | -2.52906100 | -2.39880900 | 1.49460300 |
| C | -2.24533600 | 2.83122800 | -0.99770900 |
| H | -2.32244800 | 2.90851400 | 0.08112500 |
| C | 1.65192100 | 2.04666000 | -1.22458000 |
| C | 1.58719000 | 3.41900000 | -0.90753800 |
| C | 2.62891500 | 1.67625300 | -2.17143600 |
| H | 2.72896500 | 0.62296800 | -2.41319200 |
| H | 4.22179300 | 2.24676700 | -3.49172900 |
| C | 3.46446400 | 2.59846900 | -2.78908700 |
| C | 3.34343600 | 3.95465800 | -2.48126600 |
| H | 3.99391200 | 4.69465600 | -2.95290200 |
| C | 2.40483600 | 4.36444800 | -1.53513000 |
| H | 2.32257200 | 5.41444900 | -1.25256300 |
| C | -1.31224400 | 1.91598500 | -1.52600600 |
| C | -1.22757000 | 1.86844000 | -2.93693800 |
| H | -1.92887200 | 2.59555300 | -4.83882000 |

| | | | |
|---|---|---|---|
| C | -2.02973600 | 2.67201200 | -3.75557300 |
| C | -2.94425400 | 3.55921900 | -3.19031600 |
| H | -3.56382500 | 4.18572800 | -3.83586300 |
| C | -3.04462100 | 3.64142600 | -1.79952100 |
| H | -3.73689000 | 4.34776200 | -1.33469100 |
| C | -6.19317700 | -0.53051500 | 0.91548600 |
| C | -5.35239800 | 0.34990800 | 0.22358900 |
| C | -5.90583800 | 1.39317900 | -0.53217100 |
| C | -7.28962100 | 1.55462800 | -0.58847800 |
| C | -8.12868900 | 0.67879700 | 0.10868500 |
| C | -7.57942300 | -0.36372900 | 0.85927700 |
| H | -8.23090200 | -1.05118800 | 1.40322900 |
| H | -5.76275400 | -1.34467500 | 1.50136900 |
| H | -9.21242300 | 0.80848100 | 0.06503700 |
| H | -7.71621800 | 2.36837000 | -1.17903400 |
| H | -5.24308400 | 2.07117900 | -1.07220100 |
| C | 1.21666000 | -0.15467500 | 3.07509800 |
| C | 0.89661200 | -3.24654100 | -0.68918200 |
| C | 1.31230500 | 1.35604200 | 2.80597800 |
| H | 2.21423200 | 1.59539000 | 2.22979500 |
| H | 1.35966700 | 1.92122100 | 3.74916800 |
| H | 0.46268900 | 1.72070800 | 2.22269200 |
| C | 2.51876900 | -0.62169100 | 3.75007300 |
| H | 2.46321500 | -1.68836900 | 4.01175900 |
| H | 2.70234300 | -0.04973400 | 4.67364100 |
| H | 3.37344300 | -0.48025600 | 3.07672000 |

| | | | |
|---|---|---|---|
| C | 0.03097100 | -0.44999500 | 4.00770200 |
| H | 0.04813400 | 0.25702700 | 4.85048700 |
| H | 0.07163900 | -1.46568300 | 4.41841000 |
| H | -0.92908500 | -0.34331000 | 3.49004600 |
| C | -3.40542900 | 1.53196300 | 2.39400600 |
| C | -0.23373700 | -4.28029900 | -0.53363600 |
| C | 1.09634800 | -2.95555600 | -2.18665400 |
| C | 2.18944600 | -3.85633700 | -0.10562200 |
| C | -3.53831700 | -1.40850400 | -1.65442400 |
| C | -4.42713700 | -0.64446900 | -2.64954300 |
| C | -2.24698300 | -1.80505500 | -2.36259600 |
| C | -4.25511600 | -2.66961400 | -1.14180400 |
| C | -2.15481400 | 2.28968700 | 2.84634600 |
| C | -4.53162400 | 2.56027300 | 2.18199300 |
| C | -3.82088900 | 0.52077100 | 3.47789200 |
| H | -2.35454300 | 2.82033700 | 3.78828200 |
| H | -1.32099100 | 1.60571800 | 3.02005100 |
| H | -1.83740700 | 3.02715000 | 2.09657400 |
| H | -3.99727400 | 1.03241400 | 4.43676600 |
| H | -4.74899600 | 0.00371200 | 3.19572600 |
| H | -3.03734400 | -0.23568200 | 3.62911700 |
| H | -4.59159700 | 3.20352200 | 3.07266300 |
| H | -4.32501500 | 3.20249300 | 1.31372400 |
| H | -5.51361700 | 2.09480100 | 2.04329500 |
| H | 0.15023800 | -2.70091900 | -2.67733400 |
| H | 1.78144300 | -2.11303100 | -2.32853800 |

| | | | |
|---|---|---|---|
| H | 1.52541600 | -3.83243200 | -2.69403700 |
| H | -0.04423200 | -5.10834100 | -1.23416000 |
| H | -0.27780900 | -4.70743400 | 0.47470700 |
| H | -1.21981100 | -3.86241100 | -0.77053400 |
| H | 2.46127000 | -4.77143700 | -0.65569700 |
| H | 3.02025300 | -3.14121900 | -0.16642700 |
| H | 2.04808400 | -4.13146200 | 0.94833100 |
| H | -1.81158200 | -0.95557300 | -2.89799500 |
| H | -2.43038000 | -2.61257300 | -3.08601300 |
| H | -1.50548900 | -2.14996900 | -1.63583900 |
| H | -3.97984700 | 0.33075200 | -2.89344900 |
| H | -5.44505500 | -0.48602800 | -2.27348900 |
| H | -4.50182100 | -1.22748600 | -3.58017200 |
| H | -5.18564500 | -2.41790900 | -0.61489800 |
| H | -3.60462400 | -3.23632600 | -0.45867400 |
| H | -4.51332200 | -3.32559800 | -1.98712300 |
| Br | -0.03612500 | 0.68651900 | -3.85641900 |
| Br | 0.48272500 | 4.09816800 | 0.50553600 |

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Table S21
B3LYP-D3(BJ)/def2-SVP
**3c**
G = -8174.724834 Hartree

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| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|

| Number | X | Y | Z |
|---|---|---|---|
| Si | 0.06817100 | 0.08306400 | 0.09105900 |
| Si | -0.00307900 | -0.04501700 | 2.93810500 |
| C | 0.63484000 | 0.06425300 | -2.12907100 |
| C | 1.39712900 | -1.20677600 | 3.59158200 |
| C | -1.23983300 | -1.19611700 | 1.99699200 |
| N | 0.65773100 | 0.83713100 | 1.47469400 |
| N | -0.77695500 | 0.78236600 | 4.10322700 |
| N | 1.18333000 | -0.69056500 | -1.17323200 |
| C | -1.28356500 | -1.03964300 | 0.64569300 |
| N | -0.23771000 | 0.89359500 | -1.52869600 |
| C | 0.93223100 | -0.00034000 | -3.58056600 |
| C | 0.90312200 | -2.44070000 | 4.27893300 |
| N | 2.60878400 | -0.81544000 | 3.43992900 |
| C | -2.11476100 | -2.11093000 | 2.75977000 |
| C | 1.62178300 | 1.98280100 | 1.54760100 |
| C | -0.91932600 | 1.94872500 | 4.78797500 |
| C | 2.24773400 | -1.72368700 | -1.19056400 |
| C | -2.25780200 | -1.60418100 | -0.31988700 |
| C | -1.28763800 | 1.77935400 | -2.09409700 |
| C | 1.90646400 | 0.84822500 | -4.12243800 |
| C | 0.25196700 | -0.90703100 | -4.40478600 |
| C | -0.03152900 | -2.35544700 | 5.32458000 |
| C | 1.25810100 | -3.71042900 | 3.79682600 |
| C | 3.82211000 | -1.34152600 | 4.09596500 |

| | | | |
|---|---|---|---|
| C | -2.19912500 | -3.49958900 | 2.54434500 |
| C | -2.89091800 | -1.57755700 | 3.81115700 |
| C | 2.93707600 | 1.58764900 | 0.86609400 |
| C | 1.90872800 | 2.36394500 | 3.00464700 |
| C | 1.01907600 | 3.20540600 | 0.84362000 |
| C | -1.89089300 | 2.92591800 | 4.38821600 |
| C | -0.11614100 | 2.24825100 | 5.93939100 |
| C | 2.29922800 | -2.28405000 | 0.23597100 |
| C | 1.92973900 | -2.86170600 | -2.17356500 |
| C | 3.59986000 | -1.09524500 | -1.56298500 |
| C | -3.63901400 | -1.32537100 | -0.28911600 |
| C | -1.79706600 | -2.38887100 | -1.39452600 |
| C | -2.08131600 | 2.31615100 | -0.89729600 |
| C | -2.23681200 | 0.99539800 | -3.01456200 |
| C | -0.64049700 | 2.94322100 | -2.85902700 |
| C | 2.20125600 | 0.78623100 | -5.48606900 |
| H | 2.42976500 | 1.55540100 | -3.47598700 |
| C | 0.54851900 | -0.96112500 | -5.76729200 |
| H | -0.50962400 | -1.55987300 | -3.97621700 |
| C | -0.55112100 | -3.51057100 | 5.90646300 |
| H | -0.35900400 | -1.37220600 | 5.65793300 |
| C | 0.72673300 | -4.86664800 | 4.37015600 |
| H | 1.93966500 | -3.79056100 | 2.94944300 |
| C | 3.60913000 | -2.02375600 | 5.46010700 |
| C | 4.54499300 | -2.28788000 | 3.12265300 |
| C | 4.70836200 | -0.09830900 | 4.31492900 |

| | | | |
|---|---|---|---|
| C | -3.03848500 | -4.31299300 | 3.31086000 |
| Br | -1.10405700 | -4.39529000 | 1.25043800 |
| C | -3.74013700 | -2.37583200 | 4.56919900 |
| H | -2.77624400 | -0.51427500 | 4.02170600 |
| H | 3.34282200 | 0.68967700 | 1.35178600 |
| H | 3.67633400 | 2.39982800 | 0.94493900 |
| H | 2.78024700 | 1.38418600 | -0.20462400 |
| H | 1.01164100 | 2.73548300 | 3.51390800 |
| H | 2.66457500 | 3.16381000 | 3.02423500 |
| H | 2.30890300 | 1.50233800 | 3.55213100 |
| H | 0.84336800 | 3.00655500 | -0.22364100 |
| H | 0.06615500 | 3.48369600 | 1.31553700 |
| H | 1.70212100 | 4.06558300 | 0.91705800 |
| C | -2.81590200 | 2.63851400 | 3.21672200 |
| C | -2.03209200 | 4.11405400 | 5.11174700 |
| C | 0.89334400 | 1.22780300 | 6.43687900 |
| C | -0.29623700 | 3.44971300 | 6.62950200 |
| H | 2.51240400 | -1.49762700 | 0.97163600 |
| H | 3.08986600 | -3.04365000 | 0.31210300 |
| H | 1.34441900 | -2.75668100 | 0.51014800 |
| H | 0.97106500 | -3.34318700 | -1.93603200 |
| H | 2.71238400 | -3.63023800 | -2.09155900 |
| H | 1.90725500 | -2.51745600 | -3.21543200 |
| H | 3.87645100 | -0.30767600 | -0.85174100 |
| H | 3.57807800 | -0.66991600 | -2.57671100 |
| H | 4.38299800 | -1.86779000 | -1.53918400 |

| | | | |
|---|---|---|---|
| C | -4.51025300 | -1.82946300 | -1.26253300 |
| Br | -4.38395200 | -0.17761100 | 1.03567100 |
| C | -2.65095100 | -2.89381100 | -2.37096100 |
| H | -0.73467700 | -2.61486000 | -1.43624300 |
| H | -1.44148800 | 2.87929400 | -0.20926800 |
| H | -2.87716400 | 2.98771700 | -1.24852700 |
| H | -2.55958500 | 1.50277300 | -0.33439800 |
| H | -2.64604300 | 0.11527100 | -2.50132600 |
| H | -3.07738000 | 1.64364100 | -3.30379800 |
| H | -1.73717200 | 0.66882000 | -3.93567500 |
| H | 0.05540700 | 3.49864800 | -2.21354000 |
| H | -0.09495000 | 2.59183300 | -3.74560200 |
| H | -1.42113900 | 3.64022700 | -3.19866900 |
| C | 1.52305700 | -0.11713700 | -6.30879900 |
| H | 2.96207700 | 1.44749200 | -5.90602800 |
| H | 0.01527100 | -1.66579200 | -6.40890100 |
| C | -0.17281800 | -4.77099600 | 5.43407500 |
| H | -1.27351300 | -3.42394300 | 6.72100000 |
| H | 1.00418700 | -5.84532500 | 3.97159200 |
| H | 4.58010600 | -2.12846500 | 5.96969600 |
| H | 3.16223300 | -3.02069400 | 5.37755400 |
| H | 2.95476400 | -1.41212500 | 6.09877700 |
| H | 5.52222700 | -2.58188700 | 3.53717700 |
| H | 3.96209600 | -3.20189300 | 2.94337500 |
| H | 4.71843800 | -1.79155600 | 2.15584800 |
| H | 4.87764500 | 0.42423900 | 3.36212800 |

| | | | |
|---|---|---|---|
| H | 4.21840300 | 0.60501300 | 5.00332300 |
| H | 5.68292300 | -0.38098500 | 4.74337700 |
| C | -3.82189800 | -3.74768900 | 4.31578600 |
| H | -3.06375500 | -5.38668300 | 3.12209700 |
| H | -4.33286800 | -1.92500500 | 5.36827100 |
| C | -2.97844500 | 3.82243200 | 2.25581500 |
| C | -4.18816100 | 2.16703900 | 3.72511700 |
| H | -2.36402600 | 1.80705300 | 2.65622900 |
| C | -1.24445600 | 4.39227700 | 6.22909800 |
| H | -2.78365700 | 4.84362700 | 4.79626700 |
| C | 2.25252000 | 1.83187200 | 6.80799100 |
| C | 0.31268900 | 0.42364800 | 7.61163700 |
| H | 1.05975600 | 0.52728800 | 5.60828300 |
| H | 0.32198000 | 3.65661200 | 7.50770000 |
| C | -4.01909700 | -2.61570700 | -2.30384000 |
| H | -5.57256600 | -1.58979900 | -1.20136300 |
| H | -2.25154200 | -3.51464500 | -3.17662900 |
| H | 1.75356800 | -0.16312600 | -7.37541800 |
| H | -0.59334600 | -5.67491200 | 5.88123600 |
| H | -4.48013300 | -4.38631000 | 4.90956400 |
| H | -3.49085300 | 4.67442000 | 2.73155100 |
| H | -3.57904800 | 3.53036900 | 1.37870100 |
| H | -2.00144200 | 4.18497600 | 1.89950900 |
| H | -4.87575100 | 1.94208900 | 2.89124200 |
| H | -4.09222400 | 1.26413600 | 4.34635400 |
| H | -4.66149600 | 2.94658200 | 4.34468000 |

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 H                -1.36884600    5.32762100    6.78051900
 H                 2.67613200    2.40313400    5.96768600
 H                 2.18151500    2.51198900    7.67235200
 H                 2.96840500    1.03829100    7.07936200
 H                 0.97992500   -0.40542900    7.90348700
 H                 0.16554100    1.07176600    8.49168000
 H                -0.66853400   -0.00073900    7.34980500
 H                -4.70529200   -3.00527500   -3.05902600
---------------------------------------------------------------------------------------------
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## VI. Spectra

## Supporting Information: 1H NMR spectra for all compounds

## IV. Collected $^{1}H$, $^{13}C$, $^{29}Si$, $^{31}P$ and $^{19}F$ NMR spectra of compounds 2-4

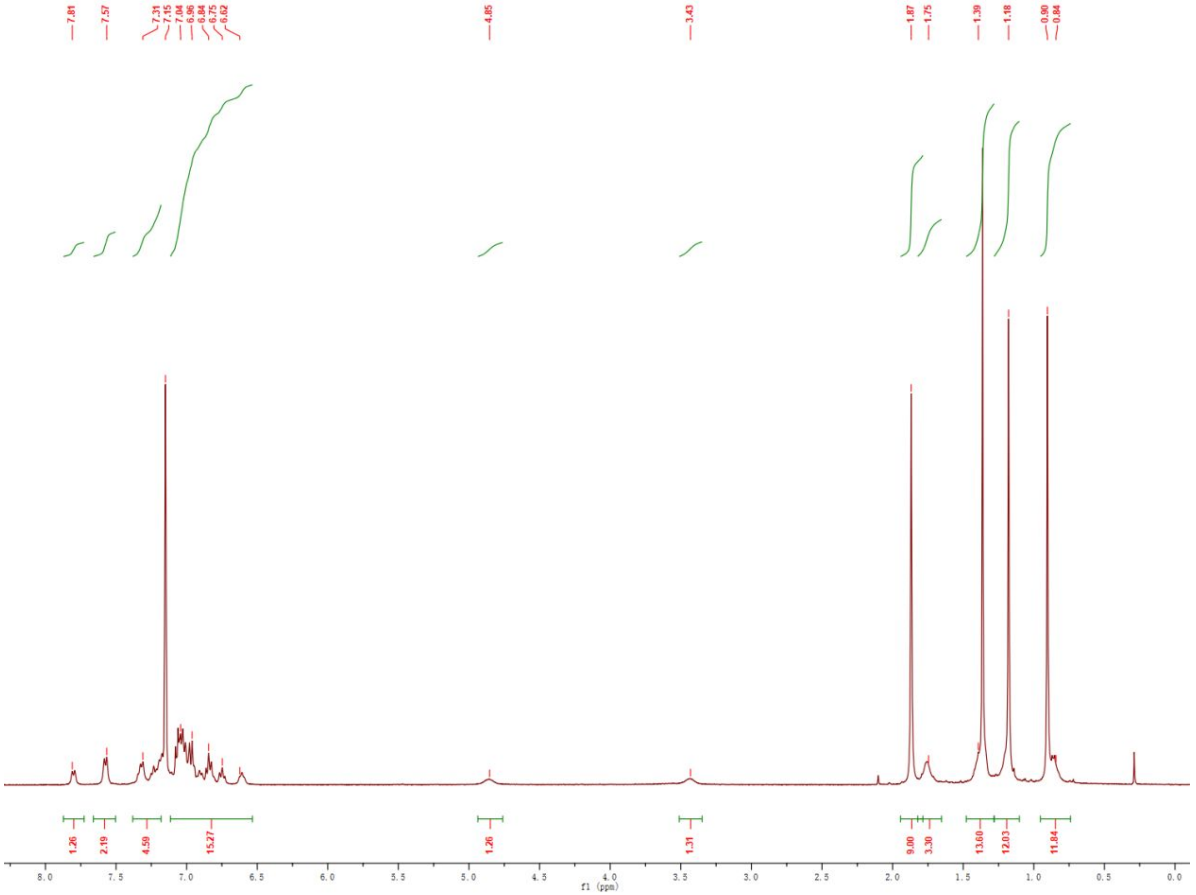


**Fig. S25.** $^{1}H$ NMR spectrum of **2a** in $C_6D_6$.

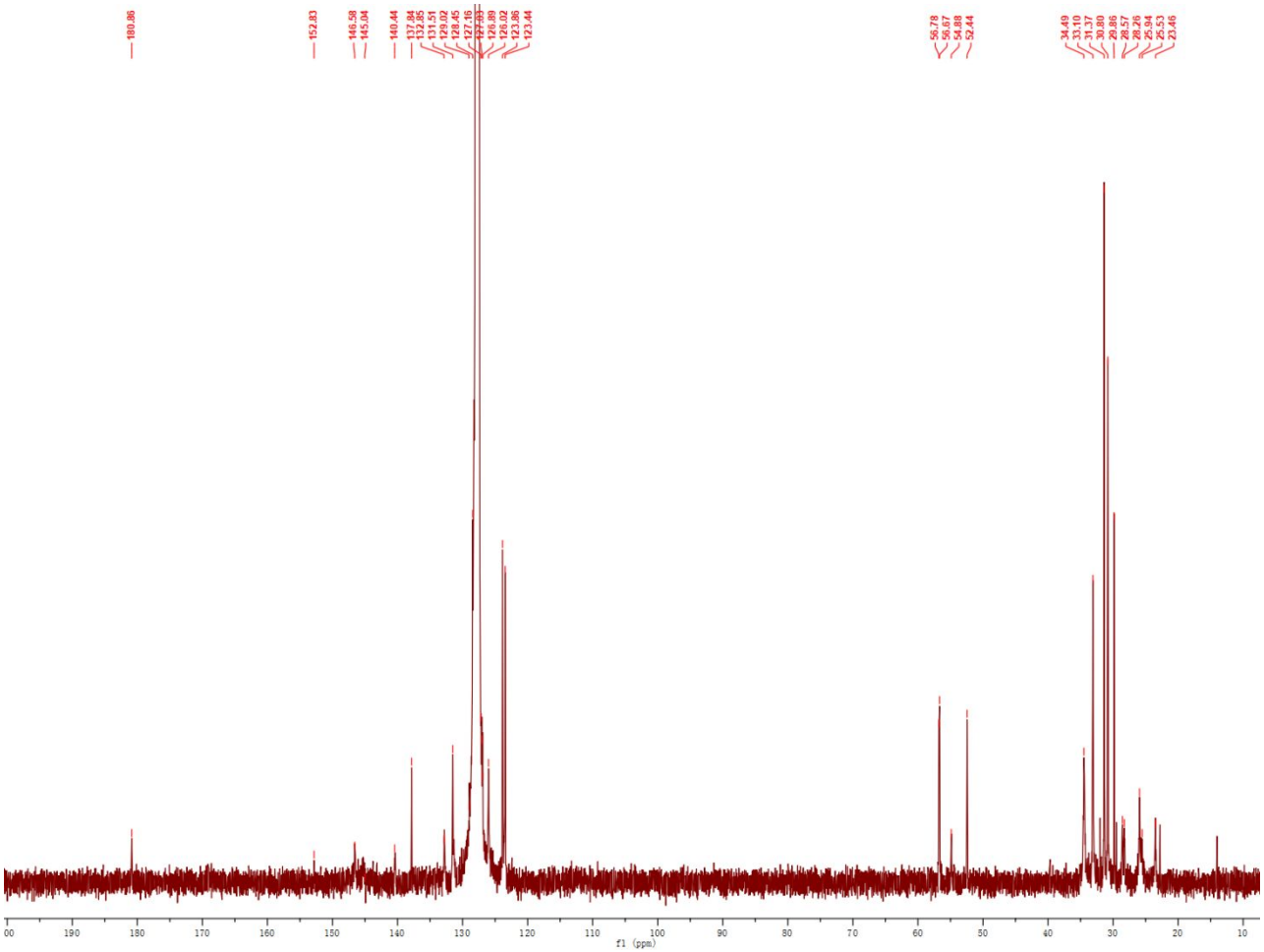


**Fig. S26.** $^{13}C$ NMR spectrum of **2a** in $C_6D_6$.

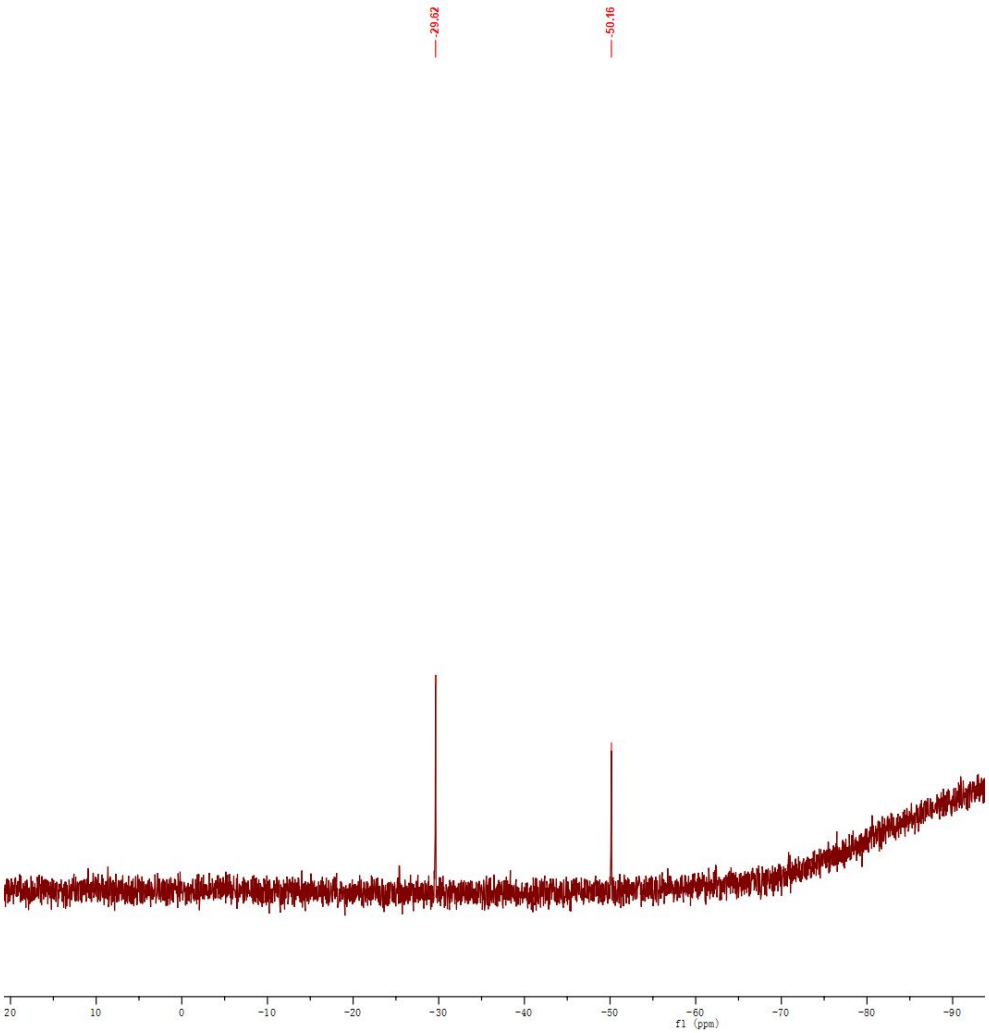


**Fig. S27.** $^{29}$Si NMR spectrum of **2a** in $C_6D_6$.

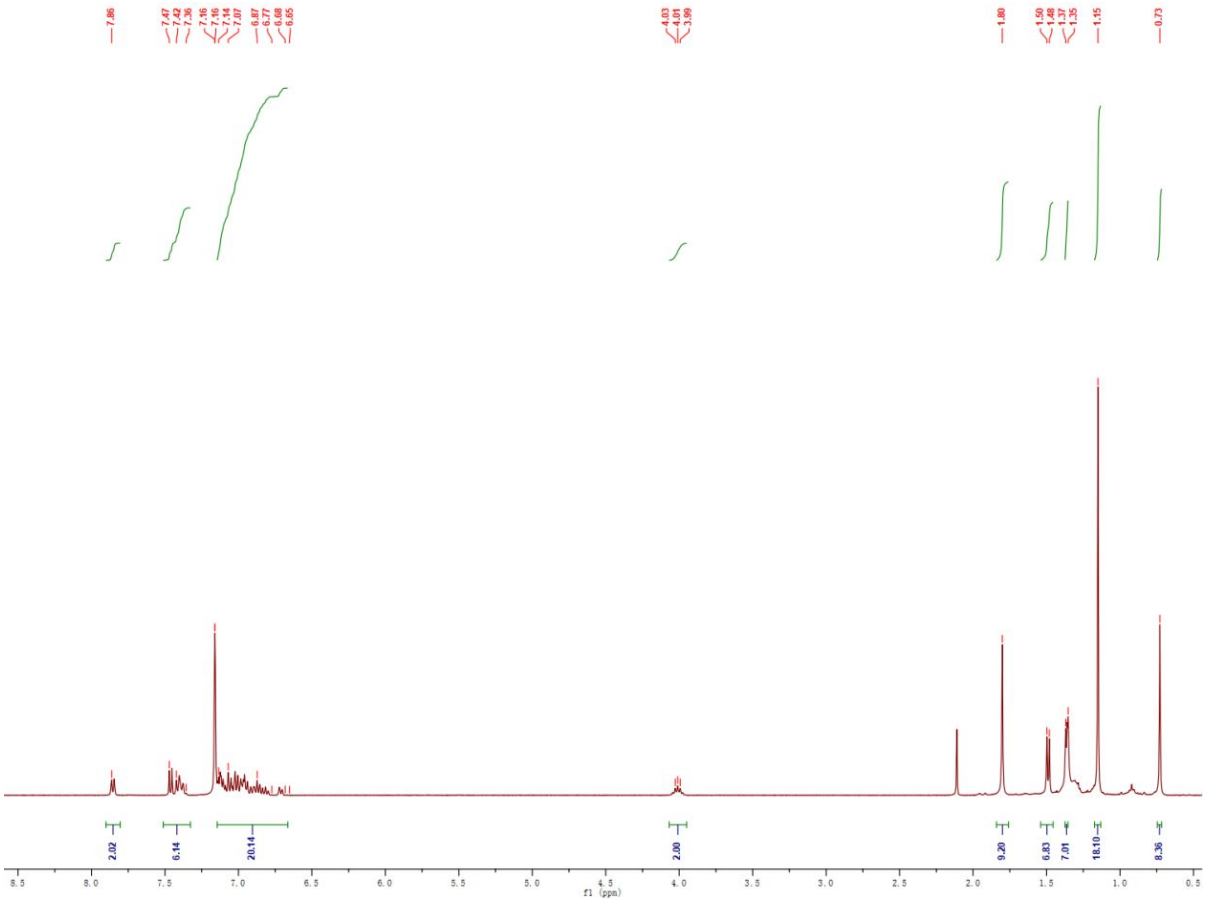


**Fig. S28.** $^{1}$H NMR spectrum of **3a** in $C_6D_6$.

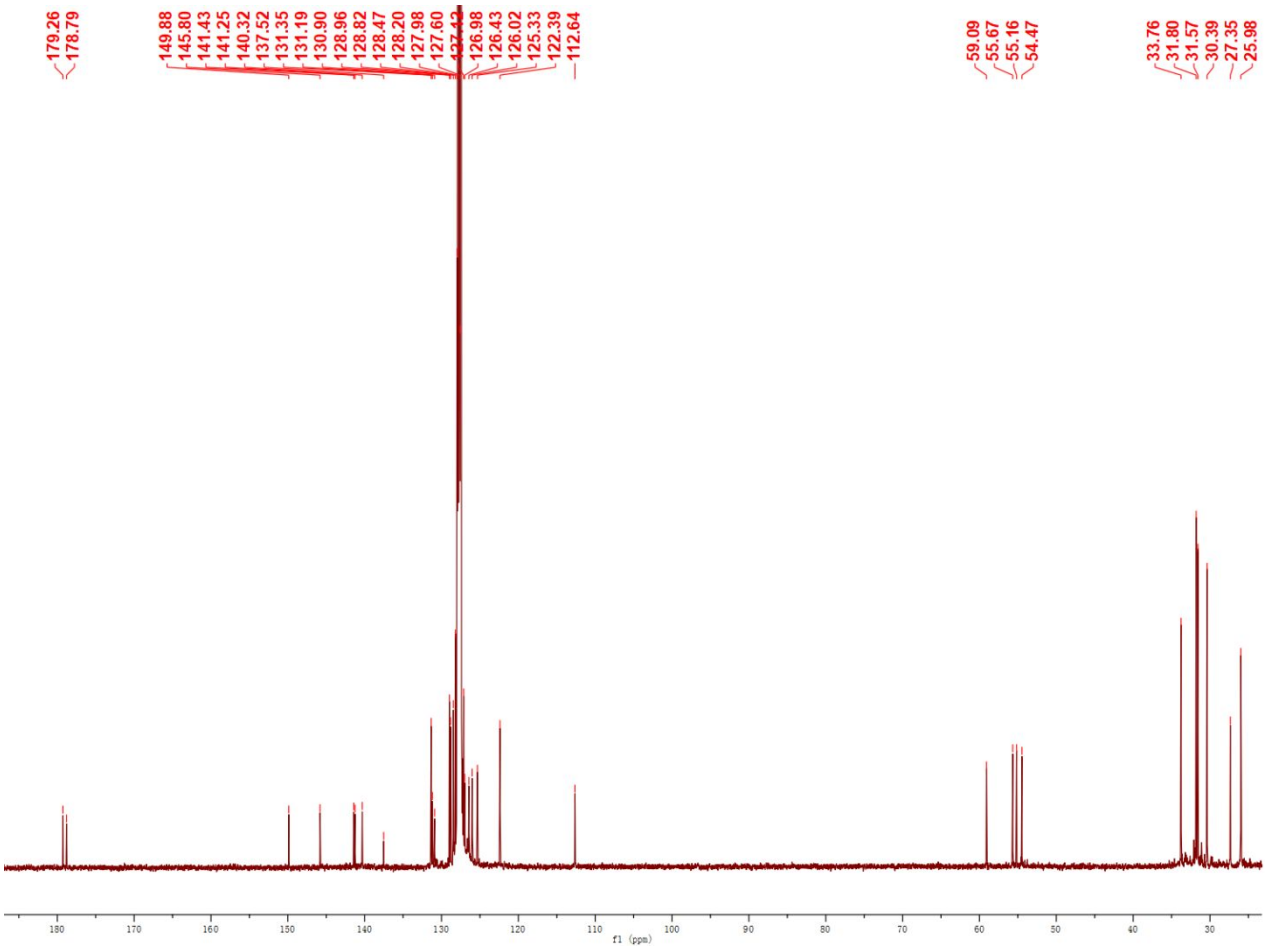


**Fig. S29.** $^{13}C$ NMR spectrum of **3a** in $C_6D_6$.

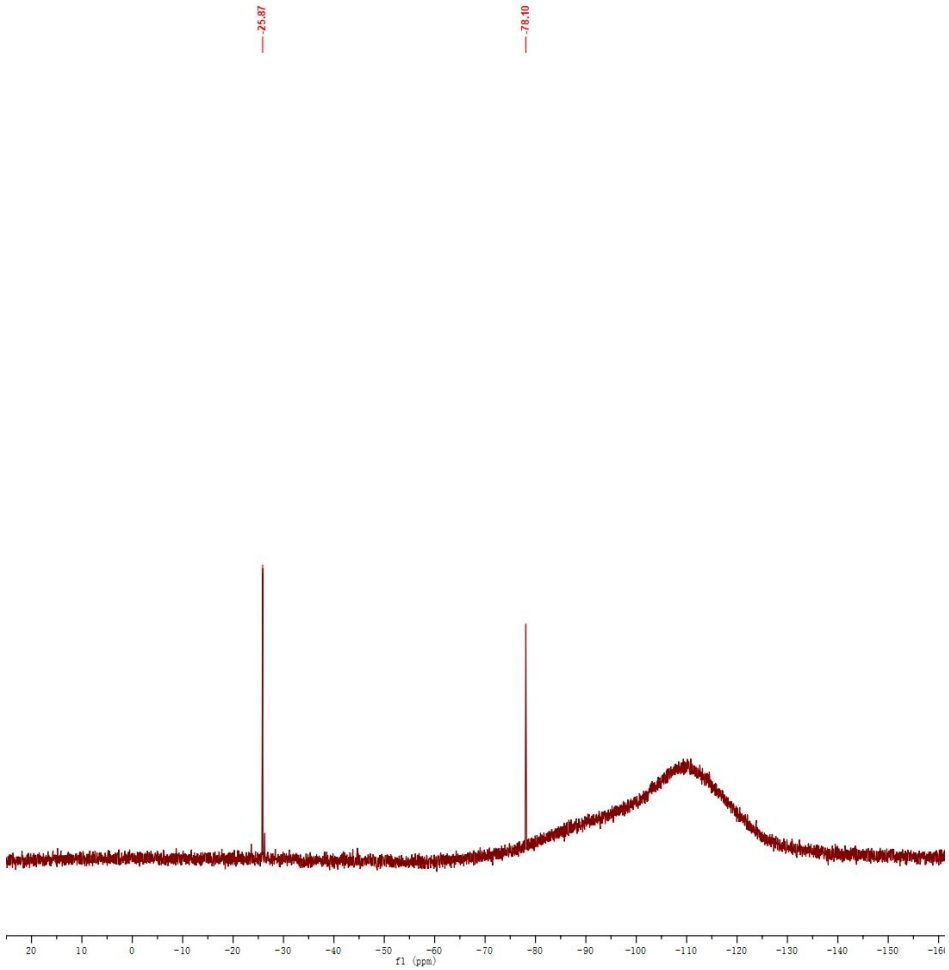


**Fig. S30.** $^{29}$Si NMR spectrum of **3a** in $C_6D_6$.

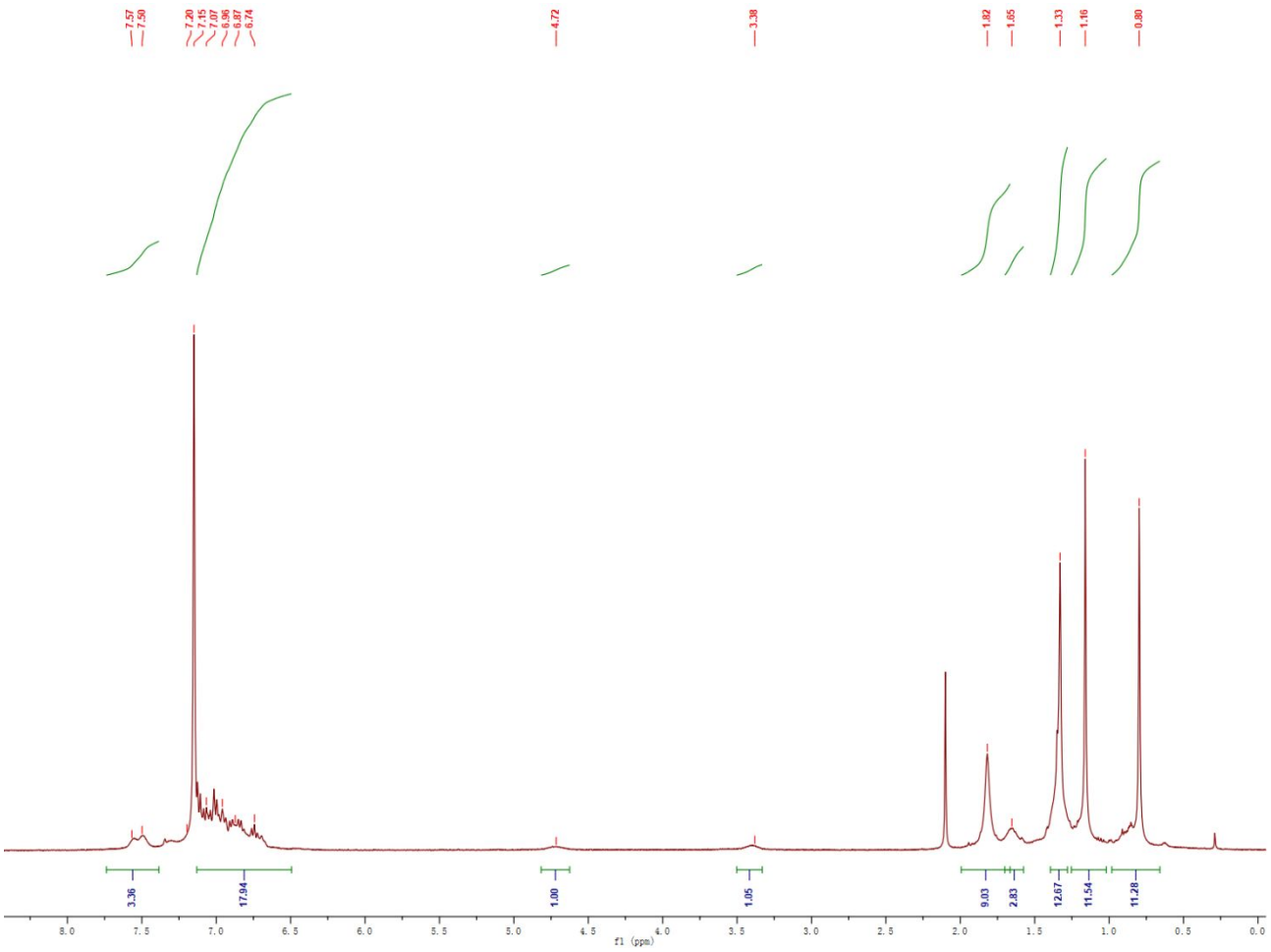


**Fig. S31.** $^{1}$H NMR spectrum of **2b** in $C_6D_6$.

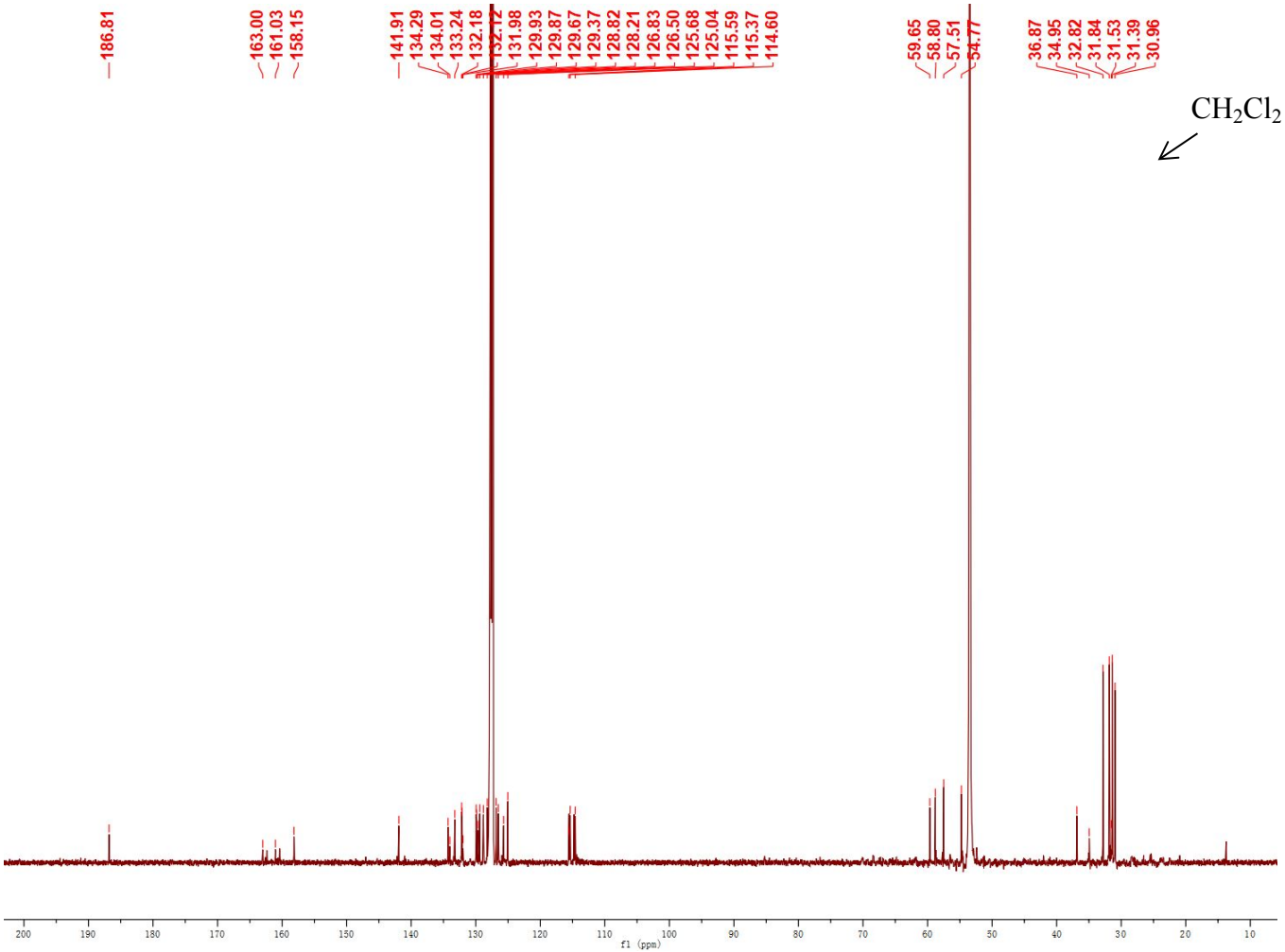


**Fig. S32.** $^{13}C$ NMR spectrum of **2b** in $C_6D_6$ (a small amount of $CH_2Cl_2$ was added to increase the solubility).

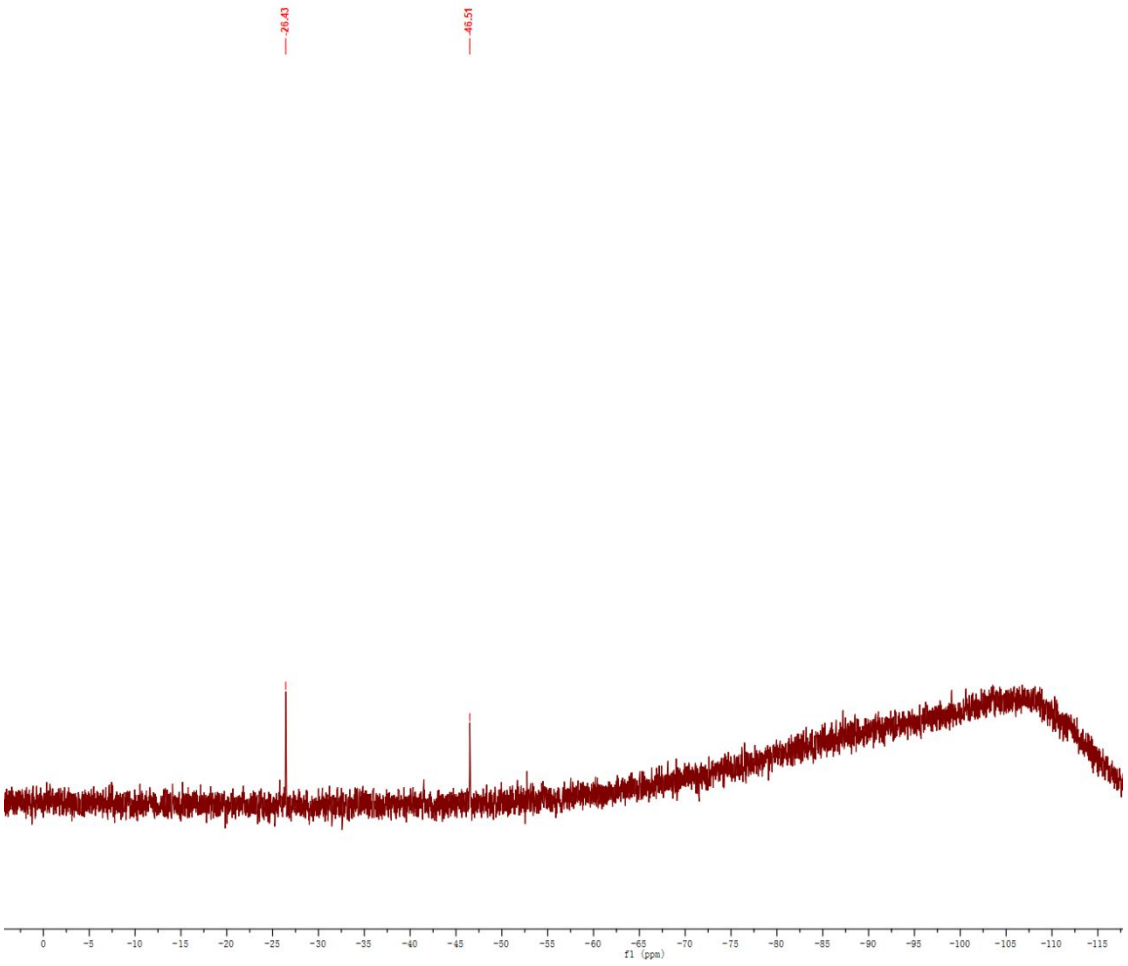


**Fig. S33.** $^{29}$Si NMR spectrum of **2b** in $C_6D_6$.

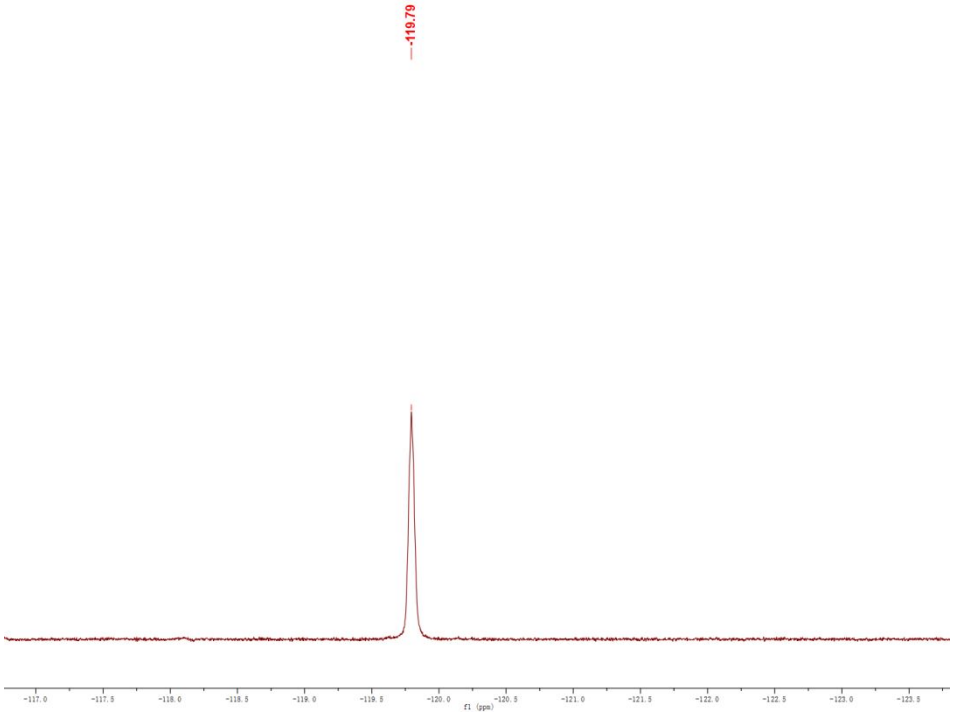


**Fig. S34.** $^{19}F$ NMR spectrum of **2b** in $C_6D_6$.

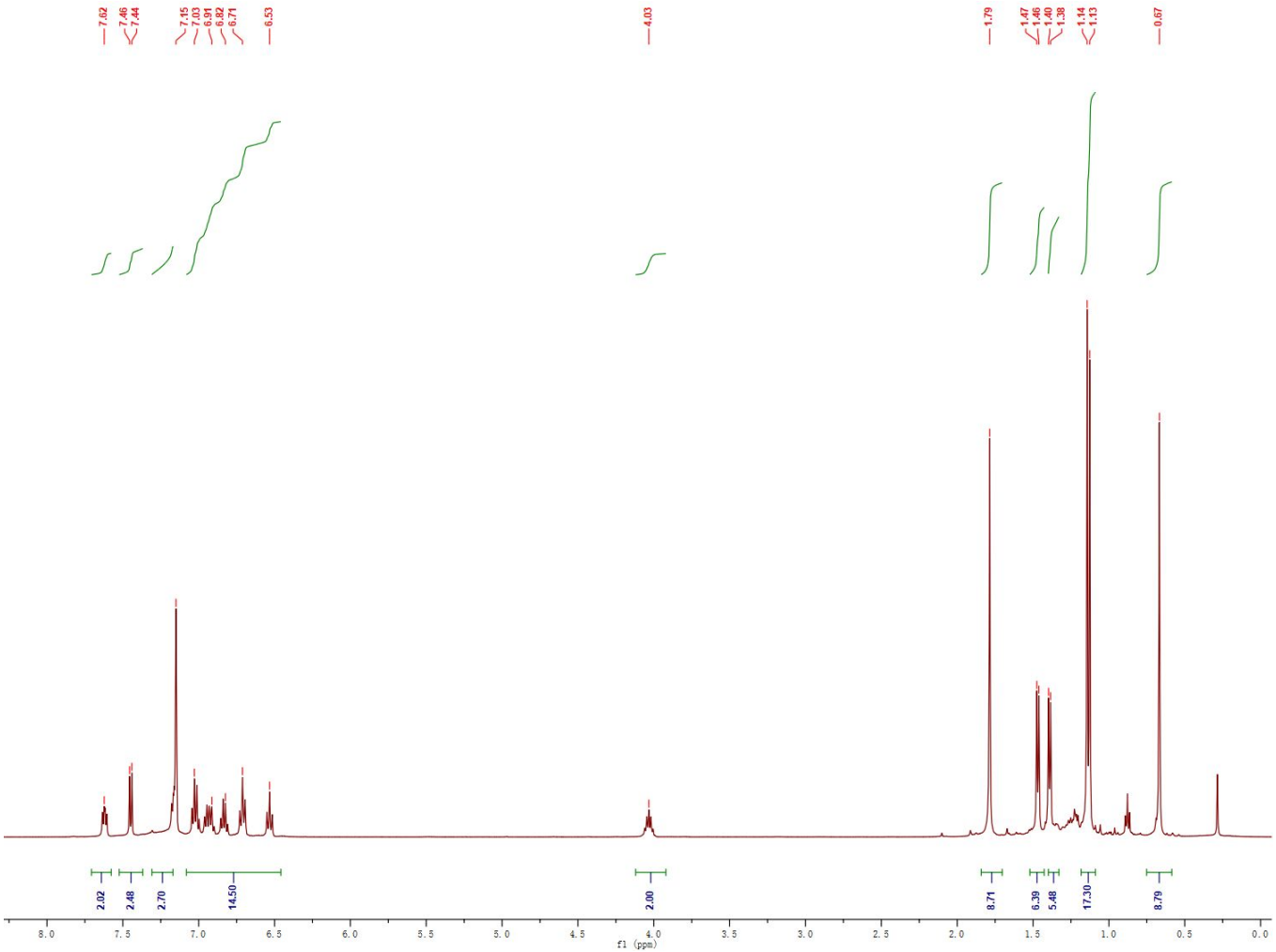


**Fig. S35.** $^{1}$H NMR spectrum of **3b** in $C_6D_6$.

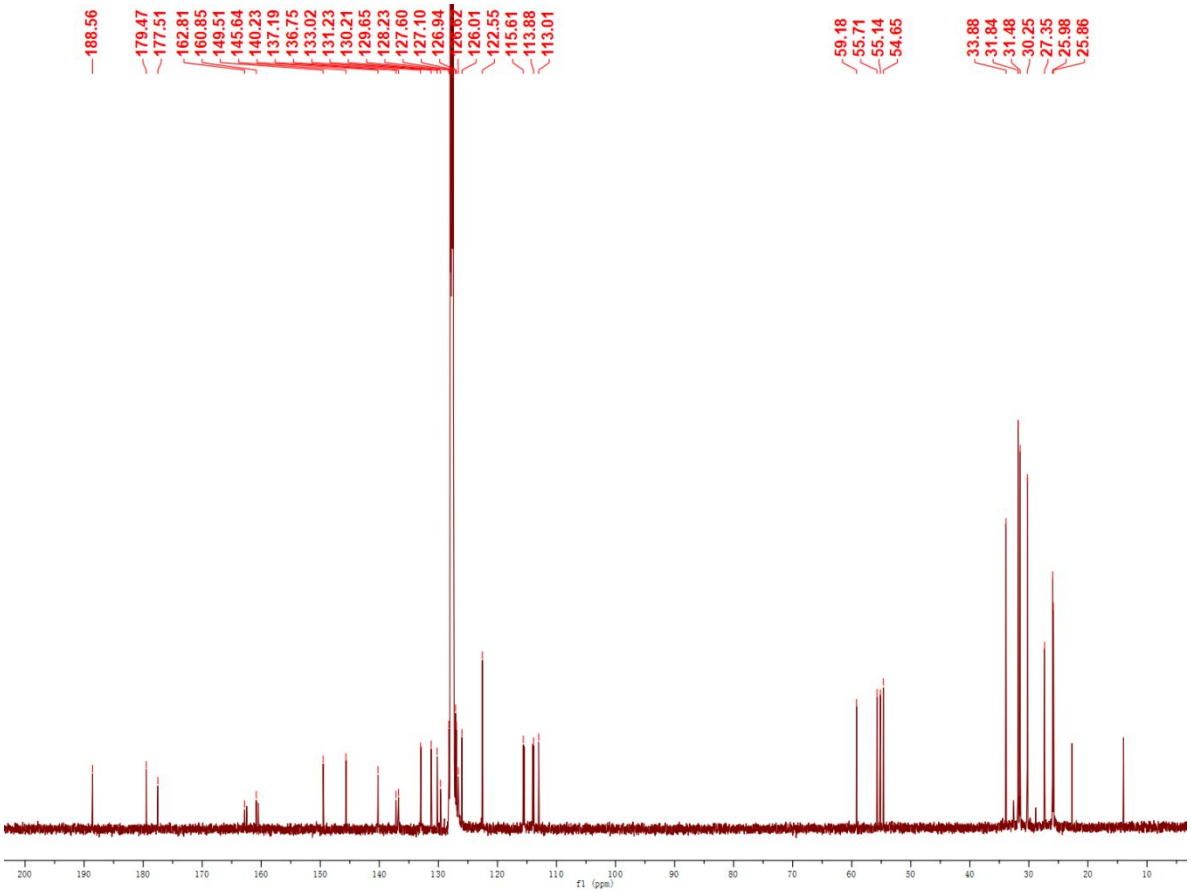


**Fig. S36.** $^{13}C$ NMR spectrum of **3b** in $C_6D_6$.

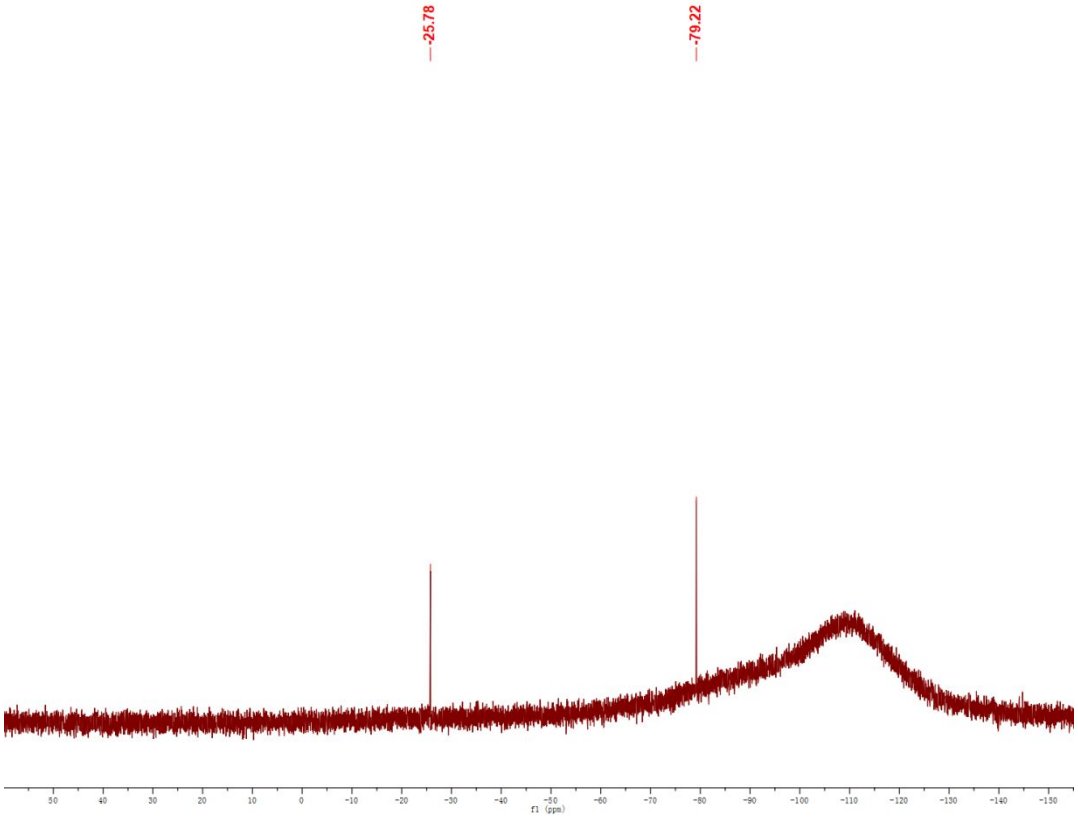


**Fig. S37.** $^{29}$Si NMR spectrum of **3b** in $C_6D_6$.

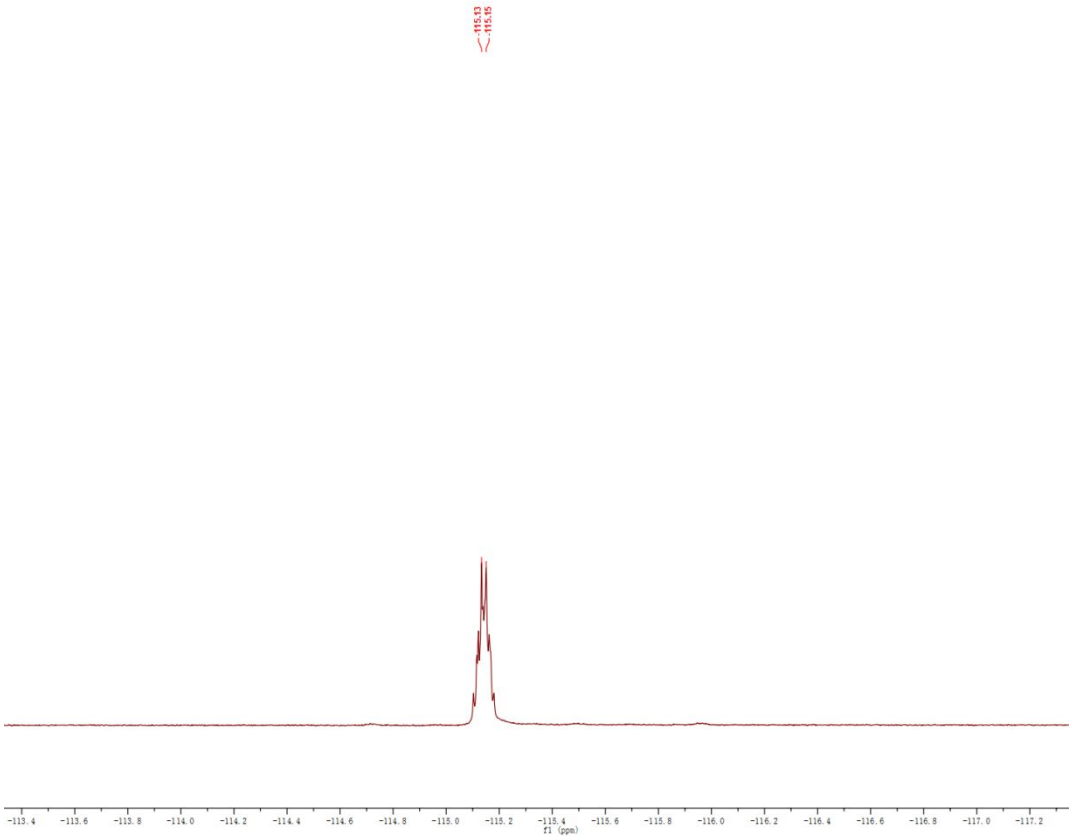


**Fig. S38.** $^{19}F$ NMR spectrum of **3b** in $C_6D_6$.

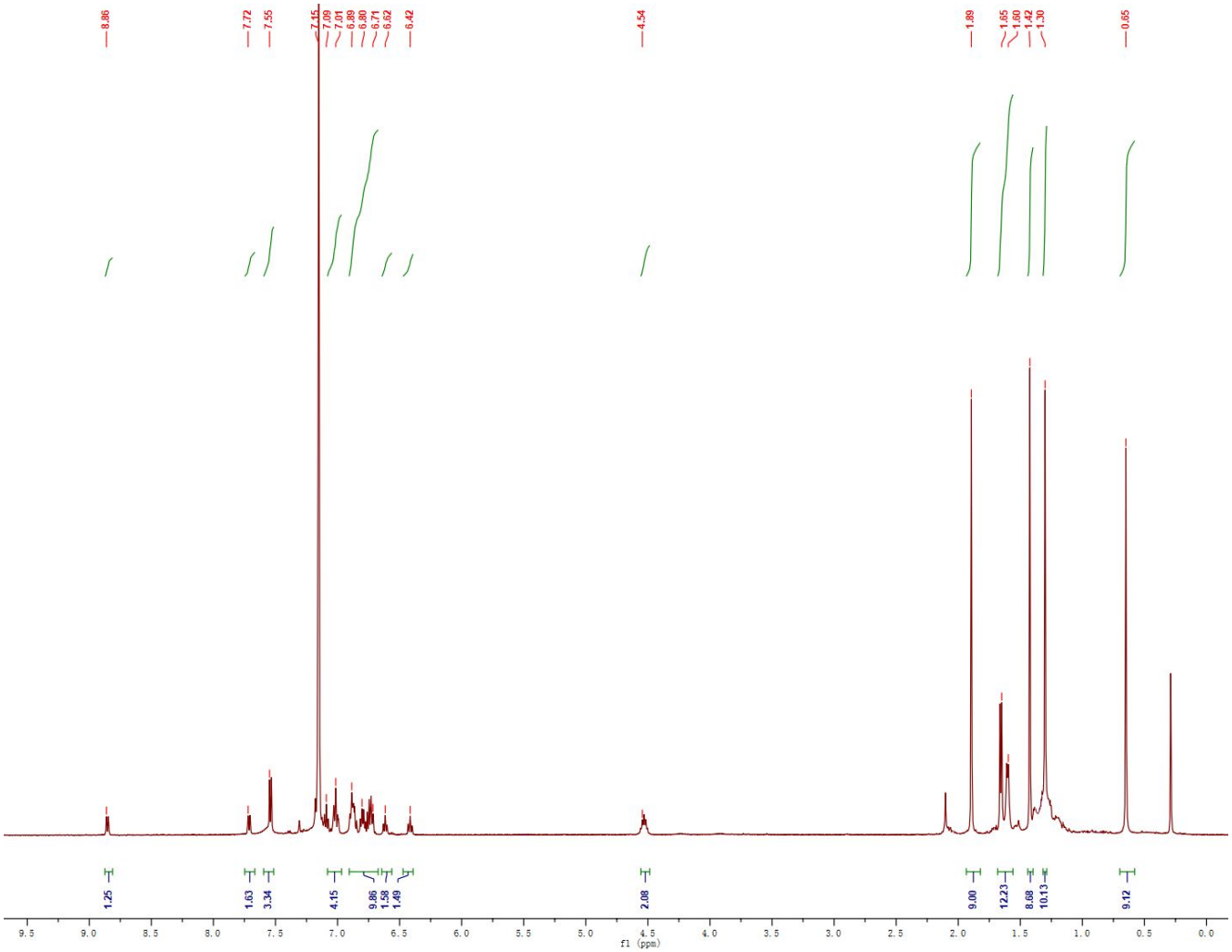


**Fig. S39.** $^{1}$H NMR spectrum of **3c** in $C_6D_6$.

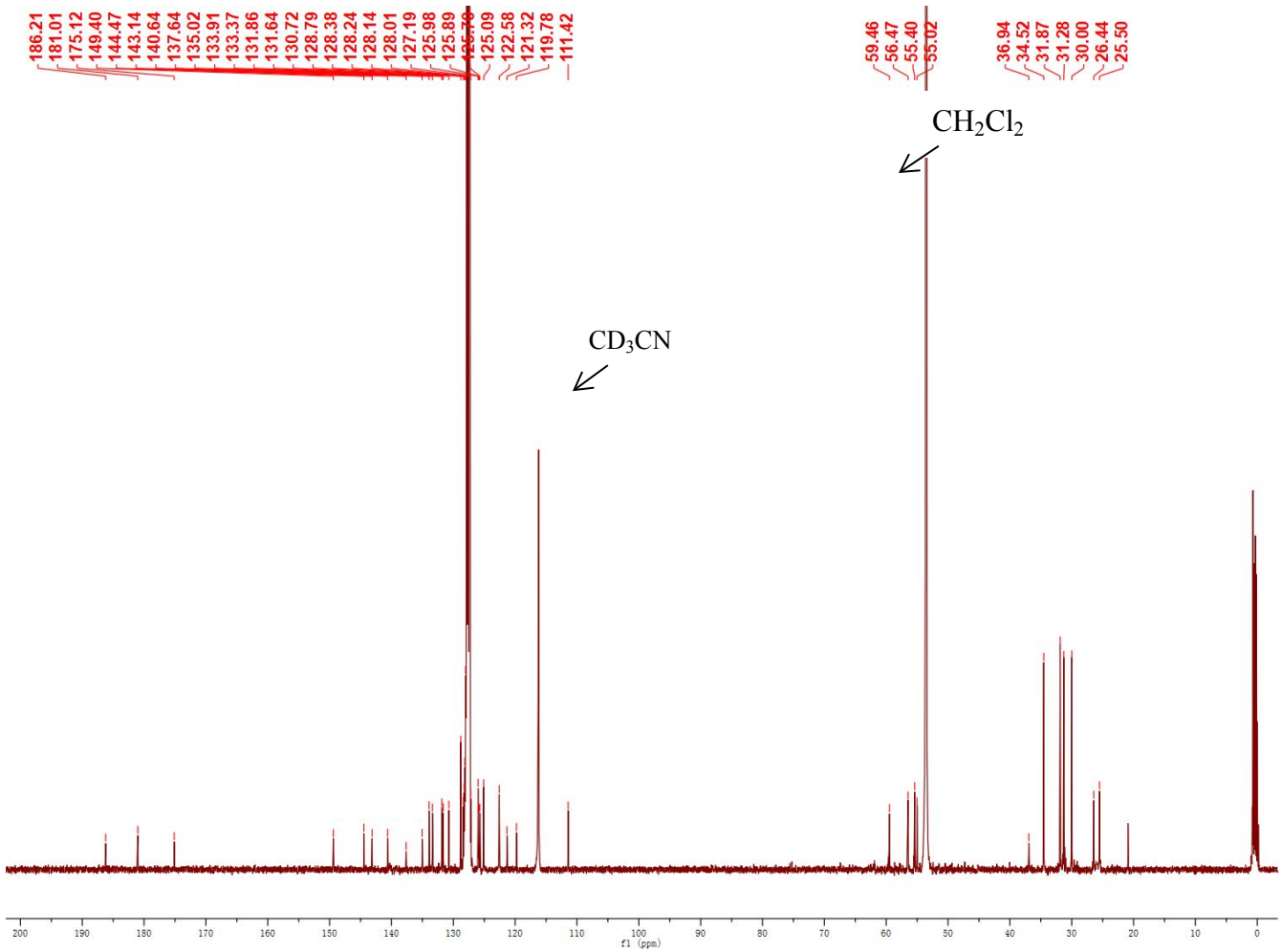


**Fig. S40.** $^{13}C$ NMR spectrum of **3c** in $CD_3CN$ (a small amount of $CH_2Cl_2$ was added to increase the solubility).

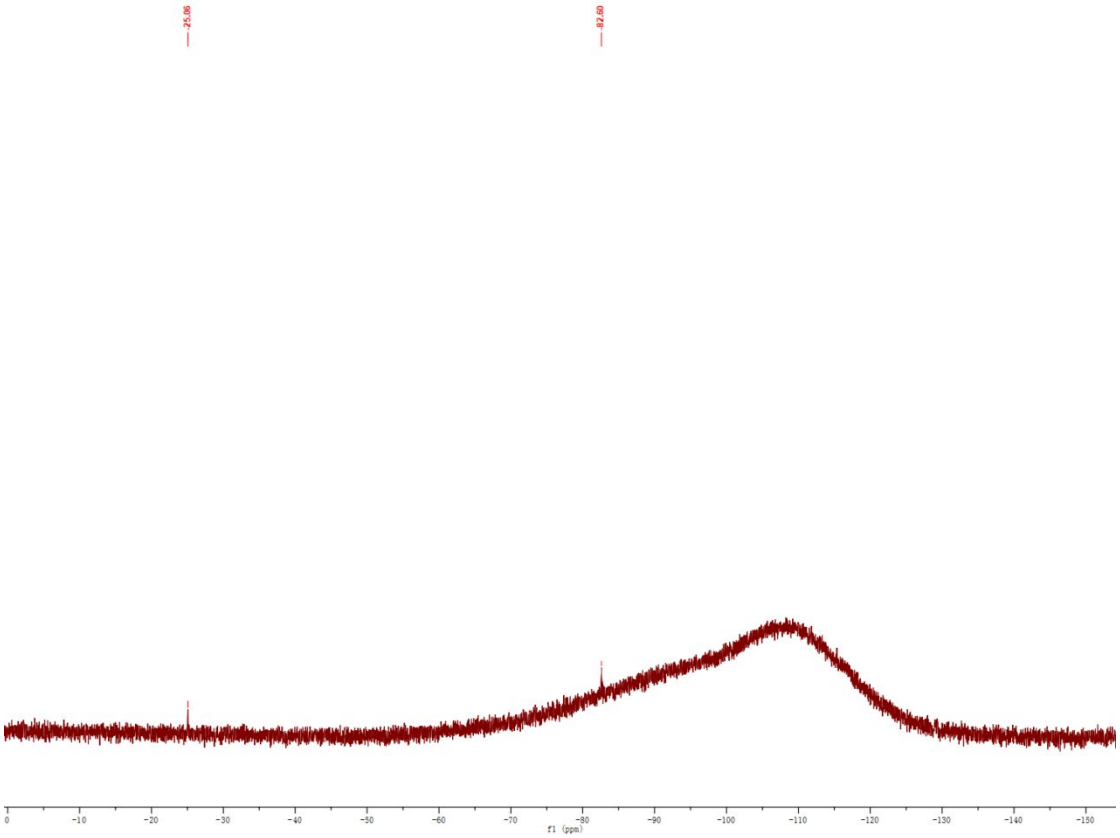


**Fig. S41.** $^{29}$Si NMR spectrum of **3c** in $C_6D_6$.

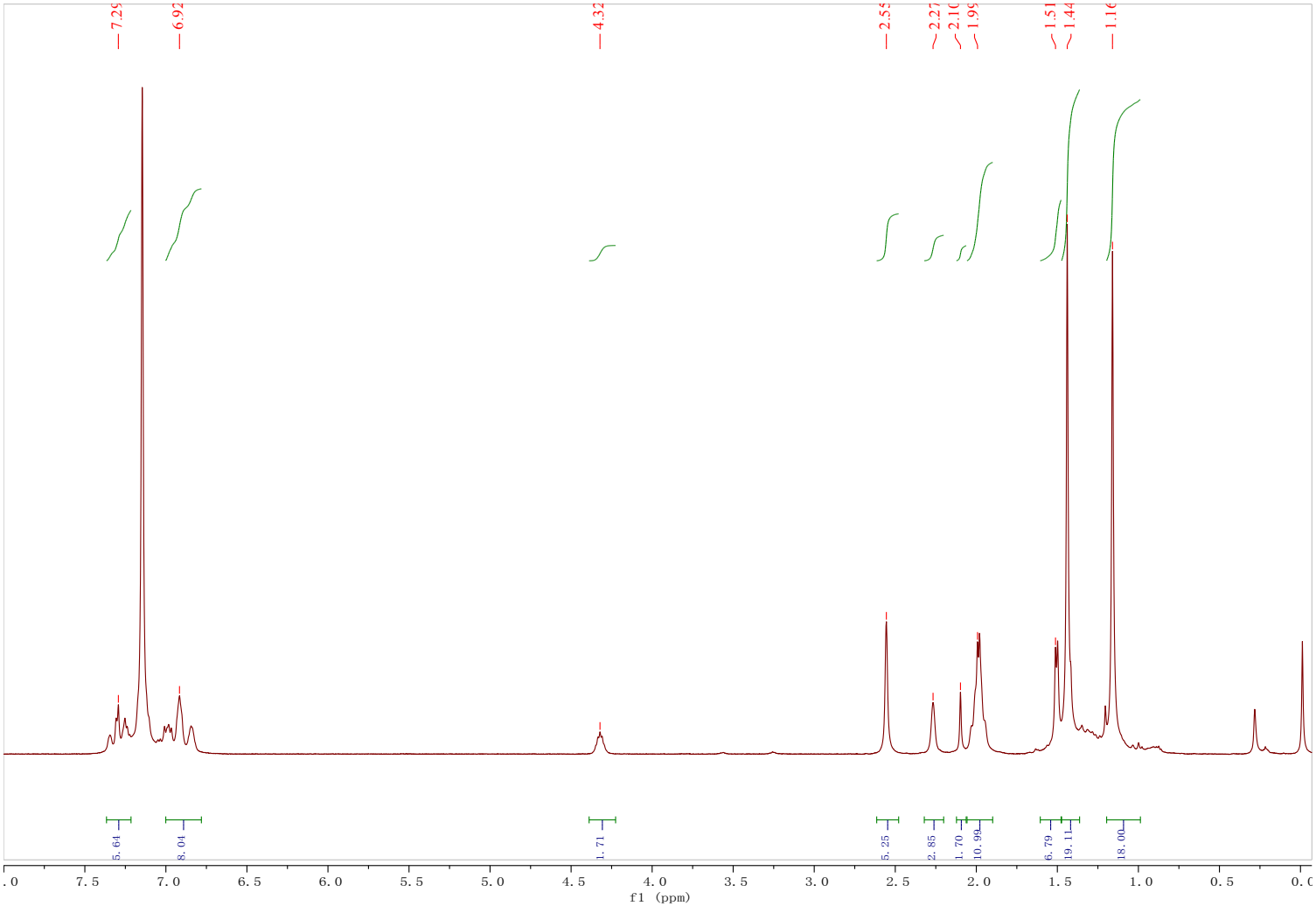


**Fig. S42.** $^{1}$H NMR spectrum of **4** in $C_6D_6$.

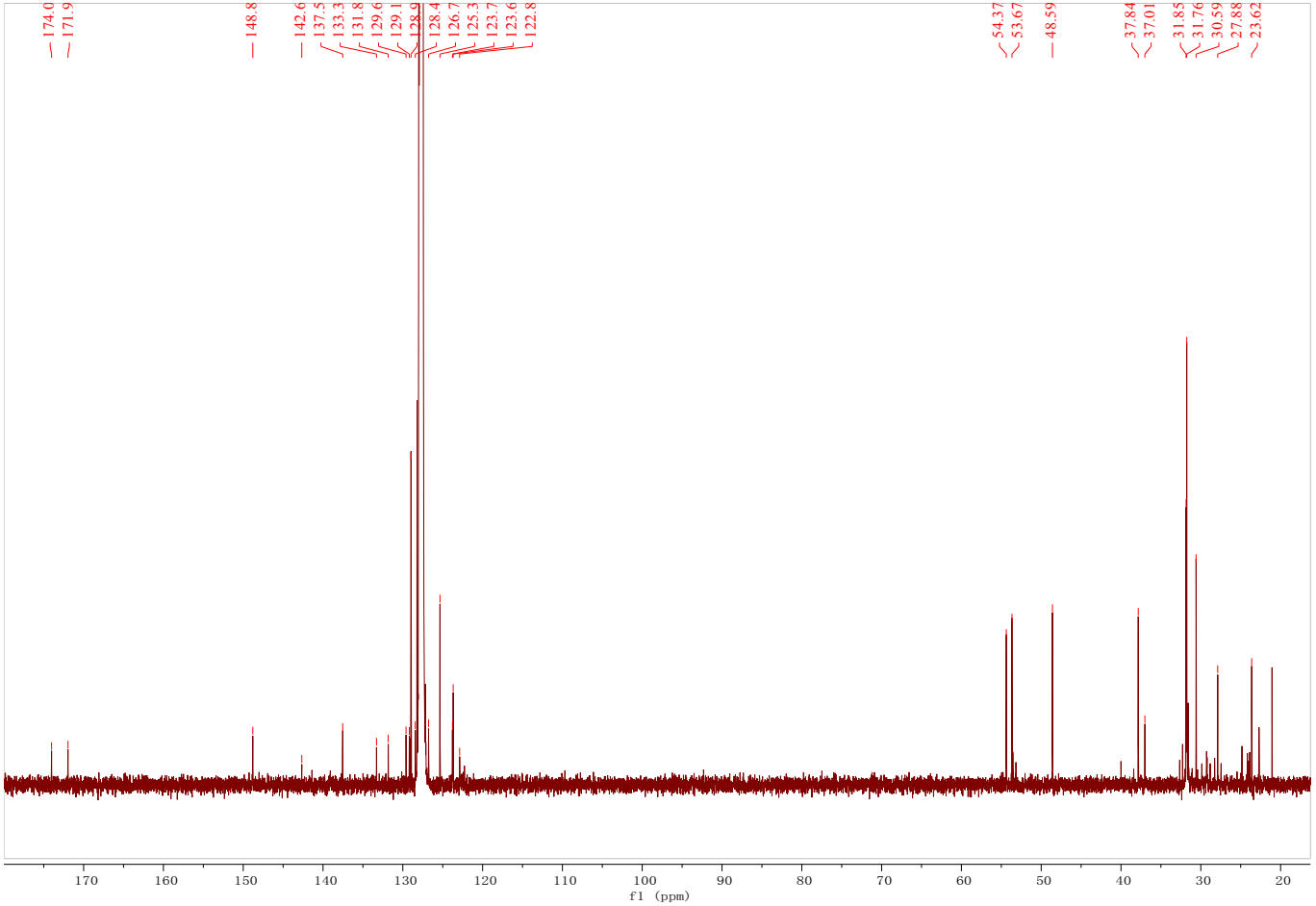


**Fig. S43.** $^{13}C$ NMR spectrum of **4** in $C_6D_6$.

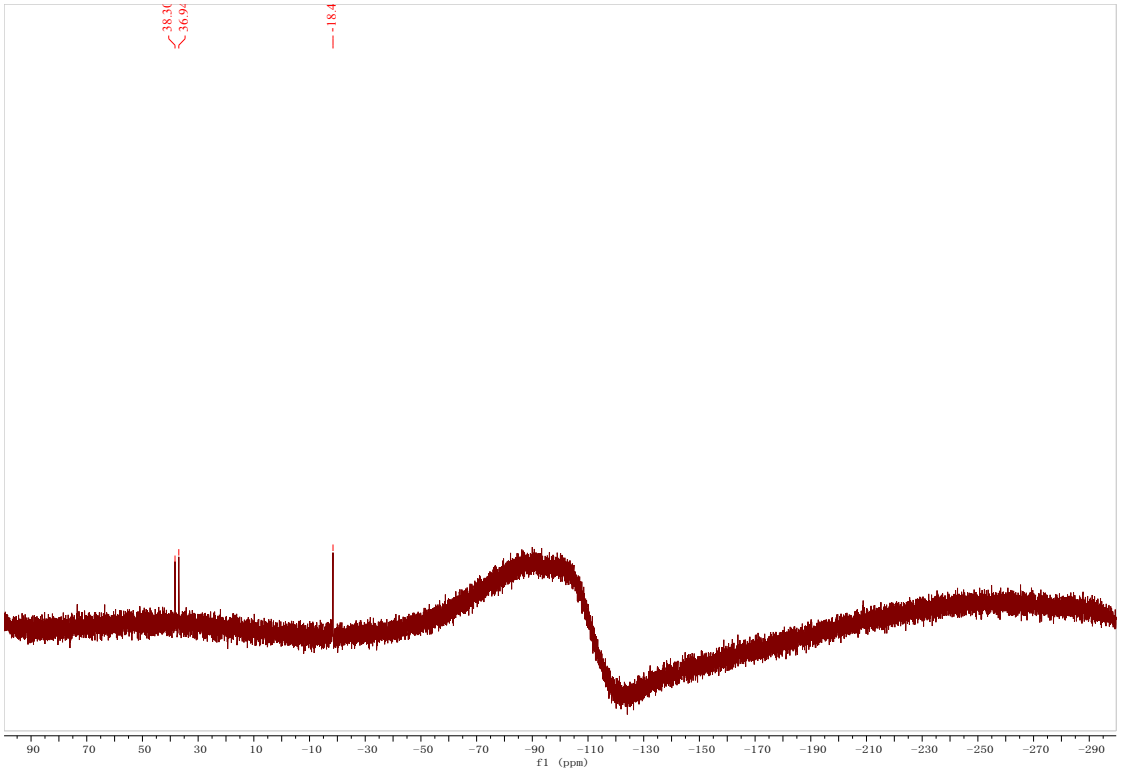


**Fig. S44.** $^{29}$Si NMR spectrum of **4** in $C_6D_6$.

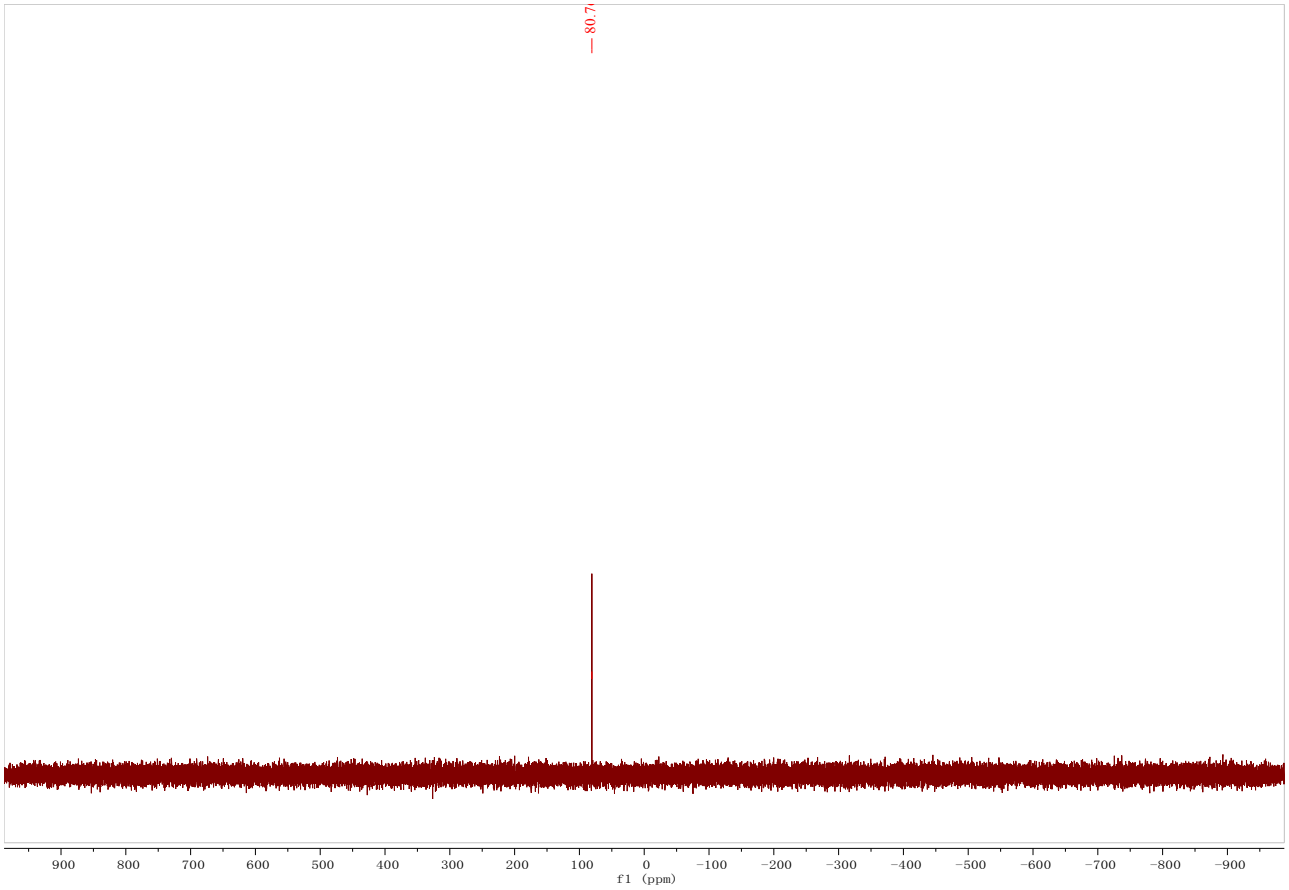


**Fig. S45.** $^{31}P$ NMR spectrum of **4** in $C_6D_6$.

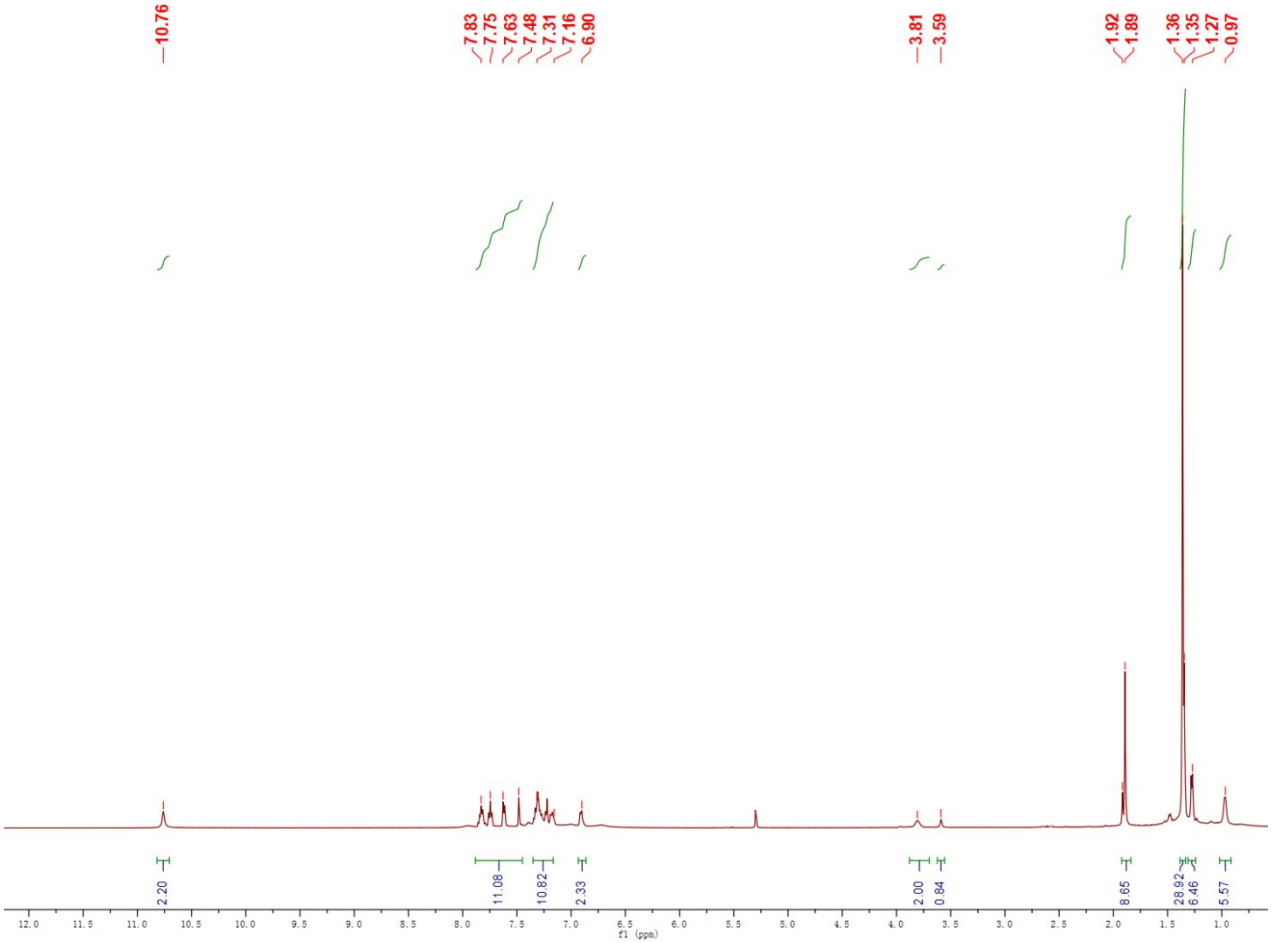


**Fig. S46.** $^{1}$H NMR spectrum of **5** in $CDCl_3$.

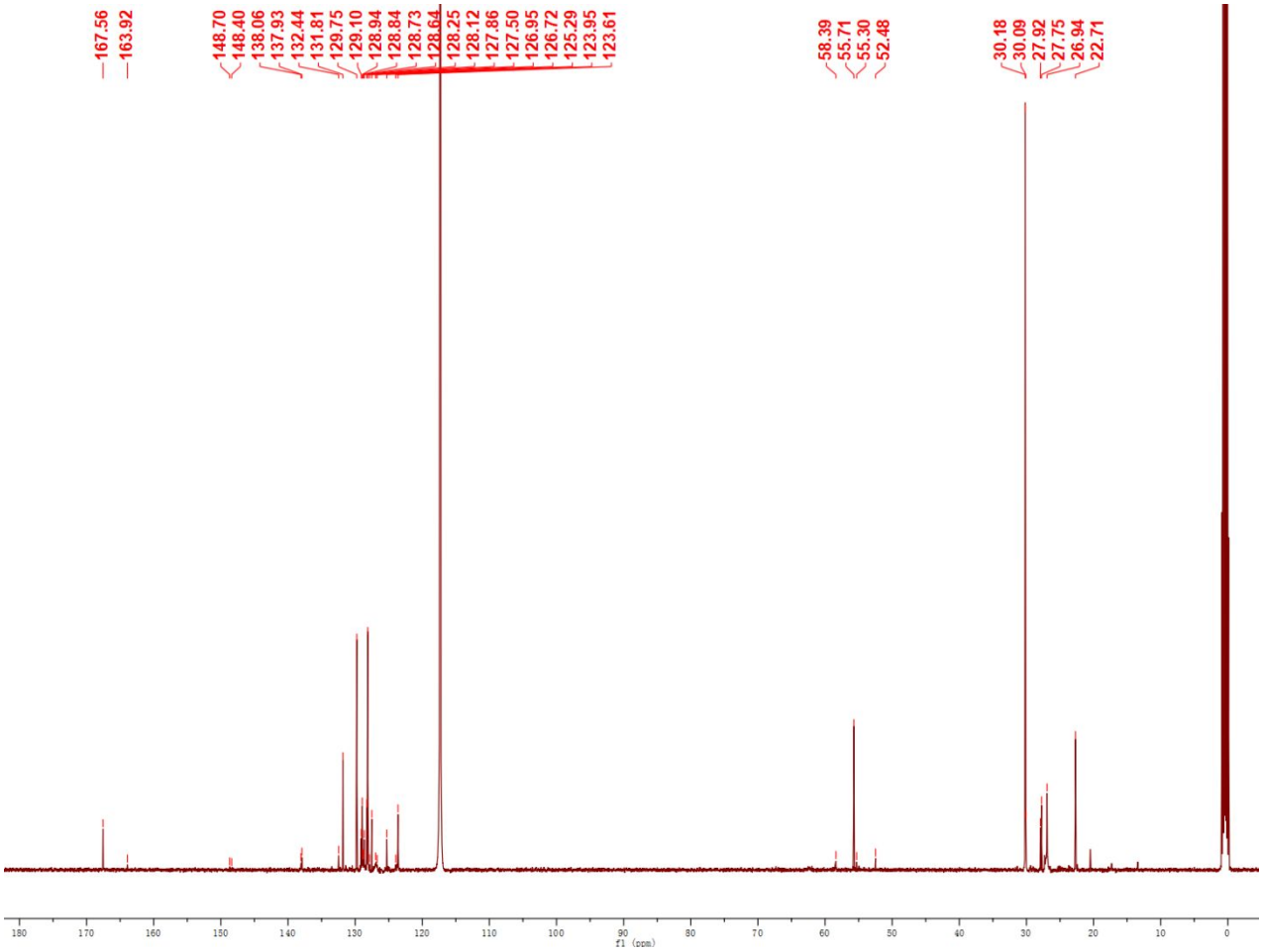


**Fig. S47.** $^{13}C$ NMR spectrum of **5** in $CD_3CN$.

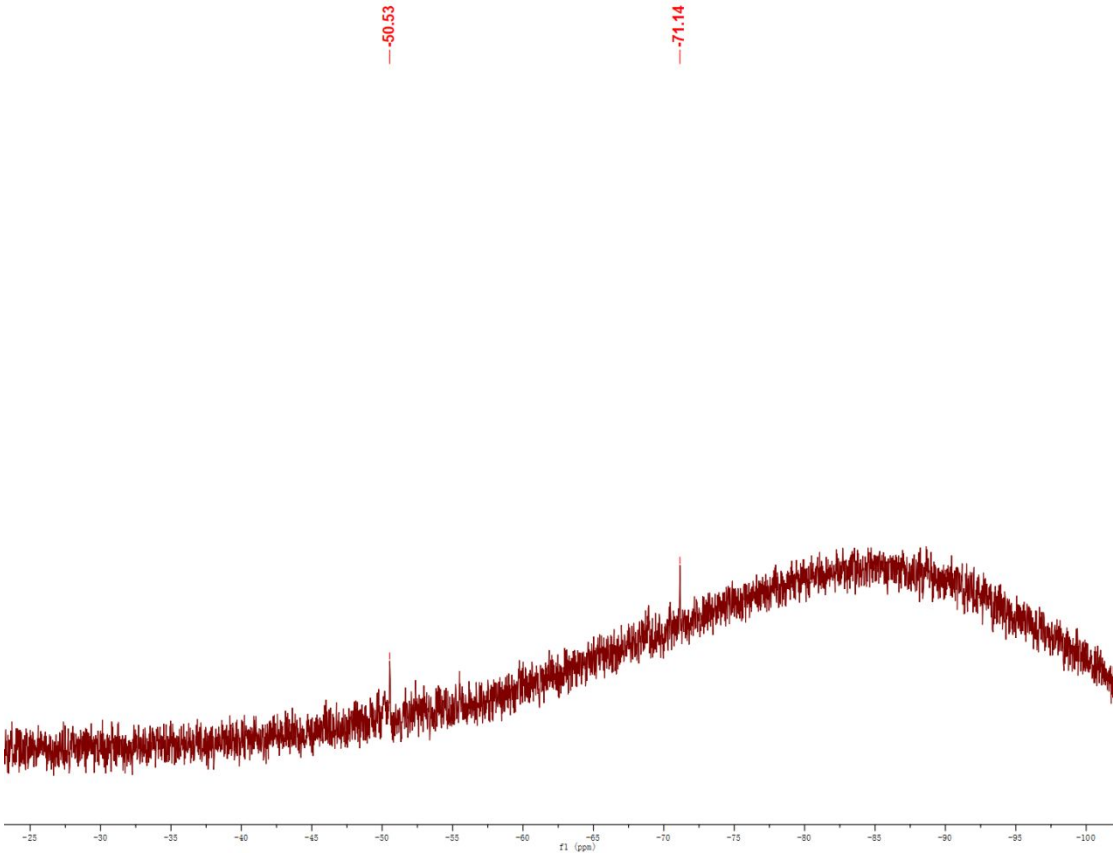


**Fig. S48.** $^{29}$Si NMR spectrum of **5** in $CD_3CN$.

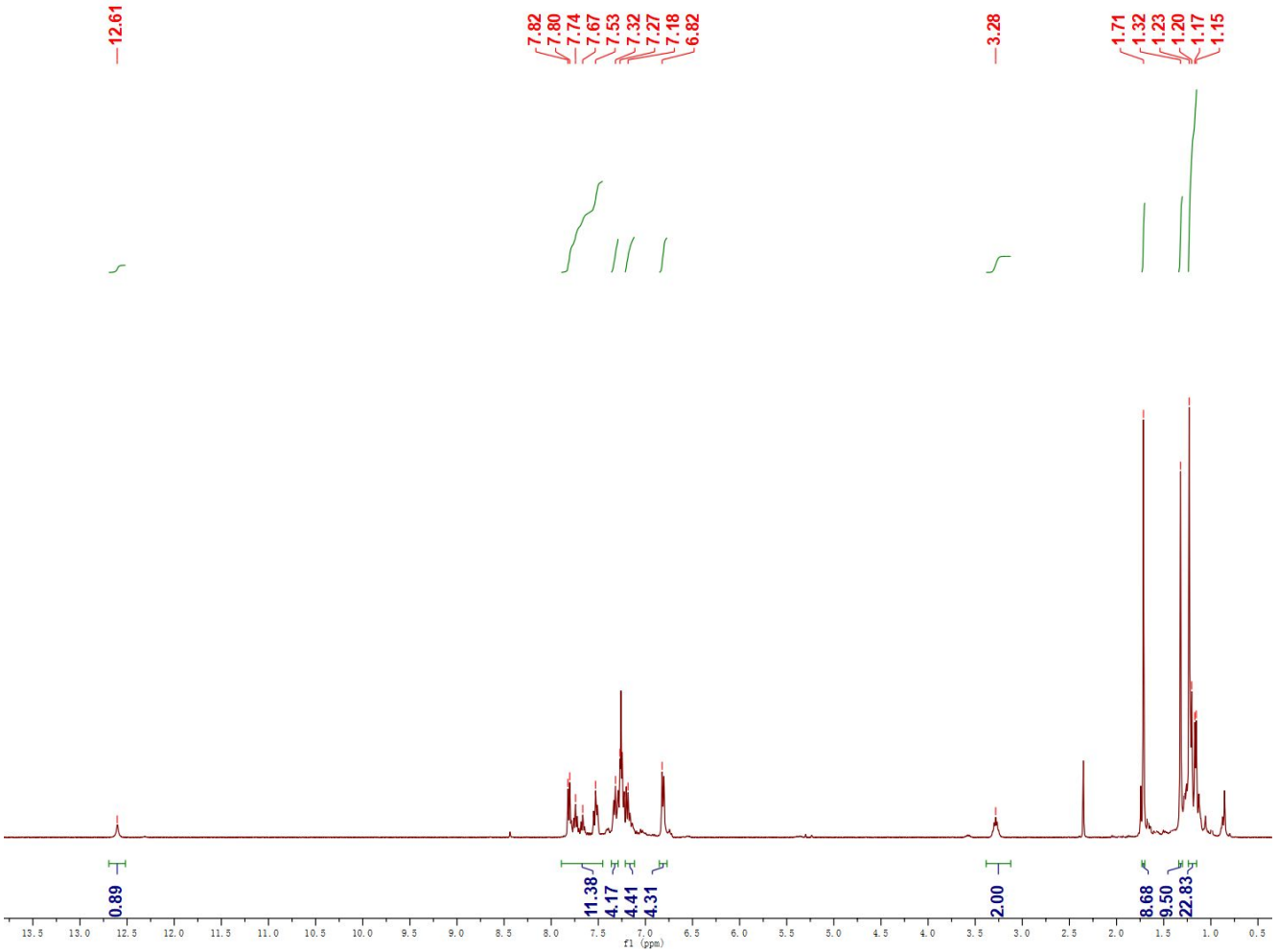


**Fig. S49** $^{1}$H NMR spectrum of **7** in $CDCl_3$.

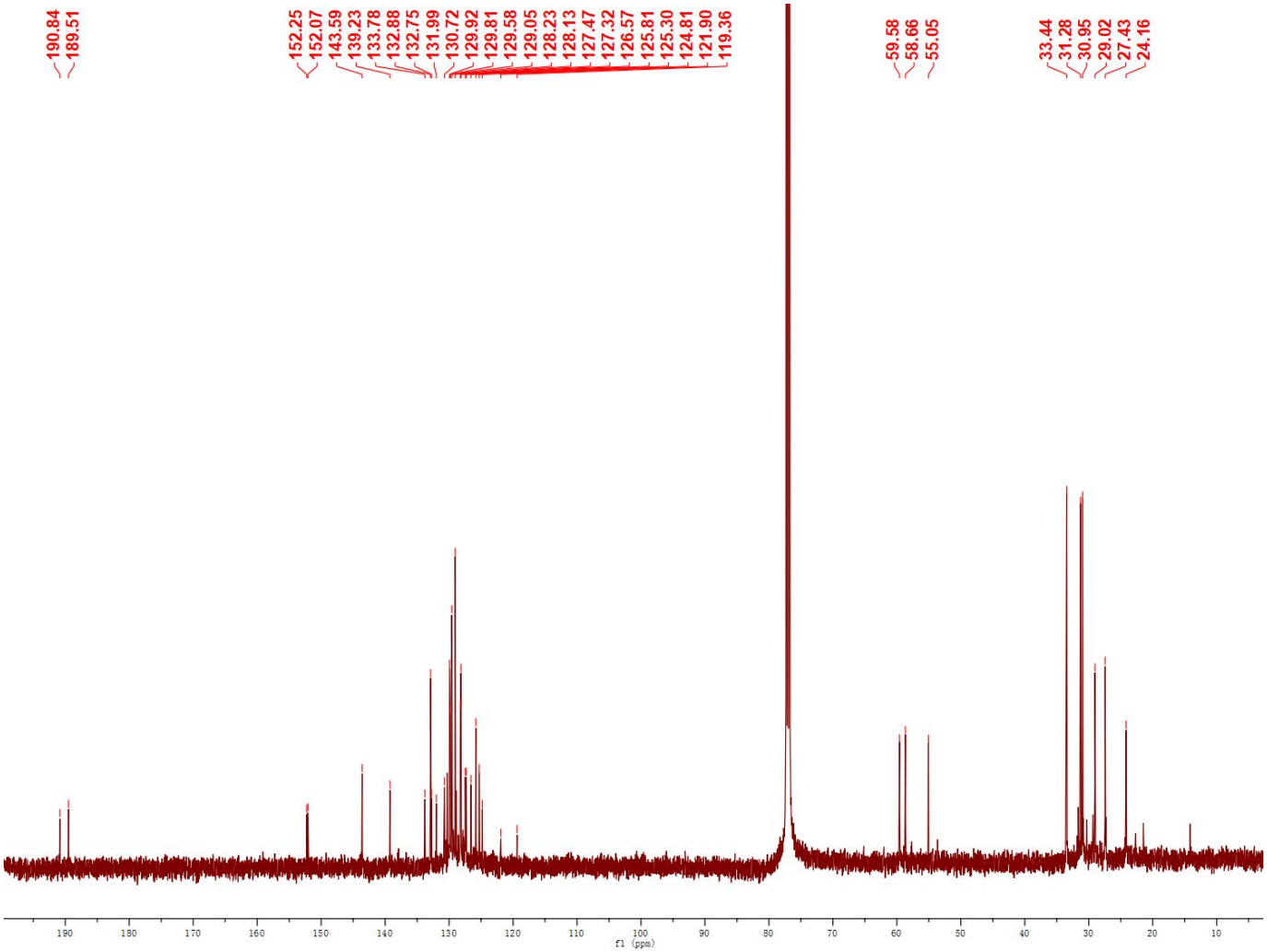


**Fig. S50.** $^{13}C$ NMR spectrum of **7** in $CDCl_3$.

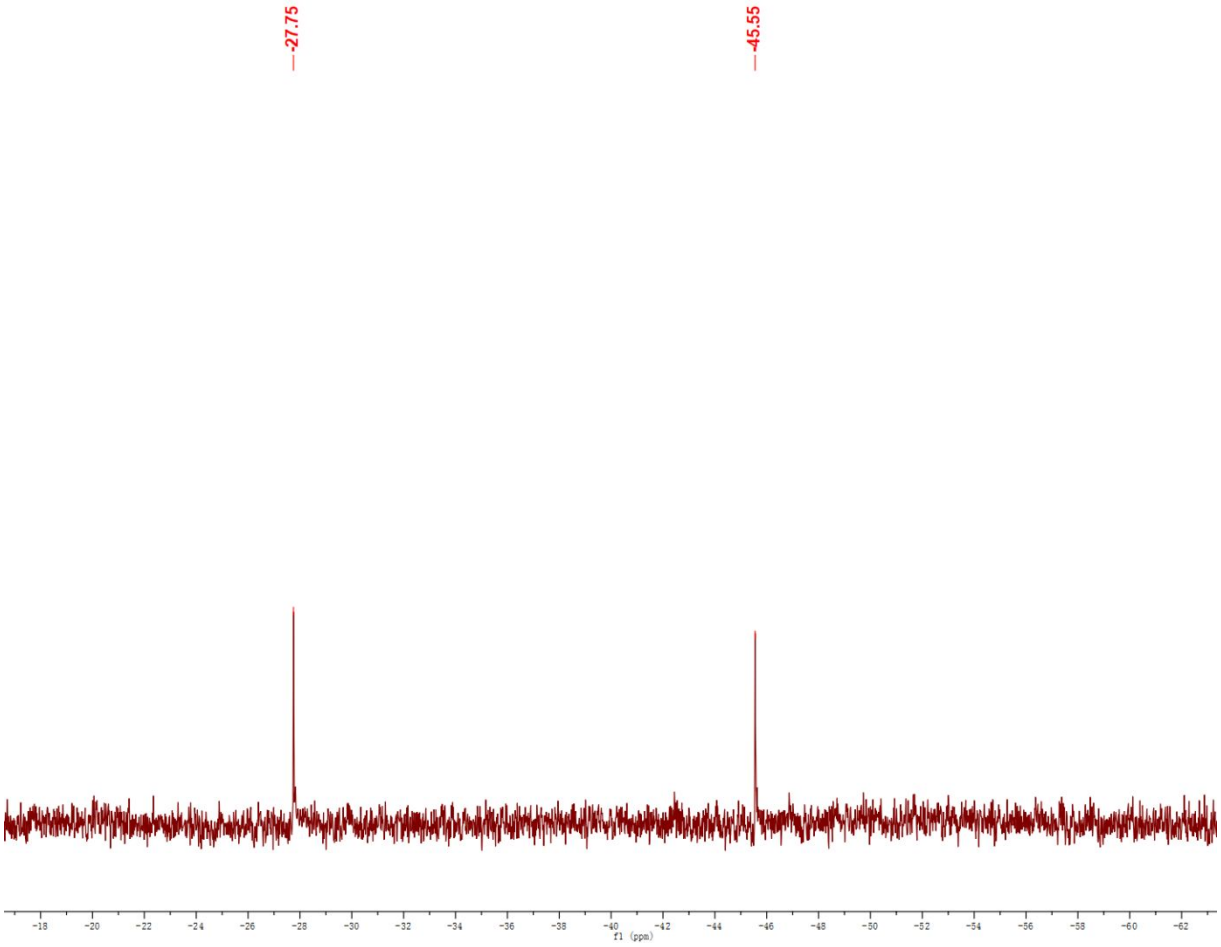


**Fig. S51.** $^{29}$Si NMR spectrum of **7** in $CDCl_3$.

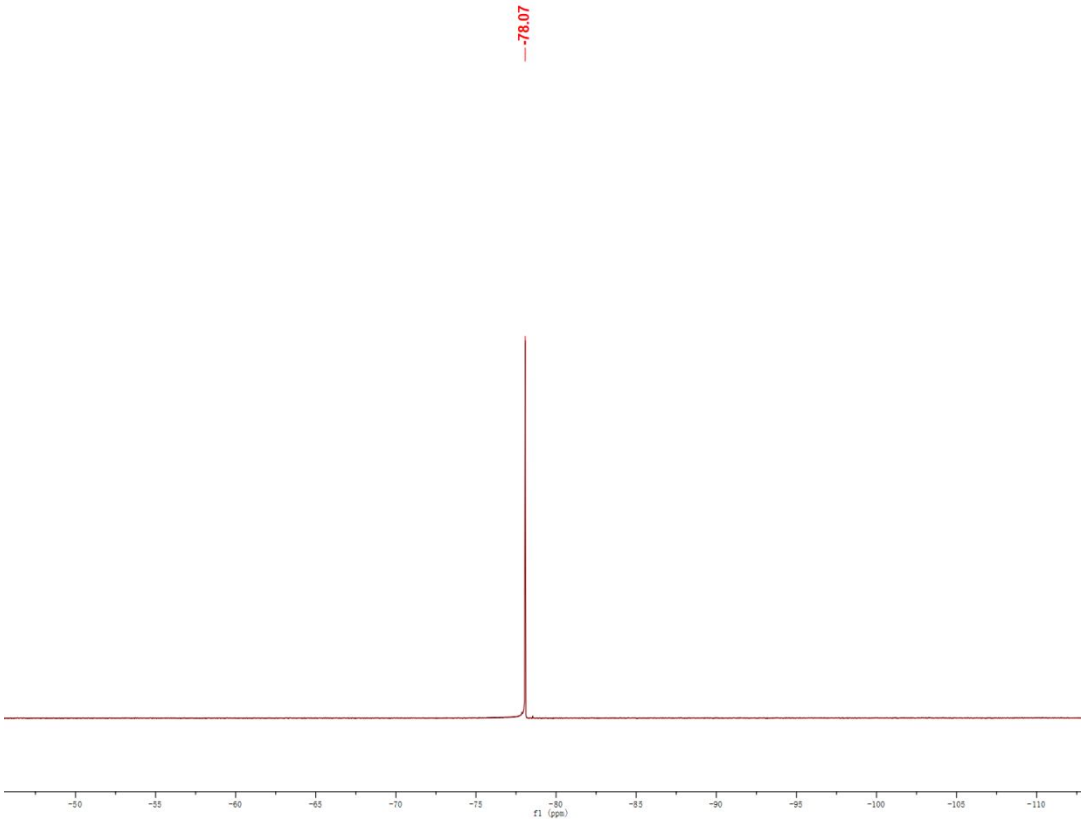


**Fig. S52.** $^{19}F$ NMR spectrum of **7** in $CDCl_3$.

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