Regiocontrolled Dimerization of Asymmetric Diazahexapentacene Derivatives Toward X-shaped Porous Semiconductors

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1. Materials and methods

Unless otherwise noted, all materials were purchased from commercial suppliers. $^1$H and $^{13}$C NMR spectra were recorded on a Bruker 400 MHz spectrometer, usually in CDCl$_3$ with TMS as an internal standard, and the chemical shifts ($\delta$) were reported in parts per million (ppm). High resolution mass spectra (HRMS) measurements were carried out on Ion Spec 9.4 Tesla Fourier Transform Mass Spectrometer.

2. Synthesis and characterization of compounds

![Chemical structures and reaction scheme]

Compound 12$^[1]$[1], 11$^[2]$[2], 7a$^[2]$[2] and tetrabrominated NDI$^[3]$[3] were synthesized according to the literatures.

**Compound 10**

To a flame-dried flask was added 12 (1.00 g, 2.98 mmol), 11 (0.97 g, 2.98 mmol), and sodium iodide (3.00 g, 20.27 mmol) in anhydrous DMF (40 mL). The mixture was stirred at 110 °C for 48 hours. The mixture was cooled to room temperature and acetone (20 mL) was added. The mixture was then filtered and the crude solid was washed by water and acetone to afford yellow solid (1.01 g, yield: 70%). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 9.10 (s, 2H), 8.63 (s, 2H). The $^{13}$C NMR spectra cannot be obtained due to the low solubility in common organic solvents. HR-MALDI-TOF (m/z): calcd. for C$_{18}$H$_4$Br$_2$F$_4$O$_2$: 485.8510, found 485.8520.

**Compound 9**

To a solution of triisopropylsilylacetylene (1 mL, 4.83 mmol) in dry Et$_2$O (28 mL), 1.24 mL of 2.5 M n-BuLi (2.99 mmol) was added dropwise at 0 °C under nitrogen. The solution was stirred at 0 °C for 1 h before the addition of compound 10 (0.35 g, 0.72 mmol) with THF (28 mL). The mixture was warmed to room temperature and stirred overnight. A solution of SnCl$_2$·2H$_2$O (5 g) in 10% HCl (28 mL) was added to the solution at room temperature and poured into water (100 mL), extracted with dichloromethane and dried over Na$_2$SO$_4$. The crude product was purified by silica chromatographic column (eluent: hexane) to provide a red solid 9 (0.51 g, 87%). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 9.48 (s, 2H), 8.96 (s, 2H), 1.31 – 1.29 (m, 42H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 131.28, 130.89, 129.21, 123.76, 119.36, 118.64, 117.46, 107.81, 17.79, 10.47. HR-MALDI-TOF
Compound 8
A mixture of tris(dibenzylideneacetone)dipalladium(0) (67.5 mg, 0.07 mmol), rac-BINAP (91.5 mg, 0.14 mmol), and anhydrous toluene (12 mL) was stirred at 110 °C for 0.5 h under nitrogen atmosphere. The mixture was cooled to room temperature and added with benzophenone imine (0.34 mL, 1.83 mmol), sodium tert-butoxide (0.18 g, 1.83 mmol), and 9 (0.5 g, 0.61 mmol). The mixture was stirred at 110 °C overnight and toluene was evaporated. The crude product was purified by silica gel column to afford a dark red solid (315 mg, 52%).

General Procedure for the Synthesis of 1a and 1b
A mixture of tetrabrominated NDI (0.4 mmol), sodium tert-butoxide (1.3 mmol), and a corresponding 7a or 7b (0.48 mmol) in toluene (40 mL) was heated at 70 °C for 3 h under nitrogen atmosphere. The reaction mixture was cooled to room temperature, poured into methanol (100 mL), and stirred for 0.5 h. After filtration, the crude product was purified by silica gel column (DCM/PE = 1/1 to 1/0, v/v) to afford the corresponding desired product. 1a: a dark blue solid (358 mg, 71%). 1H NMR (400 MHz, CDCl₃) δ 13.39 (s, 2H), 8.97 (s, 2H), 7.96 (s, 2H), 8.20 (s, 2H), 7.95 (s, 2H), 7.89 (dd, J = 6.4, 3.2 Hz, 2H), 7.41 (dd, J = 6.4, 3.2 Hz, 2H), 4.24 (t, J = 8.0 Hz, 4H), 1.85 – 1.71 (m, 4H), 1.48 – 1.36 (m, 20H), 0.90 (t, J = 7.2 Hz, 6H). 13C NMR spectra cannot be obtained due to poor solubility in organic solvents. HR-MALDI-TOF (m/z): calcd. for C₇0H₆8Br₂F₄N₄O₄Si₂: 1332.4183, found 1332.4180.

General Procedure for the Synthesis of 2a and 2b
A mixture of corresponding 1a or 1b (0.25 mmol), isopropanol (262 mmol), and sodium tert-butoxide (4.4 mmol) in toluene (50 mL) was heated at 90 °C under nitrogen atmosphere. The reaction was quenched when the starting compound completely disappeared (TLC monitoring). The reaction mixture was diluted with dichloromethane (DCM, 50 mL) and washed with water (50 mL × 3). The organic layer was separated and dried over anhydrous Na₂SO₄. The solvents were removed in vacuo and crude product was purified by column chromatography (DCM/PE=1/1, v/v) to afford the corresponding desired product. 2a: a dark blue solid (126 mg, 46%). 1H NMR (400 MHz, CDCl₃) δ 12.85 (s, 2H), 8.99 (s, 2H), 8.20 (s, 2H), 8.79 (s, 2H), 7.95 (s, 2H), 7.89 (dd, J = 6.4, 3.2 Hz, 2H), 7.41 (dd, J = 6.4, 3.2 Hz, 2H), 4.24 (t, J = 8.0 Hz, 4H), 1.76 – 1.70 (m, 4H), 1.37 – 1.36 (m, 42H), 1.28 – 1.22 (m, 20H), 0.88 (t, J = 6.5 Hz, 6H). 13C NMR (101MHz, CDCl₃) δ 164.53, 161.63, 137.73, 131.01, 130.47, 128.88, 127.09,
124.82, 124.36, 122.80, 121.79, 115.40, 108.76, 105.14, 102.70, 97.24, 39.23, 30.82, 28.25, 26.92, 26.12, 21.65, 17.99, 13.09, 10.74. HR-MALDI-TOF (m/z): calcd. for C$_7$H$_8$N$_2$O$_3$Si$_2$: 1104.6349, found 1104.6348.

2b: a dark blue solid (112 mg, 38%). $^1$H NMR (400 MHz, CDCl$_3$), $\delta$ 12.68 (s, 2H), 9.13 (s, 2H), 8.21 (s, 2H), 7.77 (s, 2H), 4.21 (t, $J$ = 7.2 Hz, 4H), 1.78 – 1.64 (m, 4H), 1.37 – 1.35 (m, 42H), 1.28 – 1.25 (m, 20H), 0.83 (t, $J$ = 6.5 Hz, 6H). $^{13}$C NMR (101MHz, CDCl$_3$), $\delta$ 164.66, 161.56, 137.65, 131.35, 129.05, 127.86, 125.25, 122.85, 122.11, 118.03, 115.69, 108.55, 106.52, 101.71, 97.74, 30.82, 28.45, 26.90, 26.10, 21.64, 17.90, 13.09, 10.63. HR-MALDI-TOF (m/z): calcd. for C$_7$H$_8$F$_3$N$_2$O$_3$Si$_2$: 1176.5972, found 1176.5976.

**General Procedure for the synthesis of dimers**

A corresponding 1 or 2 (0.08 mmol) and MnO$_2$ (68 mmol) were stirred in 10 mL CHCl$_3$ at room temperature for 10 min. After filtration, the crude material was purified by flash chromatography (DCM/PE = 1:1, v/v) as eluent to give the corresponding desired product.

5a: a yellow solid (92 mg, 93%). $^1$H NMR (400 MHz, CDCl$_3$), $\delta$ 8.84 (s, 4H), 7.81 (dd, $J$ = 6.4, 3.3 Hz, 4H), 7.41 (dd, $J$ = 6.6, 3.1 Hz, 4H), 6.57 (s, 4H), 4.34 – 4.08 (m, 8H), 1.88 – 1.71 (m, 8H), 1.50 – 1.25 (m, 124H), 0.95 – 0.91 (m, 124H), $^{13}$C NMR (101 MHz, CDCl$_3$), $\delta$ 161.35, 159.25, 158.56, 139.32, 136.14, 135.66, 132.08, 129.79, 128.15, 126.33, 121.28, 105.73, 102.11, 52.03, 46.00, 36.35, 31.88, 29.65, 29.32, 26.48, 22.65, 19.25, 14.10, 11.75. HR-MALDI-TOF (m/z): calcd. for C$_{140}$H$_{68}$Br$_4$N$_8$O$_3$Si$_2$: 2516.8806, found 2518.4418.

5b: a reddish yellow solid (89 mg, 90%). $^1$H NMR (400 MHz, CDCl$_3$), $\delta$ 9.07 (s, 4H), 6.57 (s, 2H), 4.31 – 4.09 (m, 8H), 1.89 – 1.72 (m, 8H), 1.51 – 1.17 (m, 124H), 0.95 – 0.90 (m, 124H), $^{13}$C NMR (101 MHz, CDCl$_3$), $\delta$ 161.30, 158.50, 139.04, 137.37, 136.66, 136.03, 130.32, 126.34, 121.37, 107.51, 101.01, 51.91, 46.06, 36.33, 31.89, 30.71, 29.32, 26.48, 24.60, 22.21, 19.14, 14.07, 11.65. HR-MALDI-TOF (m/z): calcd. for C$_{140}$H$_{68}$Br$_4$N$_8$O$_3$Si$_2$: 2660.8052, found 1330.4037.

6a: a yellow solid (77 mg, 90%). $^1$H NMR (400 MHz, CDCl$_3$), $\delta$ 8.82 (s, 4H), 8.70 (s, 4H), 7.78 (dd, $J$ = 6.4, 3.2 Hz, 4H), 7.37 (dd, $J$ = 6.6, 3.1 Hz, 4H), 6.59 (s, 2H), 4.30 – 4.02 (m, 8H), 1.82 – 1.70 (m, 8H), 1.51 – 1.43 (m, 84H), 1.35 – 1.30 (m, 40H), 0.90 (t, $J$ = 6.5 Hz, 12H), $^{13}$C NMR (101 MHz, CDCl$_3$), $\delta$ 162.88, 159.33, 158.89, 159.70, 136.62, 132.07, 131.62, 129.88, 128.14, 127.60, 125.68, 121.39, 105.62, 102.17, 52.12, 45.25, 36.35, 31.89, 29.64, 26.58, 22.67, 19.29, 14.09, 11.78. HR-MALDI-TOF (m/z): calcd. for C$_{140}$H$_{172}$N$_8$O$_3$Si$_2$: 2205.2386, found 1102.6194.

6b: a reddish yellow (76 mg, 85%). $^1$H NMR (400 MHz, CDCl$_3$), $\delta$ 9.05 (s, 4H), 8.74 (s, 4H), 6.59 (s, 4H), 4.21 – 4.14 (m, 8H), 1.78 – 1.71 (m, 8H), 1.45 – 1.39 (m, 124H), 0.90 (t, $J$ = 6.5 Hz, 12H), $^{13}$C NMR (400 MHz), $\delta$ 162.28, 158.92, 158.34, 139.40, 138.17, 131.69, 130.42, 126.94, 123.09, 121.66, 121.27, 119.84, 119.39, 105.23, 101.33, 101.07, 51.98, 41.14, 31.90, 29.37, 28.10, 22.67, 19.11, 14.12, 11.69. HR-MALDI-TOF (m/z): calcd. for C$_{140}$H$_{164}$F$_8$N$_8$O$_3$Si$_2$: 2349.1632, found 1174.5821.

**3. CV and UV spectra of compounds**

Cyclic voltammetry (CV) was recorded on a CHI620E electrochemical work station using glassy carbon discs as the working electrode, Pt wire as the counter electrode, and Ag/Ag$^+$ electrode as the reference electrode. The experiments were performed in nitrogen-purged DCM with tetrabutylammonium hexafluorophosphate (TBAPF$_6$, 0.1 M) as the supporting electrolyte with a scan of 100 mV/s. UV-vis absorption spectra were measured with Hitachi (model U-3010) UV-Vis spectrophotometer (chloroform solution, ~10$^{-3}$ M).
Figure S1. UV/Vis absorption of 5a, 5b, 6a, 6b, TIPS-Anthra and TIPS-F-Anthra in chloroform (~10^{-5} M).

4. X-ray crystallographic data of 2a, 5a and 5b

The measurement was made with Synchrotron Radiation (λ = 0.82653 Å). All calculations were performed using the SHELXL-97 and the crystal structure crystallographic software package.

Table S1. Crystal data and structure refinement for 2a, 5a and 5b.

| Identification code | 2a                  | 5a                  | 5b                  |
|---------------------|---------------------|---------------------|---------------------|
| Empirical formula   | C_{70}H_{88}N_{4}O_{4}Si_{2} | C_{140}H_{168}Br_{4}N_{8}O_{8}Si_{4} | C_{140}H_{168}Br_{4}F_{8}N_{8}O_{8}Si_{4} |
| Formula weight      | 1104.63             | 2516.88             | 2660.80             |
| Crystal system      | Triclinic           | Triclinic           | Monoclinic          |
| Space group         | P-1                 | P-1                 | C2/c                |
| Radiation type      | CuKα                | CuKα                | CuKα                |
| Radiation wavelength(Å) | 1.54184         | 1.54184             | 1.54178             |
| T(K)                | 223.15              | 169.99(13)          | 169.99(13)          |
| a(Å)                | 12.4231(4)          | 18.8621(3)          | 26.370(2)           |
| b(Å)                | 13.9327(5)          | 25.0420(3)          | 26.4347(10)         |
| c(Å)                | 21.1782(7)          | 34.0452(6)          | 24.2245(19)         |
| α(deg)              | 96.811(3)           | 74.2830(3)          | 90                  |
| β(deg)              | 101.236(3)          | 77.959(2)           | 120.504(8)          |
| γ(deg)              | 108.670(3)          | 68.381(2)           | 90                  |
| V(Å³)               | 3341.01(2)          | 14284.1(4)          | 14549(2)            |
| Z                   | 2                   | 4                   | 4                   |
| ρ calc. (g cm^{-3}) | 1.145               | 1.259               | 1.302               |
| θ, range(°)         | 1.573-27.484        | 4.238-151.442       | 5.128-155.69        |
| R(int)              | 3.47%               | 5.61%               | 8.63%               |
| μ(mm⁻¹)             | 0.104               | 2.152               | 2.222               |
| F(000)              | 1242                | 5696                | 5952                |
### Crystal size (mm³)

|       | 0.463 \times 0.439 \times 0.035 | 0.04 \times 0.04 \times 0.02 | 0.32 \times 0.15 \times 0.1 |
|-------|----------------------------------|-------------------------------|-------------------------------|
| Index ranges | -16 \leq h \leq 6, \quad -22 \leq h \leq 23, \quad -32 \leq h \leq 32, | -18 \leq k \leq 18, \quad -28 \leq k \leq 31, \quad -33 \leq k \leq 31, | -27 \leq l \leq 27, \quad -39 \leq l \leq 42, \quad -30 \leq l \leq 27 |
| Reflections collected | 43305 | 56672 | 83208 |
| Independent reflections | 15290 | 56672 | 14763 |
| Absorption correction | Semi-empirical from equivalents | | |
| Refinement method | Full-matrix least-squares on F² | | |
| Data / restraints / parameters | 15290 / 489 / 918 | 56672/1352/3457 | 14763/504/851 |
| Goodness-of-fit on F² | 1.026 | 1.945 | 2.092 |
| Final R indices | R₁ = 0.0818, \quad wR² = 0.2200 | R₁ = 0.1103, \quad wR² = 0.2929 | R₁ = 0.1345, \quad wR² = 0.3470 |
| R indices (all data) | R₁ = 0.1201, \quad wR² = 0.2446 | R₁ = 0.1389, \quad wR² = 0.3159 | R₁ = 0.1675, \quad wR² = 0.3635 |
| Largest diff. peak and hole | 0.997 and -0.514 | 2.61 and -1.36 | 0.99 and -0.83 |

### 5. Computational study

The density functional theory (DFT) calculations were performed with the Gaussian 09 Rev. E.01 employing the B3LYP/6-31g(d,p) level. Considering the alkyl chains on the imide positions and triisopropylsilane on the acetylene positions have negligible effect on the final structural and electronic properties of these compounds, we chose methyl substituents instead of octyl on the imide positions and hydrogen substituents instead of triisopropylsilane on the acetylene positions for better view of their structures. The dimerization mechanism has been computationally analyzed by using the density functional theory within the M06-2X functional, and, since the studied systems are quite large, the economical basis set 6-31G(d) was used (denoted as M06-2X/6-31G(d)). Frequency calculations were performed at the M06-2X/6-31G(d) level for all stationary points to differentiate them as minima or saddle points. The energies reported in this paper are at the M06-2X/6-31G(d) level of theory unless otherwise stated. Where frequency calculations were performed, unscaled zero-point vibrational energies (ZPVE) at M06-2X/6-31G(d) were added to the calculated relative energies. Time-dependent DFT (TD-DFT) calculations were performed at the (U)ωB97XD/6-311G(d,p) level of theory under vacuum.

Natural orbital occupation number (NOON)) calculations were done by spin unrestricted UCAM-B3LYP/6-31G(d,p) method based and the diradical character ($γ₀$) was calculated according to Yamaguchi’s scheme: $γ₀ = 1−(2T/(1+T²))$, and $T = (n\text{HOMO}−n\text{LUMO})/2$ ($n\text{HOMO}$ is the occupation number of the HOMO, $n\text{LUMO}$ is the occupation number of the LUMO).
Figure S2. Calculated HOMO and LUMO of $5a$, $5b$, $6a$ and $6b$ at B3LYP/6-31g(d) level.

Figure S3. Calculated dipoles of compounds.

Table S2. Calculated absolute energies (E) and Gibbs free energies (G) at 298 K in Hartrees and zeropoint vibrational energies (ZPVE) in kcal/mol of the transition states, local minima, and products at (U)M06-2X/6-31G(d).

| Name    | (U)M06-2X/6-31G(d)          |          |          |
|---------|----------------------------|----------|----------|
|         | E (Hartrees) | ZPVE(Hartrees) | G (Hartrees) |
| 4a      | -1977.978736 | -1977.511553 | -1977.578688 |
| Complex | -3956.028327 | -3955.091365 | -3955.192331 |
| T1      | -3955.978825 | -3955.057637 | -3955.143809 |
| M1      | -3956.070230 | -3955.115308 | -3955.217983 |
| T2      | -3956.068667 | -3955.105618 | -3955.212557 |
| M2      | -3956.060580 | -3955.118047 | -3955.222142 |
| T3      | -3956.060442 | -3955.115621 | -3955.218462 |
| Dimer   | -3956.051013 | -3955.126853 | -3955.227543 |
Figure S4. Calculated stick spectrum (UoB97XD/6-311G(d,p)) of 3b along with the experimental spectrum of 5b after 15s of irradiation.

Figure S5. Computational absorption spectrum obtained from TD-ωB97XD/6-31G(d) of Compound 5a, 5b, 6a and 6b.

6. Photo-induced dissociation of the dimer
In order to prove the presence of intermediates, we used $^1$H NMR and UV-Vis absorption spectra to detected the photodegradation process of 5b under nitrogen atmosphere. Toluene was refluxed over sodium, and freshly distilled prior to use. In order to find the source of hydrogen in the photo-induced dissociation process of the dimer, we used toluene-$d_8$ and D$_2$O (10/1, v/v) as solvents to detect the photolysis process. The NMR tube needs to be constantly shaken during the irradiation so that the D$_2$O can be dissolved in toluene-$d_8$. 
Figure S6. Photodissociation of 0.02 mM 5b in degassed toluene at ambient temperature (A) and possible photo-induced dissociation mechanism of the dimer (B).

Figure S7. $^1$H NMR spectrum of 5b in toluene-$d_8$ (~2 mM) with the increase of the irradiation time under nitrogen atmosphere.
Figure S8. $^1$H NMR spectrums of 5b in toluene-$d_8$ and D$_2$O after 8 hours of irradiation (red) and in toluene-$d_8$ after 4 hours of irradiation (blue) under nitrogen atmosphere.

Figure S9. ESR spectrum of 5b in degassed toluene after 10 min of irradiation at room temperature (A) and calculated spin density maps of the singlet diradicals of 3b (B).

7. Surface areas and porosities of compound 5a.
The surface areas and porosities of 5a was characterized by nitrogen adsorption and desorption analysis at 77.35 K with an auto-sorb computer-controlled surface analyzer (Micromeritics, ASAP 2460). The sample was degassed at 100 ºC (8h) before analyzed.
8. OFET fabrication and characterization

**Thin-film devices fabrication:** The SiO$_2$/Si wafers were cleaned with deionized water, piranha solution(H$_2$SO$_4$/H$_2$O$_2$=7:3), deionized water, isopropyl alcohol, and finally were blown with high purity nitrogen gas. Treatment of the SiO$_2$/Si wafers with 12-cyclohexyldodecylphosphonic acid (CDPA). Al(NO$_3$)$_3$·9H$_2$O (0.0375 g) was dissolved in ethanol (1 mL) and stirred for 4 hours under a nitrogen atmosphere, resulting a concentration of Al(NO$_3$)$_3$ in ethanol (37.5 mg/mL), which was spin-coated onto the cleaned SiO$_2$/Si substrate at 5000 rpm for 40 seconds. Then, the substrate was baked at 300 °C for half an hour to dehydrate the substrate completely. The bottom-gate top-contact (BGTC) devices based on thin film were fabricated with the “shadow mask” method. Firstly, films of the semiconductors were spin-coated from toluene solution (10 mg/mL, 4000 r/min) onto AlOx/SiO$_2$/Si substrate modified with CDPA. Secondly, silver, as the source/drain electrodes with width/length of 1000/105, were thermal evaporated (0.1 Å/s, 50 nm) on the semiconductor films through a shadow mask.

**Single-crystal devices fabrication:** The SiO$_2$/Si wafers were cleaned with deionized water, piranha solution (H$_2$SO$_4$/H$_2$O$_2$=7:3), deionized water, isopropyl alcohol, and finally were blown with high purity nitrogen gas. Treatment of the SiO$_2$/Si wafers with octadecyltrichlorosilane (OTS) was conducted by the vapor-deposition method. The clean wafers were dried under vacuum at 90 °C for 2 h to eliminate the moisture. When the temperature is decreased to room temperature, a small drop of OTS was dropped onto the wafers. Subsequently, this system was heated to 120 °C for 2 h under vacuum, after which the vacuum is maintained at approximately room temperature. The bottom-gate top-contact (BGTC) devices based on the micro/nanometer-sized single crystals were fabricated with the “gold strips” method.[4]

**Devices characterization:** All electrical characteristics of the devices were measured at room temperature using a semiconductor parameter analyzer (Keithley 4200 SCS) in nitrogen atmosphere. The mobilities of the devices were calculated in the saturation regime. The equation is listed as follows:

\[ I_{DS} = \frac{(W/2L)C_i\mu(V_{GS} - V_T)^2}{2} \]

where W/L is the channel width/length , C$_i$ is the insulator capacitance per unit area (10 nF/cm$^2$),
and $V_{GS}$ and $V_T$ are the gate voltage and threshold voltage, respectively. This equation defines the important characteristics of electron mobility ($\mu$), on/off ratio ($I_{on/off}$), and threshold voltage ($V_T$), which could be deduced by the equation from the plot of current–voltage.

**Thin film:** X-ray diffraction (XRD) was measured on a D/max2500 with a CuKα source ($\kappa = 1.541$ Å). Atomic force microscopy (AFM) measurements were carried out with a Nanoscope IIIa instrument (Digital Instruments).

**Figure S11.** AFM images (5 μm×5 μm scan area) and RMS values of CDPA-modified thin films of: (A) 5a, (B) 5b, (C) 6a and (D) 6b.

**Figure S12.** XRD images of (A) 5a, (B) 5b, (C) 6a and (D) 6b thin films.
Figure S13. Representative transfer (A), (B), (C) and (D) and output curves (E), (F), (G) and (H) of OFET devices based on thin film of 5a, 5b, 6a and 6b, respectively.

Figure S14. Optical microscopy image (A), (C), (E) and (G), and XRD image (B), (D), (F) and (H) of 5a, 5b, 6a and 6b, respectively.
**Figure S15.** Representative transfer (A), (B), (C) and (D) and output curves (E), (F), (G) and (H) of OFET devices based on single-crystalline microribbons of 5a (W/L=1/13), 5b (W/L=1/8), 6a (W/L=1/6) and 6b (W/L=1/5), respectively.

**Figure S16.** Plots showing dependence of mobilities on gate voltages of OFET devices based on single-crystalline microribbons of 5a (A) and 5b (B).

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10. $^1$H NMR, $^{13}$C NMR and HRMS spectra of compounds

**Figure S17.** $^1$H NMR spectrum of 10 in CDCl$_3$ (400 MHz, 298 K).

**Figure S18.** HR-MALDI-TOF spectra of 10.
Figure S19. $^1$H NMR spectrum of 9 in CDCl$_3$ (400 MHz, 298 K).

Figure S20. $^{13}$C NMR spectrum of 9 in CDCl$_3$ (100 MHz, 298 K).
Figure S21. HR-MALDI-TOF spectra of 9.

Figure S22. $^1$H NMR spectrum of 8 in CDCl$_2$CDCl$_2$ (400 MHz, 298 K).
Figure S23. $^{13}$C NMR spectrum of 8 in CDCl$_2$CDCl$_2$ (100 MHz, 298 K).

Figure S24. HR-MALDI-TOF spectra of 8.
Figure S25. $^1$H NMR spectrum of 1a in CDCl$_3$ (400 MHz, 298 K).

Figure S26. HR-MALDI-TOF spectra of 1a.
Figure S27. $^1$H NMR spectrum of 1b in CDCl$_3$ (400 MHz, 298 K).

Figure S28. HR-MALDI-TOF spectra of 1b.
Figure S29. $^1$H NMR spectrum of 2a in CDCl$_3$ (400 MHz, 298 K).

Figure S30. $^{13}$C NMR spectrum of 2a in CDCl$_3$ (100 MHz, 298 K).
Figure S31. HR-MALDI-TOF spectra of 2a.

Figure S32. $^1$H NMR spectrum of 2b in CDCl$_3$ (400 MHz, 298 K).
Figure S33. $^{13}$C NMR spectrum of 2b in CDCl$_3$ (100 MHz, 298 K).

Figure S34. HR-MALDI-TOF spectra of 2b.
Figure S35. $^1$H NMR spectrum of 5a in CDCl$_3$ (400 MHz, 298 K).

Figure S36. $^{13}$C NMR spectrum of 5a in CDCl$_3$ (100 MHz, 298 K).
Figure S37. HR-MALDI-TOF spectra of 5a.

Figure S38. $^1$H NMR spectrum of 5b in CDCl$_3$ (400 MHz, 298 K).
Figure S39. $^{13}$C NMR spectrum of 5b in CDCl$_3$ (100 MHz, 298 K).

Figure S40. HR-MALDI-TOF spectra of 5b.
Figure S41. $^1$H NMR spectrum of 6a in CDCl$_3$ (400 MHz, 298 K).

Figure S42. $^{13}$C NMR spectrum of 6a in CDCl$_3$ (100 MHz, 298 K).
Figure S43. HR-MALDI-TOF spectra of 6a.

Figure S44. $^1$H NMR spectrum of 6b in CDCl$_3$ (400 MHz, 298 K).
Figure S45. $^{13}$C NMR spectrum of 6b in CDCl$_3$ (100 MHz, 298 K).

Figure S46. HR-MALDI-TOF spectra of 6b.
11. Supplementary data of DFT calculations

Table S3. Selected wavelengths, oscillator strengths and comparison of major electronic transitions of the compounds.

| Name  | Transition | Energy (eV) | Wavelength (nm) | f   | Electronic Configuration       |
|-------|------------|-------------|-----------------|-----|-------------------------------|
| 5a    | $S_0 \rightarrow S_1$ | 2.5154      | 492.89          | 0.0006 | HOMO-1 $\rightarrow$ LUMO+1 (3%) |
|       |            |             |                 |     | HOMO $\rightarrow$ LUMO (75%)  |
|       |            |             |                 |     | HOMO $\rightarrow$ LUMO+1 (18%) |
| $S_0 \rightarrow S_2$ | 2.6256      | 472.22       | 0.0041          | HOMO-1 $\rightarrow$ LUMO (30%) |
|       |            |             |                 |     | HOMO-1 $\rightarrow$ LUMO+1 (16%) |
|       |            |             |                 |     | HOMO $\rightarrow$ LUMO (9%)    |
|       |            |             |                 |     | HOMO $\rightarrow$ LUMO+1 (41%) |
| $S_0 \rightarrow S_3$ | 2.7188      | 456.02       | 0.0061          | HOMO-9 $\rightarrow$ LUMO (18%) |
|       |            |             |                 |     | HOMO-8 $\rightarrow$ LUMO+1 (25%) |
|       |            |             |                 |     | HOMO-8 $\rightarrow$ LUMO+1 (11%) |
|       |            |             |                 |     | HOMO-2 $\rightarrow$ LUMO (13%) |
|       |            |             |                 |     | HOMO-2 $\rightarrow$ LUMO+1 (9%) |
| $S_0 \rightarrow S_4$ | 2.7289      | 454.34       | 0.0107          | HOMO-9 $\rightarrow$ LUMO (16%) |
|       |            |             |                 |     | HOMO-8 $\rightarrow$ LUMO (15%) |
|       |            |             |                 |     | HOMO-6 $\rightarrow$ LUMO (25%) |
|       |            |             |                 |     | HOMO-6 $\rightarrow$ LUMO+1 (8%) |
|       |            |             |                 |     | HOMO-2 $\rightarrow$ LUMO+1 (10%) |
| $S_0 \rightarrow S_5$ | 2.8153      | 440.40       | 0.0067          | HOMO-1 $\rightarrow$ LUMO (34%) |
|       |            |             |                 |     | HOMO-1 $\rightarrow$ LUMO+1 (16%) |
|       |            |             |                 |     | HOMO $\rightarrow$ LUMO (9%)    |
|       |            |             |                 |     | HOMO $\rightarrow$ LUMO+1 (32%) |
|       |            |             |                 |     | HOMO $\rightarrow$ LUMO+3 (4%)  |
| $S_0 \rightarrow S_6$ | 2.9057      | 426.69       | 0.0034          | HOMO-1 $\rightarrow$ LUMO (30%) |
|       |            |             |                 |     | HOMO-1 $\rightarrow$ LUMO+1 (54%) |
|       |            |             |                 |     | HOMO-1 $\rightarrow$ LUMO+2 (7%) |
|       |            |             |                 |     | HOMO $\rightarrow$ LUMO (3%)    |
| $S_0 \rightarrow S_7$ | 2.9192      | 424.71       | 0.1450          | HOMO-4 $\rightarrow$ LUMO (35%) |
|       |            |             |                 |     | HOMO-3 $\rightarrow$ LUMO+1 (34%) |
| $S_0 \rightarrow S_8$ | 2.9966      | 413.75       | 0.0101          | HOMO-11 $\rightarrow$ LUMO (27%) |
|       |            |             |                 |     | HOMO-11 $\rightarrow$ LUMO+1 (21%) |
|       |            |             |                 |     | HOMO-10 $\rightarrow$ LUMO (7%)  |
|       |            |             |                 |     | HOMO-10 $\rightarrow$ LUMO+1 (4%) |
| $S_0 \rightarrow S_{10}$ | 2.9996     | 413.33       | 0.0688          | HOMO-10 $\rightarrow$ LUMO+1 (29%) |
|       |            |             |                 |     | HOMO-10 $\rightarrow$ LUMO (21%) |
|      | Energy (eV) | Oscillator Strength | Probability (%) |
|------|-------------|---------------------|-----------------|
| $S_0 \rightarrow S_{11}$ | 3.0833 | 0.9837 | 9% |
|      | 3.0833 | 0.9837 | 12% |
|      | 3.0833 | 0.9837 | 3% |
|      | 3.0833 | 0.9837 | 28% |
|      | 3.0833 | 0.9837 | 20% |
|      | 3.0833 | 0.9837 | 3% |
|      | 3.0833 | 0.9837 | 2% |
| $S_0 \rightarrow S_{12}$ | 3.3734 | 0.0094 | 5% |
|      | 3.3734 | 0.0094 | 19% |
|      | 3.3734 | 0.0094 | 3% |
|      | 3.3734 | 0.0094 | 11% |
|      | 3.3734 | 0.0094 | 45% |
|      | 3.3734 | 0.0094 | 5% |
| $S_0 \rightarrow S_{13}$ | 3.3803 | 0.0089 | 3% |
|      | 3.3803 | 0.0089 | 31% |
|      | 3.3803 | 0.0089 | 19% |
|      | 3.3803 | 0.0089 | 14% |
| $S_0 \rightarrow S_{14}$ | 3.3919 | 0.2684 | 5% |
|      | 3.3919 | 0.2684 | 21% |
|      | 3.3919 | 0.2684 | 11% |
|      | 3.3919 | 0.2684 | 12% |
|      | 3.3919 | 0.2684 | 10% |
|      | 3.3919 | 0.2684 | 25% |
|      | 3.3919 | 0.2684 | 3% |
| $S_0 \rightarrow S_{15}$ | 2.5807 | 0.0013 | 3% |
|      | 2.5807 | 0.0013 | 21% |
|      | 2.5807 | 0.0013 | 11% |
|      | 2.5807 | 0.0013 | 71% |
| $S_0 \rightarrow S_2$ | 2.5943 | 0.0078 | 19% |
|      | 2.5943 | 0.0078 | 18% |
|      | 2.5943 | 0.0078 | 11% |
|      | 2.5943 | 0.0078 | 19% |
|      | 2.5943 | 0.0078 | 31% |
| $S_0 \rightarrow S_3$ | 2.6091 | 0.0091 | 10% |
|      | 2.6091 | 0.0091 | 31% |
|      | 2.6091 | 0.0091 | 31% |
|      | 2.6091 | 0.0091 | 18% |
|      | 2.6091 | 0.0091 | 11% |
| $S_0 \rightarrow S_4$ | 2.6790 | 0.0072 | 23% |
|      | 2.6790 | 0.0072 | 16% |
|      | 2.6790 | 0.0072 | 12% |
|      | 2.6790 | 0.0072 | 42% |
|      | 2.6790 | 0.0072 | 31% |
| $S_0 \rightarrow S_5$ | 2.8267 | 0.0066 | 14% |
|      | 2.8267 | 0.0066 | 14% |
|      | 2.8267 | 0.0066 | 14% |
|      | 2.8267 | 0.0066 | 42% |
|      | 2.8267 | 0.0066 | 31% |
| $S_0 \rightarrow S_1$ | 3.1219 | 422.14 | 0.0014 | HOMO-1 $\rightarrow$ LUMO+1 (23%)  
| | | | | HOMO $\rightarrow$ LUMO (9%)  
| | | | | HOMO $\rightarrow$ LUMO+1 (23%)  
| $S_0 \rightarrow S_2$ | 2.9440 | 421.14 | 0.1279 | HOMO-10 $\rightarrow$ LUMO+1 (4%)  
| | | | | HOMO-9 $\rightarrow$ LUMO (7%)  
| | | | | HOMO-9 $\rightarrow$ LUMO+1 (11%)  
| | | | | HOMO-3 $\rightarrow$ LUMO (26%)  
| | | | | HOMO-2 $\rightarrow$ LUMO+1 (27%)  
| $S_0 \rightarrow S_{10}$ | 3.0933 | 400.17 | 0.1313 | HOMO-10 $\rightarrow$ LUMO+1 (14%)  
| | | | | HOMO-9 $\rightarrow$ LUMO (5%)  
| | | | | HOMO-9 $\rightarrow$ LUMO+1 (8%)  
| | | | | HOMO-3 $\rightarrow$ LUMO (20%)  
| | | | | HOMO-2 $\rightarrow$ LUMO+1 (17%)  
| $S_0 \rightarrow S_{11}$ | 3.1337 | 395.65 | 0.9772 | HOMO-10 $\rightarrow$ LUMO+1 (6%)  
| | | | | HOMO-13 $\rightarrow$ LUMO (10%)  
| | | | | HOMO-12 $\rightarrow$ LUMO+1 (15%)  
| | | | | HOMO-11 $\rightarrow$ LUMO (9%)  
| | | | | HOMO-8 $\rightarrow$ LUMO (9%)  
| | | | | HOMO-6 $\rightarrow$ LUMO (23%)  
| | | | | HOMO-4 $\rightarrow$ LUMO (10%)  
| | | | | HOMO-2 $\rightarrow$ LUMO+5 (2%)  
| $S_0 \rightarrow S_{13}$ | 3.4165 | 362.90 | 0.0616 | HOMO-1 $\rightarrow$ LUMO+3 (54%)  
| | | | | HOMO-6 $\rightarrow$ LUMO+2 (15%)  
| | | | | HOMO-1 $\rightarrow$ LUMO+1 (7%)  
| | | | | HOMO-1 $\rightarrow$ LUMO+3 (9%)  
| $S_0 \rightarrow S_{14}$ | 3.4363 | 360.74 | 0.1749 | HOMO-1 $\rightarrow$ LUMO (4%)  
| | | | | HOMO-1 $\rightarrow$ LUMO+1 (8%)  
| | | | | HOMO-1 $\rightarrow$ LUMO+2 (59%)  
| | | | | HOMO-1 $\rightarrow$ LUMO+1 (3%)  
| | | | | HOMO $\rightarrow$ LUMO+2 (9%)  
| | | | | HOMO $\rightarrow$ LUMO+3 (11%)  

**6a**

| $S_0 \rightarrow S_1$ | 2.5092 | 489.12 | 0.0005 | HOMO-1 $\rightarrow$ LUMO+1 (5%)  
| | | | | HOMO $\rightarrow$ LUMO (79%)  
| | | | | HOMO $\rightarrow$ LUMO+1 (12%)  
| | | | | HOMO-1 $\rightarrow$ LUMO (30%)  
| | | | | HOMO-1 $\rightarrow$ LUMO+1 (11%)  
| $S_0 \rightarrow S_2$ | 2.6274 | 471.88 | 0.0047 |
|   |   |   |   |   |
|---|---|---|---|---|
| $S_0 \rightarrow S_1$ | 2.6298 | 471.46 | 0.0032 | HOMO $\rightarrow$ LUMO (6%)  
HOMO $\rightarrow$ LUMO+1 (48%)  
HOMO-9 $\rightarrow$ LUMO (2%)  
HOMO-8 $\rightarrow$ LUMO+1 (14%)  
HOMO-8 $\rightarrow$ LUMO+1 (28%)  
HOMO-2 $\rightarrow$ LUMO (16%)  
| $S_0 \rightarrow S_4$ | 2.6439 | 468.95 | 0.0041 | HOMO-9 $\rightarrow$ LUMO (16%)  
HOMO-8 $\rightarrow$ LUMO (4%)  
HOMO-7 $\rightarrow$ LUMO (22%)  
HOMO-7 $\rightarrow$ LUMO+1 (30%)  
HOMO-2 $\rightarrow$ LUMO+1 (14%)  
| $S_0 \rightarrow S_5$ | 2.7806 | 445.89 | 0.0086 | HOMO-1 $\rightarrow$ LUMO (42%)  
HOMO-1 $\rightarrow$ LUMO+1 (12%)  
HOMO $\rightarrow$ LUMO (6%)  
HOMO $\rightarrow$ LUMO+1 (31%)  
HOMO $\rightarrow$ LUMO+3 (4%)  
| $S_0 \rightarrow S_6$ | 2.9057 | 426.69 | 0.0034 | HOMO-1 $\rightarrow$ LUMO (21%)  
HOMO-1 $\rightarrow$ LUMO+1 (61%)  
HOMO-1 $\rightarrow$ LUMO+2 (5%)  
HOMO $\rightarrow$ LUMO (4%)  
HOMO $\rightarrow$ LUMO+2 (3%)  
| $S_0 \rightarrow S_8$ | 2.9535 | 419.79 | 0.303 | HOMO-4 $\rightarrow$ LUMO (51%)  
HOMO-4 $\rightarrow$ LUMO+1 (3%)  
HOMO-3 $\rightarrow$ LUMO+1 (40%)  
| $S_0 \rightarrow S_9$ | 3.0954 | 400.54 | 0.0135 | HOMO-4 $\rightarrow$ LUMO+3 (34%)  
HOMO $\rightarrow$ LUMO+2 (28%)  
HOMO-1 $\rightarrow$ LUMO+3 (14%)  
| $S_0 \rightarrow S_{10}$ | 3.1154 | 397.98 | 0.3076 | HOMO-1 $\rightarrow$ LUMO+2 (51%)  
HOMO $\rightarrow$ LUMO+1 (3%)  
HOMO $\rightarrow$ LUMO+2 (5%)  
HOMO $\rightarrow$ LUMO+3 (29%)  
| $S_0 \rightarrow S_{11}$ | 3.2282 | 384.07 | 0.6925 | HOMO-11 $\rightarrow$ LUMO+1 (24%)  
HOMO-10 $\rightarrow$ LUMO (31%)  
HOMO-8 $\rightarrow$ LUMO (13%)  
HOMO-4 $\rightarrow$ LUMO+7 (2%)  
HOMO-3 $\rightarrow$ LUMO+6 (2%)  
HOMO-2 $\rightarrow$ LUMO (18%)  
| $S_0 \rightarrow S_{14}$ | 3.4959 | 354.66 | 0.0152 | HOMO-11 $\rightarrow$ LUMO (27%)  
HOMO-10 $\rightarrow$ LUMO+1 (25%)  
HOMO-2 $\rightarrow$ LUMO+1 (18%)  
| $6b$ $S_0 \rightarrow S_1$ | 2.6540 | 467.15 | 0.0033 | HOMO-1 $\rightarrow$ LUMO+1 (12%)  

| $S_0 \rightarrow S_2$ | 2.6611 | 465.91 | 0.0023 | HOMO → LUMO (35%)  
|                 |       |        |         | HOMO → LUMO+1 (34%)  
|                 |       |        |         | HOMO-4 → LUMO (2%)  
|                 |       |        |         | HOMO-4 → LUMO+1 (28%)  
|                 |       |        |         | HOMO-6 → LUMO (44%)  
|                 |       |        |         | HOMO-8 → LUMO+1 (10%)  
| $S_0 \rightarrow S_1$ | 2.6810 | 462.45 | 0.0005 | HOMO-1 → LUMO+1 (5%)  
|                 |       |        |         | HOMO → LUMO (70%)  
|                 |       |        |         | HOMO → LUMO+1 (19%)  
| $S_0 \rightarrow S_4$ | 2.6925 | 460.47 | 0.0066 | HOMO-1 → LUMO (22%)  
|                 |       |        |         | HOMO-1 → LUMO+1 (13%)  
|                 |       |        |         | HOMO → LUMO (12%)  
|                 |       |        |         | HOMO → LUMO+1 (46%)  
| $S_0 \rightarrow S_5$ | 2.8472 | 435.46 | 0.0054 | HOMO-1 → LUMO (32%)  
|                 |       |        |         | HOMO-1 → LUMO+1 (23%)  
|                 |       |        |         | HOMO → LUMO (8%)  
|                 |       |        |         | HOMO → LUMO+1 (19%)  
| $S_0 \rightarrow S_7$ | 2.9778 | 416.35 | 0.0018 | HOMO-3 → LUMO+1 (40%)  
|                 |       |        |         | HOMO-2 → LUMO+1 (27%)  
|                 |       |        |         | HOMO-2 → LUMO (3%)  
| $S_0 \rightarrow S_5$ | 2.9925 | 414.30 | 0.3796 | HOMO-3 → LUMO (49%)  
|                 |       |        |         | HOMO-2 → LUMO+1 (43%)  
|                 |       |        |         | HOMO → LUMO+1 (2%)  
| $S_0 \rightarrow S_{10}$ | 3.1946 | 388.1 | 0.1711 | HOMO-12 → LUMO (3%)  
|                 |       |        |         | HOMO-1 → LUMO (3%)  
|                 |       |        |         | HOMO-1 → LUMO+1 (8%)  
|                 |       |        |         | HOMO-1 → LUMO+2 (50%)  
|                 |       |        |         | HOMO → LUMO+2 (9%)  
|                 |       |        |         | HOMO → LUMO+3 (12%)  
| $S_0 \rightarrow S_{11}$ | 3.2813 | 377.85 | 0.6365 | HOMO-11 → LUMO+1 (27%)  
|                 |       |        |         | HOMO-10 → LUMO (25%)  
|                 |       |        |         | HOMO-8 → LUMO (9%)  
|                 |       |        |         | HOMO-3 → LUMO+6 (5%)  
|                 |       |        |         | HOMO-2 → LUMO (16%)  
| $S_0 \rightarrow S_{14}$ | 3.6004 | 344.36 | 0.0069 | HOMO-13 → LUMO (30%)  
|                 |       |        |         | HOMO-10 → LUMO+1 (24%)  
|                 |       |        |         | HOMO-8 → LUMO+6 (23%)  
|                 |       |        |         | HOMO-4 → LUMO+1 (5%)  

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Table S4. Cartesian coordinates of the ground state optimized geometry for compound 5a.
The calculated absolute energy value for this molecule is -36535556.93 kJ/mol

|   | X          | Y          | Z          |
|---|------------|------------|------------|
| C | -0.52388900| 2.03639200 | -0.71538600|
| C | -0.52388400| 2.03658500 | 0.71480200 |
| C | -1.26499900| 2.96727200 | -1.42750100|
| C | -2.05668800| 3.95207400 | -0.72125400|
| C | -2.05668600| 3.95226500 | 0.72016400 |
| C | -1.26499200| 2.96765600 | 1.42667100 |
| C | -2.82312800| 4.90282700 | -1.40161700|
| C | -3.59237300| 5.85613900 | -0.72162100|
| C | -3.59237200| 5.85633000 | 0.72002900 |
| C | -2.82312600| 4.90319800 | 1.40027600 |
| C | -1.26115800| 2.96074900 | -2.85388500|
| C | -1.25875700| 2.95902500 | 0.71183600 |
| O | 8.48981100 | -0.08326200| -3.55738500|
| O | 4.33989460 | 1.75143900 | -3.53037700|
| C | -1.25874700| 2.96010600 | 4.06369800 |
| O | 8.48981100 | -0.08326200| 3.55741000 |
| C | -4.38090700| 6.82988900 | 1.40723400 |
| C | 8.82858200 | 0.59028000 | 0.71862100 |
| C | 8.82856700 | 0.58995600 | -0.71890300|
| C | 7.63473100 | 0.61824400 | -1.42615700|
| C | 6.40042300 | 0.79053000 | -0.71793500|
| C | 6.40043600 | 0.79082700 | 0.71762100 |
| O | 8.48981100 | -0.08326200| 3.55738500 |
| O | 4.33989460 | 1.75143900 | -3.53037700|
| O | 8.48981100 | -0.08326200| 3.55741000 |
| C | 6.36283400 | 0.84135000 | -5.01079700|
| O | 8.48981100 | -0.08326200| 3.55738500 |
| O | 4.33989460 | 1.75143900 | -3.53037700|
| O | 8.48981100 | -0.08326200| 3.55741000 |
| C | 6.36294100 | 0.84356700 | 5.01046300 |
|   | x            | y            | z            |
|---|--------------|--------------|--------------|
| N | 2.78496200   | 0.98529500   | -1.41675300  |
| C | 1.68303300   | 0.98883900   | -0.72050500  |
| C | 1.68304400   | 0.98905600   | 0.72017700   |
| N | 2.78498300   | 0.98575800   | 1.41641000   |
| C | -8.80928500  | -1.28995100  | -0.71844000  |
| C | -8.80926300  | -1.28976000  | 0.71901300   |
| C | -7.61816000  | -1.20132000  | 1.42616600   |
| C | -6.39439100  | -0.96489800  | 0.71798500   |
| C | -6.39441200  | -0.96509400  | -0.71757900  |
| C | -7.61820500  | -1.20170200  | -1.42565600  |
| C | -5.19909300  | -0.70966300  | 1.42082900   |
| C | -3.97542700  | -0.62319200  | 0.71973900   |
| C | -3.97544700  | -0.62339100  | -0.71949600  |
| C | -5.19913400  | -0.71005600  | -1.42052800  |
| C | -7.55012700  | -1.41465200  | 2.91287100   |
| N | -6.39083000  | -0.96183500  | 3.54337000   |
| C | -5.24924700  | -0.47599700  | 2.89183500   |
| C | -5.24932700  | -0.47680600  | -2.89160000  |
| N | -6.39094300  | -0.96279500  | -3.54296500  |
| C | -7.55022900  | -1.41541900  | -2.91230700  |
| O | -8.43937500  | -1.94534600  | 3.55605400   |
| O | -4.38116000  | 0.08349700   | 3.53609500   |
| O | -4.38128500  | 0.08256000   | -3.53603300  |
| O | -8.43952600  | -1.94623300  | -3.55532300  |
| C | -6.35430200  | -0.93763300  | 5.01144100   |
| C | -6.35447300  | -0.93896600  | -5.01104300  |
| N | -2.79383400  | -0.57321300  | 1.41610900   |
| C | -1.69547200  | -0.48055100  | 0.72073900   |
| C | -1.69549100  | -0.48074600  | -0.72059500  |
| N | -2.79387200  | -0.57360200  | -1.41591000  |
| C | 0.51025200   | -1.53322800  | 0.71539700   |
| C | 0.51023100   | -1.53342600  | -0.71503000  |
| C | 1.25112200   | -2.46504200  | 1.42639000   |
| C | 2.04083000   | -3.45255200  | 0.72113700   |
| C | 2.04081000   | -3.45275000  | -0.72028900  |
| C | 1.25108100   | -2.46543400  | -1.42578900  |
| C | 2.80479000   | -4.40545200  | 1.40122300   |
| C | 3.57255900   | -5.36035200  | 0.72146000   |
| C | 3.57254000   | -5.36054900  | -0.72013200  |
| C | 2.80475100   | -4.40583600  | -1.40013500  |
| C | 1.24825500   | -2.45818000  | 2.85342900   |
| C | 1.24801000   | -2.45709100  | 4.06432800   |
| C | 1.24817000   | -2.45896100  | -2.85283000  |
| C | 1.24787600   | -2.45820900  | -4.06373000  |
|  | X   | Y   | Z   |
|---|-----|-----|-----|
| C | 4.35944700 | -6.33482900 | 1.40903400 |
| C | 5.10206000 | -7.25309400 | 0.71373400 |
| C | 5.10206000 | -7.25328800 | -0.71373400 |
| C | 4.35940900 | -6.33521300 | -1.40746000 |
| C | 0.33428300 | 0.98440100 | -1.40320500 |
| C | 0.33430600 | 0.98479000 | 1.40289900 |
| C | -0.34672800 | -0.47993400 | -1.40319900 |
| C | -0.34669000 | -0.47955100 | 1.40330500 |
| H | -2.82209800 | 4.89813900 | -2.48723200 |
| H | -2.82206000 | 4.89879800 | 2.48589200 |
| H | -1.26206300 | 2.93830200 | -5.13083400 |
| H | -1.26194700 | 2.93953000 | 5.13001200 |
| H | -4.37853800 | 6.82637900 | -2.49627100 |
| H | -5.72087300 | 8.48242800 | 1.24706700 |
| H | -5.72087300 | 8.48275700 | -1.24478300 |
| H | -4.37853700 | 6.82703800 | 2.49442300 |
| H | 6.26396700 | 1.87429000 | -5.35372200 |
| H | 7.28657300 | 0.40060100 | -5.37697400 |
| H | 5.49893800 | 0.27637400 | -5.36722900 |
| H | 5.49909000 | 0.27861000 | 5.36716900 |
| H | 7.28671800 | 0.40295600 | 5.37681000 |
| H | 6.26401700 | 1.87656900 | 5.35292900 |
| H | -5.45222700 | -1.44394600 | 5.36094700 |
| H | -6.32768200 | 0.09653400 | 5.36402900 |
| H | -7.24449900 | -1.44450500 | 5.37517500 |
| H | -6.32785700 | 0.09511000 | -5.36389700 |
| H | -5.45241600 | -1.44537700 | -5.36045400 |
| H | -7.24468900 | -1.44592300 | -5.37461200 |
| H | 2.80277500 | -4.40248700 | 2.48690200 |
| H | 2.80270900 | -4.40316700 | -2.48581500 |
| H | 1.24392700 | -2.44079200 | 5.13084800 |
| H | 1.24376500 | -2.44218200 | -5.13025300 |
| H | 4.35761000 | -6.33167200 | 2.49619700 |
| H | 5.69780200 | -7.98889300 | 1.24678800 |
| H | 5.69777000 | -7.98923300 | -1.24479900 |
| H | 4.35755400 | -6.33253500 | -2.49462500 |
| H | 0.48843500 | 1.25406500 | 2.44736400 |
| H | 0.48847200 | 1.25474300 | 2.44698100 |
| H | -0.50297900 | -0.75032300 | -2.44677300 |
| H | -0.50290900 | -0.74966100 | 2.44695500 |
| Br | 10.50038600 | 0.57503200 | 1.60699700 |
| Br | 10.50035400 | 0.57428700 | -1.60730400 |
| Br | -10.47839000 | -1.39058800 | 1.60681100 |
| Br | -10.47834000 | -1.39102300 | -1.60615700 |
**Cartesian coordinates and calculated energy for 5b.**

**Table S5.** Cartesian coordinates of the ground state optimized geometry for compound 5b.

The calculated absolute energy value for this molecule is -38572280.08 kJ/mol.

|   |     X     |     Y     |     Z     |
|---|----------|----------|----------|
| C | 0.72443000 | 1.90913600 | 0.71554900 |
| C | 0.72443900 | 1.90934100 | -0.71496100 |
| C | 1.55545800 | 2.75968700 | 1.42874700 |
| C | 2.43855500 | 3.66180100 | 0.72079200 |
| C | 2.43856900 | 3.66200200 | -0.71967900 |
| C | 1.55548200 | 2.76009100 | -1.42790500 |
| C | 3.29013400 | 4.53313700 | 1.40699700 |
| C | 4.14098100 | 5.40586600 | 0.72120300 |
| C | 4.14099500 | 5.40606600 | -0.71957200 |
| C | 3.29016100 | 4.53352800 | -1.40562500 |
| C | 1.55558600 | 2.75403500 | 2.85451400 |
| C | 1.56012500 | 2.75448100 | 4.06495800 |
| C | 1.55563700 | 2.75483900 | -2.85367300 |
| C | 1.56018800 | 2.75561900 | -4.06411700 |
| C | 5.01545000 | 6.30139000 | 1.40052100 |
| C | 5.84117600 | 7.14750100 | 0.71260000 |
| C | 5.84119000 | 7.14769700 | -0.71045400 |
| C | 5.01547800 | 6.30177700 | -1.39862400 |
| C | -8.72274400 | 1.56219300 | -0.71895300 |
| C | -8.72275600 | 1.56196200 | 0.71931400 |
| C | -7.53493100 | 1.43901900 | 1.42619100 |
| C | -6.28845200 | 1.45560700 | 0.71815900 |
| C | -6.28841100 | 1.45584100 | -0.71778900 |
| C | -7.53490700 | 1.43948200 | -1.42584900 |
| C | -5.06784600 | 1.49826300 | 1.42141400 |
| C | -3.84788700 | 1.36673800 | 0.71981400 |
| C | -3.84787800 | 1.36696600 | -0.71943100 |
| C | -5.06782400 | 1.49872000 | -1.42100900 |
| C | -7.50529600 | 1.21867700 | 2.91314200 |
| N | -6.28583100 | 1.46870500 | 3.54396900 |
| C | -5.07667400 | 1.74243000 | 2.89213900 |
| C | -5.07662400 | 1.74336400 | -2.89165400 |
| N | -6.28576500 | 1.46983500 | -3.54359600 |
| C | -7.50524600 | 1.21962500 | -2.91287200 |
| O | -8.47235400 | 0.84842400 | 3.55581500 |
| O | -4.12347200 | 2.14398800 | 3.53409000 |
| O | -4.12341400 | 2.14514300 | -3.53345400 |
| O | -8.47229800 | 0.84959900 | -3.55568600 |
| C | -6.24680900 | 1.49416400 | 5.01214000 |
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
|      | -6.24671700 | 1.49576900 | -5.01175800 |
| N    | -2.67486100 | 1.21975100 | 1.41612000  |
| C    | -1.57929400 | 1.10223900 | 0.71995800  |
| C    | -1.57938800 | 1.10245400 | -0.71963100 |
| N    | -2.67484400 | 1.22018500 | -1.41576900 |
| C    | 8.63425400  | -2.18454400 | 0.71892000  |
| C    | 8.63425500  | -2.18435100 | -0.71950200 |
| C    | 7.45643300  | -1.98701700 | -1.42656800 |
| C    | 6.25934100  | -1.63982200 | -0.71812300 |
| C    | 6.25937700  | -1.64002100 | 0.71768100  |
| C    | 7.45642900  | -1.98740600 | 1.42603600  |
| C    | 5.09345600  | -1.27482500 | -1.42111800 |
| C    | 3.88320600  | -1.07394700 | -0.71971800 |
| C    | 3.88320200  | -1.07415100 | 0.71941700  |
| C    | 5.09344700  | -1.27522300 | 1.42077000  |
| C    | 7.36930100  | -2.19120900 | -2.91367100 |
| N    | 6.25522800  | -1.63482000 | -3.54404000 |
| C    | 5.16529300  | -1.04476400 | -2.89215500 |
| C    | 5.16527100  | -1.04557500 | 2.89187200  |
| N    | 6.25521200  | -1.63579700 | 3.54359900  |
| C    | 7.36929500  | -2.19199900 | 2.91308400  |
| O    | 8.20695400  | -2.79855400 | -3.55768100 |
| O    | 4.35287200  | -0.40424300 | -3.53390600 |
| O    | 4.35283700  | -0.40524800 | 3.53380000  |
| O    | 8.20695500  | -2.79950400 | 3.55693300  |
| C    | 6.22252600  | -1.60544400 | -5.01241200 |
| C    | 6.22249800  | -1.60682500 | 5.01197900  |
| N    | 2.71164400  | -0.91191600 | -1.41587400 |
| C    | 1.62753300  | -0.71432000 | -0.72021200 |
| C    | 1.62752900  | -0.71452600 | 0.71999900  |
| N    | 2.71163500  | -0.91232100 | 1.41561100  |
| C    | -0.67627000 | -1.53161700 | -0.71557000 |
| C    | -0.67621000 | -1.53182500 | 0.71511500  |
| C    | -1.50670200 | -2.38355000 | -1.42765800 |
| C    | -2.38727900 | -3.28933400 | -0.72073800 |
| C    | -2.38728100 | -3.28954200 | 0.71976700  |
| C    | -1.50670500 | -2.38396500 | 1.42695300  |
| C    | -3.23487800 | -4.16466400 | -1.40666100 |
| C    | -4.08229700 | -5.04111700 | -0.72104200 |
| C    | -4.08230000 | -5.04132300 | 0.71956100  |
| C    | -3.23488300 | -4.16506800 | 1.40543500  |
| C    | -1.50688500 | -2.37839900 | -2.85413500 |
| C    | -1.51215600 | -2.38017200 | -4.06482500 |
| C    | -1.50689100 | -2.37922500 | 2.85343200  |
### Cartesian coordinates and calculated energy for 6a.

**Table S6.** Cartesian coordinates of the ground state optimized geometry for compound 6a.

The calculated absolute energy value for this molecule is -10150908.72 kJ/mol

|  | X (Å) | Y (Å) | Z (Å) |
|---|-------|-------|-------|
| C | 0.76563500 | 1.82157500 | 0.71538900 |
| C | 0.76555100 | 1.82180600 | -0.71506800 |
| C | 1.62079300 | 2.64962400 | 1.42706500 |
| C | 2.52906500 | 3.52785600 | 0.72091300 |
| C | 2.52892300 | 3.52812700 | -0.72032000 |
| C | 1.62054600 | 2.65013200 | -1.42661800 |
| C | 3.40636700 | 4.37761000 | 1.40123700 |
| C | 4.28509000 | 5.23103700 | 0.72122000 |
| C | 4.28494300 | 5.23131400 | -0.72033500 |
| C | 3.40608300 | 4.37814700 | -1.40049800 |
| C | 1.61916200 | 2.64111400 | 2.85354900 |
| C | 1.62012600 | 2.63614700 | 4.06421300 |
| C | 1.61862400 | 2.64211900 | -2.85310200 |
| C | 1.61932600 | 2.63757500 | -4.06377100 |
| C | 5.18422600 | 6.10320100 | 1.40871400 |
| C | 6.03150700 | 6.92600000 | 0.71349200 |
| C | 6.03136500 | 6.92626900 | -0.71230600 |
| C | 5.18394500 | 6.10373800 | -1.40767300 |
| C | -8.68919300 | 1.56271500 | -0.70398000 |
| C | -8.68916500 | 1.56272400 | 0.70466300 |
| C | -7.50057400 | 1.56490700 | 1.40415100 |
| C | -6.24972000 | 1.55982300 | 0.71856700 |
| C | -6.24975100 | 1.55986000 | -0.71796900 |
| C | -7.50062700 | 1.56491900 | -1.40350800 |
| C | -5.03797000 | 1.54422100 | 1.43487300 |
| C | -3.82315500 | 1.39489400 | 0.72400600 |
| C | -3.82314000 | 1.39488800 | -0.72353300 |
| C | -5.03803200 | 1.54435600 | -1.43432200 |
| C | -7.55749200 | 1.54193700 | 2.88859400 |
| N | -6.33029200 | 1.58824900 | 3.54648000 |
| C | -5.06977100 | 1.71049900 | 2.92245300 |
| C | -5.06989500 | 1.71077200 | -2.92188600 |
| N | -6.33042200 | 1.58847100 | -3.54587800 |
| C | -7.55758900 | 1.54192000 | -2.88795200 |
| O | -8.61842700 | 1.49839000 | 3.49739600 |
| O | -4.09685200 | 1.95011700 | 3.61295800 |
| O | -4.09701100 | 1.95057600 | -3.61237600 |
| O | -8.61853500 | 1.49820900 | -3.49672200 |
|     |          |          |          |
|-----|----------|----------|----------|
| C   | -1.58044400 | -2.40427700 | 2.85270400 |
| C   | -1.58131800 | -2.40155000 | 4.06355200 |
| C   | -5.14004300 | -5.87168400 | -1.40926700 |
| C   | -5.98627400 | -6.69560000 | -0.71405600 |
| C   | -5.98643300 | -6.69568300 | 0.71167900 |
| C   | -5.14035200 | -5.87185400 | 1.40717400 |
| C   | -0.22227600 | 0.89089400  | 1.40378800 |
| C   | -0.22236100 | 0.89122200  | -1.40357700 |
| C   | 0.25888700  | -0.64990600 | 1.40376200 |
| C   | 0.25900000  | -0.64949800 | -1.40397200 |
| H   | 3.40475200  | 4.37373400  | 2.48687700 |
| H   | 3.40424300  | 4.37467500  | -2.48613800 |
| H   | 1.62160800  | 2.61086800  | 5.13044700 |
| H   | 1.62062400  | 2.61259500  | -5.13001400 |
| H   | 5.18141900  | 6.10052800  | 2.49590400 |
| H   | 6.71078700  | 7.58562400  | 1.24649200 |
| H   | 6.71054600  | 7.58609000  | -1.24518900 |
| H   | 5.18092600  | 6.10147300  | -2.49486300 |
| H   | -9.61773800 | 1.55083500  | -1.26429900 |
| H   | -9.61768900 | 1.55086600  | 1.26494900 |
| H   | -6.03650500 | 2.66084800  | 5.34216200 |
| H   | -7.33404900 | 1.42912600  | 5.35529600 |
| H   | -5.60533800 | 0.94398300  | 5.40732400 |
| H   | -5.60515400 | 0.94469600  | -5.40675500 |
| H   | -7.33413600 | 1.42889800  | -5.35468400 |
| H   | -6.03727600 | 2.66132200  | -5.34152800 |
| H   | 9.40320900  | 2.89949600  | 1.26444500 |
| H   | 9.40346600  | 2.89844100  | -1.26480000 |
| H   | 5.40302500  | 2.27672800  | -5.40439200 |
| H   | 6.31622300  | 0.75974300  | -5.34905800 |
| H   | 7.19782200  | 2.31686200  | -5.35347800 |
| H   | 6.31476500  | 0.76370900  | 5.34969000 |
| H   | 5.40227000  | 2.28115700  | 5.40385800 |
| H   | 7.19707300  | 2.32045600  | 5.35316300 |
| H   | -3.36247300 | -4.14059900 | -2.48709700 |
| H   | -3.36296200 | -4.14097800 | 2.48561000 |
| H   | -1.57576800 | -2.38066000 | -5.13084600 |
| H   | -1.57649000 | -2.38164800 | 5.12997900 |
| H   | -5.13718700 | -5.86924100 | -2.49645100 |
| H   | -6.66460500 | -7.35612100 | -1.24707100 |
| H   | -6.66489000 | -7.35626000 | 1.24446600 |
| H   | -5.13773500 | -5.86953900 | 2.49435900 |
| H   | -0.33994300 | 1.17894500  | 2.44773900 |
| H   | -0.34018100 | 1.17951000  | -2.44743600 |
The calculated absolute energy value for this molecule is -12187638.65 kJ/mol.

|   |      |      |      |
|---|------|------|------|
| C | 1.16232500 | -1.53551900 | -0.71559700 |
| C | 1.16238400 | -1.53572300 | 0.71506800  |
| C | 2.19282800 | -2.12912800 | -1.42834000 |
| C | 3.28648100 | -2.76055200 | -0.72076500 |
| C | 3.28653800 | -2.76075900 | 0.71972000  |
| C | 2.19294200 | -2.12953600 | 1.42760500  |
| C | 4.34192700 | -3.36914700 | -1.40678800 |
| C | 5.39764300 | -3.97860800 | -0.72119400 |
| C | 5.39769900 | -3.97881500 | 0.71963600  |
| C | 4.34203600 | -3.36955000 | 1.40548600  |
| C | 2.19401100 | -2.11879400 | -2.85423600 |
| C | 2.20138800 | -2.11178200 | -4.06468800 |
| C | 2.19423800 | -2.11960500 | 2.85346100  |
| C | 2.20172800 | -2.11293400 | 4.06391400  |
| C | 6.48262000 | -4.60283800 | -1.40042600 |
| C | 7.50756400 | -5.19206300 | -0.71250000 |
| C | 7.50761900 | -5.19226700 | 0.71043300  |
| C | 6.48272800 | -4.60324000 | 1.39860700  |
| C | -8.03358500 | -3.70546000 | 0.70428300  |
| C | -8.03366000 | -3.70524300 | -0.70458100 |
| C | -6.88777400 | -3.39063300 | -1.40400500 |
| C | -5.68303600 | -3.05218400 | -0.71872100 |
| C | -5.68295900 | -3.05241300 | 0.71837000  |
| C | -6.88762300 | -3.39107100 | 1.40368000  |
| C | -4.51935600 | -2.71622500 | -1.43596000 |
| C | -3.38417500 | -2.25908500 | -0.72398000 |
| C | -3.38410100 | -2.25931200 | 0.72363200  |
| C | -4.51920100 | -2.71668600 | 1.43558800  |
| C | -6.94918700 | -3.38704800 | -2.88853500 |
| N | -5.75468700 | -3.10381300 | -3.54750300 |
| C | -4.50887300 | -2.87638400 | -2.92558100 |
| C | -4.50855000 | -2.87733500 | 2.92515500  |
| N | -5.75429700 | -3.10493700 | 3.54714500  |
| C | -6.94887600 | -3.38793700 | 2.88821900  |
| O | -7.98302400 | -3.63100900 | -3.49581300 |
| O | -3.50927500 | -2.83290100 | -3.61835400 |
| O | -3.50887400 | -2.83406500 | 3.61782900  |
O      -7.98265200  -3.63206500   3.49553300
C      -5.73435500  -3.17181600  -5.01388200
C      -5.73380300  -3.17340100  -5.01388200
N      -2.29278800  -1.79531000  -1.41410300
C      -1.27341200  -1.37653900  -0.71944400
C      -1.27334700  -1.37674900   0.71916100
N      -2.29265300  -1.79573400   1.41379100
C       7.70028800   4.48595100  -0.70404600
C       7.70034900   4.48574900   0.70466100
C       6.67313700   3.88810300  1.40393300
C       5.58874300   3.26357900   0.71877100
C       5.58868400   3.26378000  -0.71832000
C       6.67301700   3.88850100  -1.40339900
N       5.67193600   3.28622600   3.54769800
C       4.63949800   2.55202400   2.92654800
C       4.63927200   2.55282100  -2.92621400
C       7.63948200   3.93684600  2.88832700
C       5.67157900   3.26226000   3.94670800
N       5.67162800   3.28723600  -3.54724800
C       6.71240700   3.93767400 -2.88778200
O       7.61089300   4.50412900   3.49529200
O       5.70191900   3.23235200   5.01443100
C       5.70154200   3.23379600  -5.01399900
N       2.32624500   1.70297100   1.41371400
C       1.32913400   1.23323000   0.71960500
C       1.32907900   1.23343200  -0.71937900
N       2.32613300   1.70336800 -1.41343600
C      -1.10940800   1.40299100   0.71560800
C      -1.10946200   1.40320000  -0.71513900
C      -2.13885800   1.99914200   1.42766700
C      -3.23165300   2.63162600   0.72073400
C      -3.23170300   2.63337500  -0.71975300
C      -2.13896100   1.99956100 -1.42695100
C      -4.28525500   3.24503700  1.40657400
C      -5.33956900   3.85728000   0.72109800
C      -5.33961800   3.85749300 -0.71961100
C      -4.28535200   3.24545300 -1.40534000
C      -2.13850400   1.99222100   2.85404700
|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| C | -2.144511 | 1.989879  | 4.064690  |
| C | -2.138712 | 1.993054  | -2.853320 |
| C | -2.144803 | 1.991045  | -4.063975 |
| C | -6.422551 | 4.484706  | 1.400372  |
| C | -7.445783 | 5.077081  | 0.712474  |
| C | -7.445831 | 5.077292  | -0.710484 |
| C | -6.422645 | 4.485121  | -1.398626 |
| C | -0.022203 | -0.872825 | -1.403962 |
| C | -0.022086 | -0.873219 | 1.403715  |
| C | 0.074147  | 0.739300  | -1.403669 |
| C | 0.074259  | 0.738904  | 1.403859  |
| H | 4.343959  | -3.368622 | -2.490170 |
| H | 4.344154  | -3.369333 | 2.488869  |
| H | 2.205387  | -2.087708 | -5.131177 |
| H | 2.206031  | -2.089151 | 5.130408  |
| H | -5.161464 | -4.042922 | -5.343021 |
| H | -6.764353 | -3.246755 | -5.354589 |
| H | -5.255236 | -2.275257 | -5.411057 |
| H | -5.254650 | -2.276961 | 5.410906  |
| H | -6.763762 | -3.248457 | 5.354297  |
| H | -5.160865 | -4.044603 | 5.342301  |
| H | 4.722065  | 3.510329  | 5.406339  |
| H | 5.932254  | 2.217614  | 5.350266  |
| H | 6.468601  | 3.924704  | 5.354276  |
| H | 5.931784  | 2.219158  | -5.350156 |
| H | 4.721597  | 3.511880  | -5.405734 |
| H | 6.468114  | 3.926255  | -5.353120 |
| H | -4.287025 | 3.245948  | 2.489973  |
| H | -4.287198 | 3.246681  | -2.488738 |
| H | -2.143001 | 1.974595  | 5.131437  |
| H | -2.143287 | 1.975820  | -5.130723 |
| H | -0.065819 | -1.180568 | -2.448032 |
| H | -0.065618 | -1.181253 | 2.447704  |
| H | 0.119527  | 1.048470  | -2.447191 |
| H | 0.119724  | 1.047787  | 2.447462  |
| F | -8.464393 | 5.666534  | -1.344308 |
| F | -6.435690 | 4.492726  | -2.742141 |
| F | -8.464301 | 5.666135  | 1.346542  |
| F | -6.435507 | 4.491914  | 2.743889  |
| F | 8.528238  | -5.778011 | -1.346616 |
| F | 8.528343  | -5.778397 | 1.344302  |
| F | 6.496188  | -4.610910 | 2.742134  |
| F | 6.495978  | -4.610124 | -2.743956 |
| H | -8.931452 | -3.942741 | 1.264399  |
Table S8. Cartesian coordinates of the ground state optimized geometry for compound 4a.

|    | x         | y         | z          |
|----|-----------|-----------|------------|
| C  | -6.932562 | -0.712572 | -0.25871   |
| C  | -6.93257  | 0.712533  | -0.25869   |
| C  | -5.765402 | 1.404008  | -0.13951   |
| C  | -4.50456  | 0.724377  | -0.02013   |
| C  | -4.50459  | -0.724385 | -0.02013   |
| C  | -5.765386 | -1.404033 | -0.13953   |
| C  | -3.32735  | 1.437065  | 0.098399   |
| C  | -2.072132 | 0.733343  | 0.102471   |
| C  | -2.072129 | -0.73336  | 0.102477   |
| C  | -3.327342 | -1.437063 | 0.098411   |
| C  | -5.826799 | 2.890811  | -0.16597   |
| N  | -4.617721 | 3.54572   | -0.000709  |
| C  | -3.379932 | 2.926356  | 0.25100    |
| C  | -3.379918 | -2.92635  | 0.251048   |
| N  | -4.617668 | -3.54573  | -0.000804  |
| C  | -5.826757 | -2.890838 | -0.16605   |
| O  | -6.875417 | 3.487247  | -0.312134  |
| O  | -2.441616 | 3.614045  | 0.577982   |
| O  | -2.44163  | -3.614013 | 0.578160   |
| O  | -6.875362 | -3.487288 | -0.312244  |
| N  | -0.939684 | 1.415961  | 0.059456   |
| C  | 0.214038  | 0.722776  | 0.0480060  |
| C  | 0.21404  | -0.722774 | 0.048005   |
| N  | -0.939682 | -1.415958 | 0.059459   |
| C  | 1.428609 | 1.415426  | 0.019538   |
| C  | 2.643589 | 0.727733  | 0.001540   |
| C  | 2.643591 | -0.72773  | 0.001540   |
| C  | 1.428611 | -1.415424 | 0.019535   |
| C  | 3.887328 | 1.424544  | -0.016622  |
| C  | 5.105807 | 0.725110  | -0.03344   |
| C  | 5.105809 | -0.725094 | -0.033437  |
| C  | 3.887335 | -1.424534 | -0.016624  |
| C  | 6.349396 | 1.404653  | -0.049765  |
| C  | 7.548094 | 0.724827  | -0.064773  |
| C  | 7.548095 | -0.724808 | -0.064768  |
| C  | 6.349399 | -1.404636 | -0.049758  |
| C  | 3.884361 | 2.852379  | -0.01604   |
| C  | 3.872629 | 4.060045  | -0.015348  |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | 3.88438500| -2.85236900| -0.01601900|
| C       | 3.87275800| -4.06003800| -0.01510900|
| C       | 8.81322600| 1.41191200 | -0.08070100|
| C       | 9.97962800| 0.71959600 | -0.09530200|
| C       | 9.97962900| -0.71957500| -0.09530200|
| C       | 8.81322800| -1.41189200| -0.08068900|
| C       | -4.61827600| 5.06179000| 0.06823000|
| C       | -4.61820700| -5.00619400| 0.06811900|
| H       | -7.85730200| -1.27070800| -0.36239400|
| H       | -7.85731800| 1.27066100 | -0.36234700|
| H       | 1.40166200| 2.49958000 | 0.02085500|
| H       | 1.40166300| -2.49957700| 0.02085300|
| H       | 6.34554100| 2.49060600 | -0.04961100|
| H       | 6.34554300| -2.49058900| -0.04959900|
| H       | 3.85700600| 5.12733300 | -0.01322600|
| H       | 3.85728900| -5.12732900| -0.01310400|
| H       | 8.80670000| 2.49839900 | -0.08056200|
| H       | 10.92827600| 1.24702300 | -0.10734100|
| H       | 10.92827700| -1.24700000| -0.10732800|
| H       | 8.80670300| -2.49837800| -0.08054100|
| H       | -3.82428800| 5.39258200 | -0.57130700|
| H       | -5.59248800| 5.35397000 | -0.26512200|
| H       | -4.42670800| 5.33196100 | 1.09309000|
| H       | -5.59236900| -5.35399900| -0.26536900|
| H       | -3.82412600| -5.39257100| -0.57131700|
| H       | -4.42677400| -5.33199000| 1.09300000|

Table S9. Cartesian coordinates of the ground state optimized geometry for compound Complex.
| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| H    | 0.45910200 | -3.17375800 | 1.11923100 |
| H    | 0.54422000 | 1.76957600 | 1.87142200 |
| C    | 3.00775700 | 0.64908600 | 1.81962800 |
| C    | 2.96360800 | -2.16670000 | 1.38650200 |
| C    | 4.19056700 | -1.50448500 | 1.56840200 |
| C    | 4.21170000 | -0.07193800 | 1.79169800 |
| C    | -3.00743200 | -0.64985100 | -1.82002400 |
| C    | -2.96399500 | 2.16569500 | -1.38592600 |
| C    | -4.19080400 | 1.50342100 | -1.56878000 |
| C    | -4.21156200 | 0.07094500 | -1.79243900 |
| C    | 2.98686300 | 1.34724300 | -1.30682700 |
| C    | -2.98704200 | -1.34667000 | 1.30693900 |
| C    | 2.95726700 | -0.10326700 | -1.52632100 |
| C    | -2.95712200 | 0.10381200 | 1.52638400 |
| C    | 4.19290000 | -0.83961100 | -1.59281600 |
| C    | 4.25800300 | 2.00513700 | -1.14216500 |
| C    | 5.42735300 | -2.19750300 | 1.51075200 |
| H    | 5.41430600 | -3.26889400 | 1.32816900 |
| C    | 5.46188200 | 0.57632100 | -1.95892200 |
| H    | 5.46916300 | 1.65118800 | 2.12374500 |
| C    | -4.25823800 | -2.00433900 | 1.14231800 |
| C    | -4.19256900 | 0.84037100 | 1.59296700 |
| C    | -5.42770200 | 2.19623400 | -1.51159700 |
| H    | -5.41508200 | 3.26760100 | -1.32882500 |
| C    | -5.46152500 | -0.57753500 | -1.96019000 |
| H    | -5.46855200 | -1.65239400 | -2.12506700 |
| C    | -6.65154400 | 0.11484200 | -1.91074800 |
| C    | -6.63372100 | 1.54592300 | -1.67264700 |
| C    | 5.38899600 | -0.17447100 | -1.40703900 |
| C    | 5.41924600 | 1.25570100 | -1.17049300 |
| C    | 6.63355200 | -1.54737900 | 1.67097000 |
| C    | 6.65174000 | -0.11627400 | 1.90902600 |
| C    | -5.41934000 | -1.25464000 | 1.17020700 |
| C    | -5.38876500 | 0.17552900 | 1.40654600 |
| C    | 6.63908300 | -0.88566600 | -1.43717600 |
| C    | 6.69885900 | 1.87208200 | -0.94642300 |
| C    | 7.82823200 | -0.24214100 | -1.28144400 |
| H    | 8.74181700 | -0.82664400 | -1.30153300 |
| C    | 7.89116700 | -2.24171900 | 1.57281400 |
| H    | 7.87647400 | -3.30714200 | 1.36279400 |
| C    | 7.92184600 | 0.54468500 | 2.05899100 |
| H    | 7.92766100 | 1.61936300 | 2.22476000 |
| C    | 9.06408200 | -1.57253400 | 1.70909800 |
| H    | 10.00660200 | -2.10395500 | 1.62274000 |
| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| C    | -6.69901900 | -1.87081700 | 0.94610200 |
| C    | -6.63862700 | 0.88707400  | 1.43592800 |
| C    | -7.85609000 | -1.15681900 | 0.93514000 |
| H    | -8.79412700 | -1.66900100 | 0.83647700 |
| C    | -7.89148500 | 2.24005200  | -1.57514400 |
| H    | -7.87709200 | 3.30547300  | -1.36512100 |
| C    | -7.92144500 | -0.54637600 | 1.43592800 |
| H    | -7.90542000 | 0.15374200  | 1.96574200 |
| C    | -10.03487700| -0.35265100 | 2.07322400 |
| C    | 7.85607900  | 1.15840400  | -0.02403400 |
| C    | 8.79402500  | 1.67075200  | -0.83728000 |
| C    | 9.08076300  | -0.15565700 | 0.96300700 |
| H    | 10.03524300 | 0.35054400  | 2.07012900 |
| C    | -7.82792300 | 0.24382000  | 1.28009000 |
| H    | -8.74135200 | 0.82858000  | 1.29952000 |
| C    | -9.06422200 | 1.57062900  | -1.71941000 |
| H    | -10.00687300| 2.10189800  | -1.62605300 |
| C    | -6.79160300 | -3.29894500 | 0.55201900 |
| C    | -6.64087000 | 2.36764500  | 1.57256000 |
| C    | 6.79123700  | 3.00010300  | -0.55194800 |
| C    | 6.66495800  | -2.36620800 | -1.57432500 |
| N    | 5.59830400  | 4.00135200  | -0.55625800 |
| N    | -5.43476300 | 2.97834100  | 1.73719500 |
| N    | -5.59868500 | -4.00024400 | 0.55598300 |
| N    | 5.43559400  | -2.97732000 | -1.73630500 |
| C    | 4.34214000  | 3.48519100  | -0.93488900 |
| C    | -4.19707300 | 2.31808400  | 1.85391500 |
| C    | 4.19755900  | -2.31758100 | 1.85222200 |
| C    | -4.34269700 | -3.48445900 | 0.93580600 |
| O    | -7.84951100 | -3.81425200 | 0.24007800 |
| O    | -3.42093300 | -4.25724000 | 1.05630900 |
| O    | -3.22482900 | 2.97138200  | 2.14979600 |
| O    | 3.41987700  | 4.25764500  | -1.05385600 |
| O    | 7.84906300  | 3.81543000  | -0.23976200 |
| O    | 7.70421100  | -2.99837900 | -1.53290600 |
| O    | 3.22510600  | -2.97162300 | -2.14577200 |
| O    | -7.70307300 | 3.00013800  | 1.52904500 |
| C    | -5.62587800 | -5.42855000 | 0.25156100 |
| H    | -4.90414300 | -5.64348700 | -0.53849300 |
| H    | -5.34528000 | -6.00245300 | 1.13669000 |
| H    | -6.63369800 | -5.68112100 | -0.06735800 |
| C    | -5.38783600 | 4.42981700  | 1.89799200 |
| H    | -5.06581400 | 4.68241100  | 2.91044600 |
Table S10. Cartesian coordinates of the ground state optimized geometry for T1

|   | [x]       | [y]       | [z]       |
|---|-----------|-----------|-----------|
| C | -0.13104000 | -1.78711600 | 0.54707500 |
| C | -1.38159800 | -1.21426800 | 0.94323100 |
| C | -1.36014100 | 0.16811300  | 1.40366600 |
| C | -0.10431100 | 0.77629800  | 1.64653400 |
| C | 1.11290800  | 0.05299200  | 1.61194600 |
| C | 1.08330000  | -1.32900500 | 1.15081300 |
| C | 1.41301100  | 1.32902600  | -1.32869600 |
| C | 0.20393600  | 2.05158300  | -1.30965800 |
| C | 1.37178800  | -0.11878800 | -1.51003400 |
| C | -1.04641300 | 1.44348800  | -1.53582900 |
| H | 0.24230300  | 3.12969000  | -1.16945600 |
| C | 0.09120300  | -0.78375500 | -1.53785000 |
| C | -1.10920700 | -0.00332200 | -1.71899200 |
| H | 0.07676500  | -1.79863400 | -1.92724000 |
| H | -0.14983900 | -2.81945600 | 0.19970100  |
H  -0.08116700  1.82105800  1.94917300
C   2.33976900  0.61397800  1.94361200
C   2.22937500 -2.08352000  1.17240100
C   3.47725800 -1.55080900  1.61443100
C   3.54211800 -0.14720000  1.94326300
C  -2.33416000 -0.58446500 -1.95878700
C  -2.21479200  2.19158500 -1.57520200
C  -3.48248800  1.59708800 -1.79025100
C  -3.54577600  0.17167000 -1.99984000
C   3.86101200  1.25531500 -1.17173300
C  -3.82945900 -1.21067600  0.99902600
C   3.82665300 -0.17145500 -1.37885500
C  -3.81853300  0.19544900  1.32329300
C   5.01927200 -0.88723600 -1.33855900
C   5.08788900  1.88673100 -0.96203300
C   4.63570800 -2.31804900  1.66070000
H   4.57987300 -3.37895400  1.42214800
C   4.78344700  0.41722100  2.23903300
H   4.84560100  1.48241300  2.45354200
C  -5.04514400 -1.86739000  0.84529900
C  -5.03437800  0.87427000  1.41202900
C  -4.66361900  2.34057900 -1.78338500
H  -4.61177200  3.41740200 -1.63405500
C  -4.78924500 -0.43072000 -2.16481500
H  -4.84469500 -1.50986600 -2.29485500
C  -5.97891500  0.31193600 -2.13431100
C  -5.91360400  1.73258200 -1.94734300
C   6.25050300 -0.25726000 -1.10408600
C   6.28621800  1.16477400 -0.91968300
C   5.87847100 -1.75732000  1.99444800
C   5.95599400 -0.35155400  2.26516800
C  -6.26907500 -1.19181500  0.97120400
C  -6.26068100  0.21717700  1.23605600
C   7.46981300 -0.99040200 -1.01760700
C   7.54492000  1.79498300 -0.68479900
C   8.65590200 -0.35397500 -0.78235700
H   9.57518900 -0.92650000 -0.70388400
C   7.07055900 -2.53605700  2.05718600
H   7.00283700 -3.60358400  1.86168900
C   7.22956500  0.21957400  2.55761600
H   7.28802500  1.29012400  2.73687800
C   8.27164800 -1.95589400  2.35714400
H   9.17294600 -2.55991600  2.40380300
C  -7.52159100 -1.85673900  0.82796000
C  -7.50700100  0.90563300  1.31612300
C  -8.69718200 -1.16592000  0.92762600
H  -9.64544500  2.47800900 -1.92100200
C  -7.13028700  2.47800900 -1.92100200
H  -7.07465300  3.55577900 -2.36809000
C  -7.25789700  0.44001300 -2.21956500
H  -7.30288800 -0.30490900 -2.36809000
C  -8.40278500 -0.30490900 -2.36809000
H  -9.37109900 -0.30490900 -2.36809000
C  -8.69451100  1.05998500 -0.62034500
H  -9.64595600  1.55019600 -0.43665400
C  -9.63090200  0.77368400  1.22595900
C  -8.35321400 -0.55702400  2.82236500
C  -8.33732100  1.85271100 -2.02912400
C  -8.68914700 -0.57702400  1.22595900
C  -8.40278500 -0.30490900 -2.36809000
C  -8.25675300  2.43000100 -2.36809000
H  -2.07384300  4.90599400 -1.21981700
C  -2.07384300  4.90599400 -1.21981700
C  -2.01882500  5.96553600 -1.08109600
C  -2.13560700  3.71653400 -1.37554700
C  -2.18337500  2.14749500 -0.59281800
C  -2.14749500  2.14749500 -0.59281800
C  -2.11553300 -0.57039700  1.54641900
C  -2.09897000  2.09939200  2.34405600
C  -2.01882500  5.96553600 -1.08109600
N  -6.24601300 -4.09807500  0.45692000
N  -6.20903800  3.12976300  1.71243900
N  -6.12862400 -3.19078400 -1.40239100
N  -6.32867300  4.09643800 -0.57265600
N  -2.56068900 -0.81227700 -1.54650200
N  -2.63551400  1.96585200 -1.16670400
N  -2.57984200 -1.85965800  0.76738200
N  -2.56809400  0.84244400  1.53024800
C  -5.04972700 -3.37136500  0.51418300
C  -5.03233000  2.38550700  1.70827100
C  -4.98616600 -2.41630800 -1.51867500
Table S11. Cartesian coordinates of the ground state optimized geometry for M1

|   |   |   |   |
|---|---|---|---|
| C | -0.08278300 | 1.28707700 | 0.81784700 |
| C | 1.16801700 | 0.66497600 | 1.36389200 |
| C | 1.24969900 | -0.77141700 | 1.28747000 |
| C | 0.02732800 | -1.51700900 | 0.82511300 |
| C | -1.23415000 | -0.89368200 | 1.36292200 |
| C | -1.31752200 | 0.53576800 | 1.28455900 |
| C | -1.24970700 | -0.77126100 | -1.28751600 |
| C | -0.02731800 | -1.51690300 | -0.82526400 |
| C | -1.16801800 | 0.66513800 | -1.36381500 |
| C | 1.23416500 | -0.89350100 | -1.36299300 |
| H | -0.12340800 | -2.56210600 | -1.12011900 |
| C | 0.08276800 | 1.28718500 | -0.81770000 |
| C | 1.31750300 | 0.53594600 | -1.28451400 |
| H | 0.13162600 | 2.33371600 | -1.11914900 |
| H | -0.13165200 | 2.33357100 | 1.11942200 |
| H | 0.12342300 | -2.56224800 | 1.11984200 |
|   | x       | y       | z       |
|---|---------|---------|---------|
| C | -2.34258400 | -1.65001400 | 1.66357000 |
| C | -2.52240400 | 1.17186700  | 1.48550600 |
| C | -3.71463300 | 0.41134700  | 1.78875400 |
| C | -3.62151800 | -1.01607600 | 1.88870500 |
| C | 2.52235500  | 1.17210200  | -1.48543900 |
| C | 2.34263700  | -1.64977200 | -1.66366400 |
| C | 3.62155200  | -1.01577300 | -1.88875700 |
| C | 3.71460900  | 0.41164900  | -1.78874500 |
| C | -3.50789200 | -0.64029300 | -1.53272200 |
| C | 3.40955500  | 0.78337700  | 1.70109000 |
| C | -3.40954700 | 0.78359500  | -1.70100400 |
| C | 3.50787800  | -0.64050000 | 1.53270800 |
| C | -4.57633700 | 1.57195500  | -1.72735300 |
| C | -4.76758100 | -1.24773200 | -1.35201600 |
| C | -4.95772400 | 1.02646600  | 1.93482700 |
| H | -5.02623400 | 2.10852900  | 1.85295700 |
| C | -4.77760700 | -1.76082000 | 2.11457800 |
| H | -4.70544400 | -2.84394100 | 2.17502500 |
| C | 4.57636600  | 1.57170900  | 1.72746700 |
| C | 4.76754800  | -1.24795000 | 1.35192400 |
| C | 4.77767800  | -1.76045500 | -2.11464000 |
| H | 4.70556800  | -2.84357700 | -2.17512000 |
| C | 4.95766900  | 1.02681300  | -1.93478800 |
| H | 5.02613000  | 2.10889600  | -1.85287100 |
| C | 6.11755400  | 0.28265600  | -2.17848200 |
| C | 6.02620200  | -1.14552400 | -2.26071700 |
| C | -5.80418100 | 0.97661900  | -1.42337000 |
| C | -5.90260600 | -0.43649800 | -1.23701400 |
| C | -6.11757100 | 0.28222800  | 2.17851700 |
| C | -6.02615400 | -1.14595200 | 2.26071000 |
| C | 5.80419300  | 0.97636900  | 1.42342300 |
| C | 5.90258500  | -0.43673600 | 1.23695300 |
| C | -6.97020100 | 1.77553300  | -1.22850000 |
| C | -7.17213300 | -0.99397000 | -0.90010900 |
| C | -8.17158200 | 1.20364400  | -0.90714900 |
| H | -9.02744900 | 1.85143000  | -0.74688400 |
| C | -7.39394300 | 0.90265400  | 2.34363600 |
| H | -7.45685000 | 1.98636300  | 2.28091900 |
| C | -7.21971800 | -1.90081200 | 2.47546500 |
| H | -7.14983200 | -2.98534200 | 2.50796600 |
| C | -8.51057600 | 0.14734300  | 2.56285800 |
| H | -9.47686000 | 0.62692400  | 2.68691700 |
| C | 6.97023100  | 1.77526500  | 1.22858900 |
| C | 7.17208800  | -0.99421800 | 0.89996800 |
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| C       | 8.17159100   | 1.20336800   | 0.90717000   |
| H       | 9.02747200   | 1.85114400   | 0.74694200   |
| C       | 7.21980800   | -1.90032100  | -2.47546100  |
| H       | 7.14996900   | -2.98485300  | -2.50800200  |
| C       | 7.39390100   | 0.90314800   | -2.34356600  |
| H       | 7.45675600   | 1.98685700   | -2.28080400  |
| C       | 8.51057300   | 0.14789500   | -2.56277600  |
| H       | 9.47683800   | 0.62752500   | -2.68680100  |
| C       | -8.27674400  | -0.19951300  | -0.75276200  |
| H       | -9.21644900  | -0.66695600  | -0.47758800  |
| C       | -8.42389200  | -1.27454900  | 2.61868900   |
| H       | -9.32608500  | -1.85923400  | 2.76735300   |
| C       | 8.27671800   | -0.19978200  | 0.75267000   |
| H       | 9.21641000   | -0.66722500  | 0.47744800   |
| C       | 8.42395700   | -1.27400000  | -2.61864300  |
| H       | 9.32618000   | -1.85863900  | -2.76730200  |
| N       | -2.19076900  | 1.41034900   | -1.63937000  |
| N       | -2.37561800  | -1.40262300  | 1.40141200   |
| N       | 2.19078000   | 1.41015200   | 1.63950800   |
| N       | 2.37559900   | -1.40280300  | 1.40141200   |
| C       | -6.89359900  | 3.25889100   | -1.30322200  |
| C       | -7.31617800  | -2.45081700  | -0.63901000  |
| C       | 7.31607200   | -2.45105000  | 0.63874800   |
| C       | 6.89367000   | 3.25861800   | 1.30343100   |
| C       | 2.63551500   | 2.58258700   | -1.26641200  |
| C       | 2.27341500   | -3.07945300  | -1.62710100  |
| C       | 2.22449500   | -4.28465900  | -1.58155100  |
| H       | 2.17011000   | -5.34932500  | -1.52653400  |
| C       | 2.73417900   | 3.76340600   | -1.03412900  |
| H       | 2.80175900   | 4.80779000   | -0.82317100  |
| C       | -2.27330100  | -3.07968900  | 1.62696400   |
| C       | -2.22435400  | -4.28489300  | 1.58137700   |
| H       | -2.16989700  | -5.34955600  | 1.52638700   |
| C       | -2.63561800  | 2.58236100   | 1.26655700   |
| C       | -2.73433500  | 3.76318800   | 1.03434100   |
| H       | -2.80198100  | 4.80757200   | 0.82340400   |
| N       | -6.14791500  | -3.19536100  | -0.71405100  |
| N       | -5.66070700  | 3.78700700   | -1.66158700  |
| N       | 5.66080500   | 3.78673600   | 1.66188900   |
| N       | 6.14775700   | -3.19553100  | 0.71358700   |
| C       | 4.90929500   | -2.73082600  | 1.19473300   |
| C       | 4.52000500   | 3.03899300   | 2.00401900   |
| C       | -4.51993900  | 3.03925700   | -2.00379900  |
| C       | -4.90936200  | -2.73061300  | -1.19492300  |
|   | x             | y             | z             |
|---|---------------|---------------|---------------|
| O | 4.04600500    | -3.53640400   | 1.45130900    |
| O | 8.38623800    | -2.95686100   | 0.36204100    |
| O | 7.85498900    | 3.96462500    | 1.06729800    |
| O | 3.57604700    | 3.60442200    | 2.50477000    |
| O | -3.57597800   | 3.60469000    | -2.50453900   |
| O | -7.85489500   | 3.96490900    | -1.06703500   |
| O | -4.04598600   | -3.53617600   | -1.45127100   |
| O | -8.38638000   | -2.95659400   | -0.36237500   |
| C | -6.22129000   | -4.63152500   | -0.45887300   |
| H | -6.15367800   | -5.18835200   | -1.39646900   |
| H | -5.37925500   | -4.91715500   | 0.17384600    |
| H | -7.17074400   | -4.83463700   | 0.03049700    |
| C | -5.55047800   | 5.23078100    | -1.85635100   |
| H | -4.67034000   | 5.59721200    | -1.32612000   |
| H | -5.42958100   | 5.46596000    | -2.91811800   |
| H | -6.45700100   | 5.68901100    | -1.46977100   |
| C | 5.55061100    | 5.23049500    | 1.85678500    |
| H | 4.67062600    | 5.59704800    | 1.32638000    |
| H | 5.42946200    | 5.45618700    | 2.91854700    |
| H | 6.45725200    | 5.68871500    | 1.47047000    |
| C | 6.22111600    | -4.63166200   | 0.45823400    |
| H | 6.15437000    | -5.18861900   | 1.39582100    |
| H | 5.37859500    | -4.91730300   | -0.17381800   |
| H | 7.17020400    | -4.83462300   | -0.03191600   |

Table S12. Cartesian coordinates of the ground state optimized geometry for T2
|   |   |   |   |
|---|---|---|---|
| C | 3.36460200 | 0.72880300 | 1.78616100 |
| C | -3.35498800 | 0.79296000 | -1.74780200 |
| C | -3.43016100 | -0.63807000 | -1.63948300 |
| C | 2.43731100 | -1.55440600 | -1.58728600 |
| C | 2.55380500 | 1.26776900 | -1.40380000 |
| C | -2.55957100 | 1.20029600 | 1.46396100 |
| C | -2.42454800 | -1.62576500 | 1.57439100 |
| C | 3.75975300 | 0.53736900 | -1.72248700 |
| C | -3.69409500 | -0.97839400 | 1.81583800 |
| C | 3.69926300 | -0.89090600 | -1.82800000 |
| C | -3.76446800 | 0.45199200 | 1.74618100 |
| C | 4.86791600 | -1.60503900 | -2.09351000 |
| C | 4.98489500 | 1.18374000 | -1.88727400 |
| H | 5.02839800 | 2.26631500 | -1.79567600 |
| C | 4.68039200 | -1.33502000 | 1.48564800 |
| C | 4.54678400 | 1.49451900 | 1.77838800 |
| C | -4.86072800 | -1.70929200 | 2.03803900 |
| H | -4.80681200 | -2.79435000 | 2.07500700 |
| C | -4.99761800 | 1.08346000 | 1.90744400 |
| H | -5.04930400 | 2.16763500 | 1.84427300 |
| C | -4.53423300 | 1.56310500 | -1.74085300 |
| C | -4.67971500 | -1.27102200 | -1.48839700 |
| C | -5.82452000 | -0.48392700 | -1.32141700 |
| C | -5.75054100 | 0.93630200 | -1.45146100 |
| C | 6.09542100 | -0.95754400 | -2.27391600 |
| C | 6.15487100 | 0.47164200 | -2.16993400 |
| C | 5.82199300 | -0.54900800 | 1.30207100 |
| C | 5.75620700 | 0.86916000 | 1.45674100 |
| C | -6.09727400 | -1.07728000 | 2.21007900 |
| C | -6.16681200 | 0.35366900 | 2.14719700 |
| C | 7.29984700 | -1.67861400 | -2.54476200 |
| H | 7.25784400 | -2.76314100 | -2.59475100 |
| C | 7.41213900 | 1.12661200 | -2.35379600 |
| H | 7.45162100 | 2.20954900 | -2.26400400 |
| C | 8.48217900 | -1.01904300 | -2.71306900 |
| H | 9.39148800 | -1.57802700 | -2.90932000 |
| C | 7.05536900 | -1.13771200 | 0.89526600 |
| C | 6.92851000 | 1.63918000 | 1.19892400 |
| C | 8.16571500 | -0.36917000 | 0.67267100 |
| H | 9.07370000 | -0.85510900 | 0.33196600 |
| C | -7.30093300 | -1.81595100 | 2.43046700 |
| H | -7.24918300 | -2.90133600 | 2.45059400 |
| C | -7.43306400 | 0.99216000 | 2.32524300 |
| H | -7.47989100 | 2.07710800 | 2.27006600 |
C   -8.49303600  -1.17200600  2.59124900
H   -9.40190500  -1.74420000  2.74708300
C   -6.92401900   1.70755100 -1.20239300
C   -7.07420700  -1.07447400  -0.96686300
C   -8.18756400  -0.30418200  -0.76575700
H   -9.11003800  -0.79362000  -0.47215300
C    8.53841700   0.40392800 -2.62290100
H    9.48924400   0.90940300 -2.76185800
C    8.10065200   1.03635000  0.82764000
H    8.96016000   1.66266600  0.61313300
C   -8.55904500   0.25369000  2.54606700
H   -9.51691000   0.74577500  2.68000300
C   -8.10977400  1.10490700  0.67948500
H   -8.97086500  1.73181800  0.67237800
H    4.82125300   2.68874900  0.16386400
C   -6.85644200   3.19129700 -1.19645500
C   -7.17654800  -2.53782000 -0.72054000
C    7.13191400  -2.59389900  0.60711600
C    6.88001100   3.12452700  1.23566200
N   -5.63319400   3.75546000 -1.52479700
N    5.66887500   3.68486600  1.61952000
N    5.99082500  -3.33551800  0.87254700
N   -6.00364800  -3.26231900 -0.87916100
N    2.15815500   1.37751000  1.71095600
N    2.29216900  -1.44391000  1.50861600
N   -2.14830400  1.43663500 -1.64498100
N   -2.28968800  -1.38786800 -1.50730000
C   -2.37950400  -3.05463100  1.48854100
C   -2.34897800  -4.25784000  1.39444000
H   -2.30750900  -5.32022000  1.29784700
C   -2.65466800   2.61437500  1.25810000
C   -2.74294000   3.79740100  1.03213300
H   -2.80448500   4.84309800  0.82503400
C    2.40898400  -2.98484000 -1.52556500
C    2.40999700  -4.18920500 -1.44306300
H    2.38216700  -5.25285300 -1.35439300
C    2.63793400   2.67676600  1.16220700
C    2.71014800   3.85562300 -0.91048400
H    2.75329100   4.89790200  0.68320200
C    4.52379100   2.96971800  2.01320200
C    4.79037500  -2.82842800  1.40860600
C   -4.49593600   3.04290900  1.95167800
C   -4.79827700  -2.76083600 -1.40396100
O   -3.56938800   3.62752300 -2.46120100
|  | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| O | -7.81407700 | 3.88756000 | -0.91768400 |
| O | -8.21934000 | -3.06616000 | -0.38611800 |
| O | -3.94202800 | -3.53925600 | -1.75122500 |
| O | 3.92968600  | 3.56647700  | 2.52054300  |
| C | 5.89688800  | 5.13522800  | 1.77406200  |
| H | 4.70025500  | 5.50169900  | 1.25998900  |
| H | 5.05414000  | 3.80723400  | 2.83159800  |
| H | 6.49128800  | 5.56554500  | 1.34629500  |
| C | 6.07180600  | -4.77807200 | 0.65197000  |
| H | 7.09048200  | -5.10424800 | 0.85319800  |
| H | 5.36223500  | -5.26524100 | 1.31593100  |
| H | 5.82121100  | -5.01129500 | -0.38737900 |
| C | -6.04379600 | -4.70753800 | -0.67203200 |
| H | -5.17220300 | -4.99975500 | -0.08421700 |
| H | -6.96766400 | -4.94356200 | -0.15000900 |
| H | -6.00683500 | -5.23007600 | -1.63059100 |
| C | -5.59346000 | 5.21424600  | -1.59298200 |
| H | -4.55445800 | 5.51929200  | -1.68795800 |
| H | -6.16181700 | 5.57076400  | -2.45579400 |
| H | -6.04632500 | 5.61815500  | -0.68768100 |

**Table S13.** Cartesian coordinates of the ground state optimized geometry for M2
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -3.520226 | 0.862967  | -1.430158 |
| C    | -3.626178 | -0.570386 | -1.335880 |
| C    | 2.086690  | -1.586626 | -1.528686 |
| C    | 2.301199  | 1.229312  | -1.306109 |
| C    | -2.342074 | 1.191424  | 2.257519  |
| C    | -2.168353 | -1.633949 | 2.390981  |
| C    | 3.443842  | 0.474116  | -1.769931 |
| C    | -3.355712 | -0.981695 | 2.892874  |
| C    | 3.331221  | -0.949972 | -1.896374 |
| C    | -3.450610 | 0.446236  | 2.808467  |
| C    | 4.444829  | -1.689237 | -2.291518 |
| C    | 4.663138  | 1.090363  | -2.047945 |
| H    | 4.747344  | 2.169112  | -1.941311 |
| C    | 4.819232  | -1.322480 | 1.194856  |
| C    | 4.724649  | 1.486390  | 1.666320  |
| C    | -4.425722 | -1.706918 | 3.411931  |
| H    | -4.353068 | -2.789568 | 3.465536  |
| C    | -4.611982 | 1.080859  | 3.244288  |
| H    | -4.680155 | 2.163158  | 3.175017  |
| C    | -4.641680 | 1.633560  | -1.793197 |
| C    | -4.860550 | -1.202949 | -1.569083 |
| C    | -5.944565 | -0.439103 | -2.022614 |
| C    | -5.833717 | 0.979954  | -2.140400 |
| C    | 5.667602  | -1.072272 | -2.578156 |
| C    | 5.779177  | 0.351989  | -2.456446 |
| C    | 5.944239  | -0.524526 | 0.957075  |
| C    | 5.897174  | 0.882073  | 1.200968  |
| C    | -5.588870 | -1.071848 | 3.856370  |
| C    | -5.684772 | 0.355556  | 3.770187  |
| C    | 6.818416  | -1.820760 | -2.973715 |
| H    | 6.737750  | -2.902882 | -3.039932 |
| C    | 7.029928  | 0.974699  | -2.753932 |
| H    | 7.107729  | 2.055029  | -2.658270 |
| C    | 7.999592  | -1.192307 | -3.243047 |
| H    | 8.870483  | -1.773651 | -3.528082 |
| C    | 7.146602  | -1.089665 | 0.436489  |
| C    | 7.048755  | 1.667531  | 0.896758  |
| C    | 8.240194  | -0.308079 | 0.179597  |
| H    | 9.127220  | -0.777350 | -0.232799 |
| C    | -6.692846 | -1.805061 | 4.392551  |
| H    | -6.613155 | -2.887011 | 4.455566  |
| C    | -6.880633 | 0.994413  | 4.223585  |
| H    | -6.946558 | 2.077070  | 4.156123  |
| C    | -7.817947 | -1.160378 | 4.814829  |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | -8.651177 | -1.725402 | 5.221082  |
| C    | -6.959694 | 1.711565  | -2.617207 |
| C    | -7.171655 | -1.063531 | -2.390148 |
| C    | -8.231238 | -0.327037 | -2.850362 |
| H    | -9.140246 | -0.847966 | -3.131863 |
| C    | 8.104404  | 0.226126  | -3.140966 |
| H    | 9.051606  | 0.708013  | -3.363960 |
| C    | 8.187749  | 1.088100  | 0.405531  |
| H    | 9.032593  | 1.725992  | 0.167369  |
| C    | -7.913414 | 0.260929  | 4.728814  |
| H    | -8.817761 | 0.754708  | 5.070669  |
| C    | -8.124221 | 1.077281  | -2.963185 |
| H    | -8.949539 | 1.677150  | -3.319900 |
| H    | 4.360790  | -2.770007 | -2.374806 |
| C    | -6.892176 | 3.187831  | -2.778374 |
| C    | -7.324946 | -2.541674 | -2.313892 |
| C    | 7.223221  | -2.537084 | 0.103674  |
| C    | 7.018263  | 3.147021  | 1.044947  |
| N    | -5.703220 | 3.786580  | -2.385951 |
| N    | 5.843479  | 3.683301  | 1.553880  |
| N    | 6.064260  | -3.268299 | 0.320350  |
| N    | -6.235751 | -3.240790 | -1.813917 |
| N    | 2.340066  | 1.362395  | 1.843959  |
| N    | 2.451660  | -1.447827 | 1.527093  |
| N    | -2.327455 | 1.487648  | -1.160999 |
| N    | -2.523302 | -1.335356 | -1.041204 |
| C    | -2.110591 | -3.064191 | 2.357985  |
| C    | -2.058815 | -4.269372 | 2.327366  |
| H    | -2.016448 | -5.334849 | 2.284471  |
| C    | -2.483353 | 2.594266  | 2.015117  |
| C    | -2.609749 | 3.758097  | 1.720999  |
| H    | -2.730075 | 4.773730  | 1.415359  |
| C    | 2.017791  | -3.016822 | -1.513134 |
| C    | 1.972064  | -4.222658 | -1.482044 |
| H    | 1.921800  | -5.287978 | -1.436697 |
| C    | 2.449094  | 2.633351  | -1.066576 |
| C    | 2.583951  | 3.807479  | -0.819311 |
| H    | 2.685244  | 4.845447  | -0.591037 |
| C    | 4.729082  | 2.944655  | 1.991386  |
| C    | 4.916373  | -2.802801 | 0.989454  |
| C    | -4.611287 | 3.133405  | -1.786489 |
| C    | -5.060780 | -2.663997 | -1.299947 |
| O    | -3.727649 | 3.805802  | -1.307556 |
| O    | -7.824385 | 3.830704  | -3.218820 |
Table S14. Cartesian coordinates of the ground state optimized geometry for T3

| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| O    | -8.346922 | -3.099890 | -2.660439 |
| O    | -4.294284 | -3.356598 | -0.673347 |
| O    | 4.090119  | -3.604738 | 1.355538  |
| O    | 8.232607  | -3.046128 | -0.343378 |
| O    | 7.967129  | 3.843414  | 0.739584  |
| O    | 3.854992  | 3.510048  | 2.606188  |
| C    | 5.788086  | 5.120960  | 1.812678  |
| H    | 5.465200  | 5.181310  | 2.350570  |
| H    | 6.076039  | -4.697314 | 0.019375  |
| H    | 5.108490  | -5.280179 | 0.941840  |
| H    | 5.043300  | -4.952902 | -0.495787 |
| H    | 5.812854  | -5.308254 | 2.888436  |
| H    | 6.502711  | -5.417682 | 1.153567  |
| H    | 5.703160  | 5.673837  | -2.891805 |
| H    | 5.082111  | 5.243712  | -2.456015 |
| C    | -0.137445 | -1.540586 | -0.220118 |
| C    | 1.078218  | -1.015478 | -0.949516 |
| C    | 1.169123  | 0.409359  | -1.085858 |
| C    | -0.018584 | 1.239008  | -0.621022 |
| C    | -1.298902 | 0.557124  | -1.004108 |
| C    | -1.372498 | -0.864467 | -0.763646 |
| C    | -1.229544 | 0.822301  | 1.664917  |
| C    | -0.038790 | 1.471995  | 0.988971  |
| C    | -1.152120 | -0.580330 | 1.942045  |
| C    | 1.247960  | 0.906007  | 1.515710  |
| C    | 0.045393  | -1.306149 | 1.383923  |
| C    | 1.310168  | -0.528313 | 1.640815  |
| C    | -3.554450 | -0.844689 | -1.423454 |
| C    | -3.494423 | 0.583411  | -1.602041 |
| C    | 3.511003  | 1.023167  | 1.633974  |
| C    | 3.581312  | -0.412073 | 1.669436  |
| C    | -2.196402 | -1.238010 | 2.547490  |
| C    | -2.386220 | 1.519909  | 1.925978  |
| C    | 2.350457  | 0.993427  | -1.486933 |
C  2.15413500  -1.82217000  -1.23739200
C  -3.49860700   0.87103400   2.58018900
C   3.40282400  -1.24532300  -1.68098600
C  -3.39395100  -0.51855000   2.91663800
C   3.50536700   0.18019300  -1.79745100
C  -4.46428700  -1.14912100   3.54770100
H  -4.38313700  -2.20301900   3.79908900
C  -4.67173100   1.56047200   2.87997300
H  -4.74698800   2.61262200   2.61890000
C  -4.75856000  -1.53387500  -1.65579000
C  -4.65385200   1.30860400  -1.94372600
C   4.52808500  -2.03222100  -1.92057700
C   4.45155600  -3.11162800  -1.81604900
C   4.72610900   0.74909100  -2.15907900
H   4.80358000   1.83066800  -2.23976200
C   4.67913600   1.78101800   1.42359800
C   4.81136200  -1.06669800   1.45573300
C   5.93170400  -0.30686600   1.09895100
C   5.86245700   1.11973900   1.08131400
C  -5.63944600  -0.45771200   3.85617600
C  -5.74685700   0.92942000   3.51225600
C  -5.91840200  -0.80299400  -1.94954500
C  -5.86673900   0.61808300  -2.09412500
C   5.75206300  -1.46389300  -2.28944500
C   5.85207200  -0.03979800  -2.41948200
C  -6.74487500  -1.09474600   4.50098800
H  -6.65713700  -2.14649800   4.75985100
C  -6.95508200   1.62591600   3.82606500
H  -7.02905300   2.67784700   3.56351000
C  -7.88253400  -0.39762400   4.78283700
H  -8.71684900  -0.89019600   5.27223700
C  -7.17688600  -1.46011300  -2.08076900
C  -7.07482600   1.31098200  -2.39823100
C  -8.31835400  -0.75708000  -2.36175000
H  -9.25487400  -1.29882900  -2.44102100
C   6.91430200  -2.25992200  -2.52728900
H   6.84190600  -3.33711000  -2.39934800
C   7.10206400   0.53180400  -2.80934800
H   7.17088400   1.61265200  -2.90695200
C   8.09490300  -1.67840400  -2.88888100
H   8.97425100  -2.29240500  -3.05538700
C   7.00259100   1.85420600   0.63913900
C   7.15000100  -0.93640600   0.70434000
C   8.23392400  -0.19743700   0.31430200
| Atom | x       | y       | z       |
|------|---------|---------|---------|
| H    | 9.130671 | -0.72173 | 0.000856 |
| C    | -7.989333 | 0.983593 | 4.440177 |
| H    | -8.903231 | 1.520462 | 4.674168 |
| C    | -8.264061 | 0.643755 | -2.532315 |
| H    | -9.155429 | 1.217862 | -2.761612 |
| C    | 8.187551  | -0.263666 | -3.041766 |
| H    | 9.133825  | 0.179148 | -3.338022 |
| C    | 8.156545  | 1.215517 | 0.273661 |
| H    | 8.991344  | 1.813490 | -0.077485 |
| H    | -0.254361 | -2.614876 | -0.365099 |
| H    | 0.005633  | 2.228369 | -1.078440 |
| H    | -0.052366 | 2.550652 | 1.146667 |
| H    | 0.156907  | -2.297094 | 1.824706 |
| C    | -7.084098 | 2.786774 | -2.570948 |
| C    | -7.293796 | -2.930140 | -1.882624 |
| C    | 6.929515  | 3.330193 | 0.488160 |
| C    | 7.249835  | -2.418511 | 0.637242 |
| C    | 2.491056  | 2.418358 | -1.469481 |
| C    | 2.621493  | 3.616946 | -1.400378 |
| H    | 2.720646  | 4.677837 | -1.329489 |
| C    | 2.093623  | -3.228922 | -0.978203 |
| C    | 2.057268  | -4.411817 | -0.740606 |
| H    | 2.012747  | -5.454474 | -0.516186 |
| C    | -2.528824 | 2.861393 | 1.450115 |
| C    | -2.654066 | 3.959718 | 0.964710 |
| H    | -2.766604 | 4.911853 | 0.494883 |
| C    | -2.126993 | -2.650857 | 2.772827 |
| C    | -2.067822 | -3.841917 | 2.958617 |
| H    | -2.009739 | -4.896032 | 3.115738 |
| N    | 6.095866  | -3.117342 | 0.961279 |
| N    | 5.744838  | 3.933866 | 0.880079 |
| N    | -5.861143 | 3.420993 | -2.414002 |
| N    | -6.109867 | -3.604340 | -1.624211 |
| C    | 4.926960  | -2.558599 | 1.511788 |
| C    | 4.655378  | 3.275343 | 1.483083 |
| C    | -4.634833 | 2.800849 | -2.112460 |
| C    | -4.825913 | -3.032018 | -1.632143 |
| O    | 8.272770  | -2.984359 | 0.303228 |
| O    | 4.097916  | -3.295917 | 1.990480 |
| O    | 7.852154  | 3.988496 | 0.046960 |
| O    | 3.779480  | 3.913812 | 2.016862 |
| O    | -3.653758 | 3.500634 | -2.007407 |
| O    | -8.101591 | 3.397447 | -2.832923 |
| O    | -3.862230 | -3.760886 | -1.631363 |
| Element | X     | Y     | Z     |
|---------|-------|-------|-------|
| O       | -8.36263800 | -3.50389500 | -1.95071300 |
| C       | 6.12910400   | -4.57636000  | 0.90742900  |
| H       | 6.19312200   | -4.99480200  | 1.91475400  |
| H       | 5.20607400   | -4.92886000  | 0.44413700  |
| H       | 6.99973300   | -4.86079000  | 0.32518200  |
| C       | 5.71263500   | 5.39251100   | 0.90742900  |
| H       | 6.19312200   | -4.99480200  | 1.91475400  |
| H       | 5.20607400   | -4.92886000  | 0.44413700  |
| H       | 6.99973300   | -4.86079000  | 0.32518200  |

Table S15. Cartesian coordinates of the ground state optimized geometry for Dimer
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | -1.95669500 | 2.11164600 | -1.68546500 |
| C       | 3.69657500  | 1.43774200 | -0.86286000 |
| C       | 0.12413500  | 1.02500400 | 1.29462300  |
| C       | -2.01302700 | 2.36881100 | 1.13631600  |
| C       | -3.03079900 | 2.85758000 | -1.07160300 |
| C       | 3.69498700  | 1.54475700 | 0.57317700  |
| H       | 0.20270300  | 1.44790900 | 2.29650600  |
| C       | -3.06276500 | 2.98181100 | 0.35605700  |
| C       | 4.09038700  | -3.18716400| 1.74166300  |
| C       | 5.11684800  | -3.91547100| 1.13400900  |
| C       | 5.09341800  | -4.10584900| -0.28627100 |
| C       | -4.91968800 | -1.36657000| 1.60690200  |
| C       | -6.10651500 | -1.66754100| 0.91977300  |
| C       | -6.08745700 | -1.93938700| -0.48334000 |
| C       | -4.10884400 | 3.67958800 | 0.95720600  |
| C       | -5.12489400 | 4.26622700 | 0.19793900  |
| C       | -5.09230700 | 4.14278100 | -1.22954800 |
| C       | 4.90759400  | 1.69840600 | 1.27170600  |
| C       | 6.11484300  | 1.65947700 | 0.55919200  |
| C       | 6.11351900  | 1.58357300 | -0.86709800 |
| C       | -4.04500100 | 3.43851600 | -1.83011100 |
| C       | -4.88219100 | -1.91668800| -1.19869300 |
| C       | 4.04551500  | -3.55835500| -1.03151500 |
| C       | 4.90590100  | 1.53017800 | -1.57582900 |
| H       | -4.01794700 | 3.34031100 | -2.91177400 |
| H       | -4.13059600 | 3.76896700 | 2.03979500  |
| H       | 4.10386400  | -3.04018500| 2.81809000  |
| H       | 4.02615400  | -3.69820900| -2.10878500 |
| C       | -7.32075100 | -2.20979800| -1.14563800 |
| C       | -8.50474600 | -2.23740900| -0.45769200 |
| H       | -9.41861600 | -2.43841000| -1.00649000 |
| C       | -8.52083300 | -2.00221900| 0.93468000  |
| C       | -6.20122600 | 4.98731500 | 0.80276700  |
| C       | -7.18057900 | 5.54769500 | 0.03710700  |
| C       | -7.14809900 | 5.42462400 | -1.38442900 |
| C       | 6.19379500  | -4.47787300| 1.88726600  |
| C       | 7.18283900  | -5.18291800| 1.26757700  |
| C       | 7.16032800  | -5.37173800| -0.14681700 |
| C       | 7.36744000  | 1.68359500 | 1.23803400  |
| C       | 8.54973000  | 1.63662000 | 0.54697000  |
| C       | 8.54760700  | 1.56268800 | -0.86431400 |
| C       | -7.35720200 | -1.72203500| 1.60165800  |
| C       | 6.14893000  | -4.85085900| -0.89872800 |
| C       | 7.36258600  | 1.53783800 | -1.55149600 |
| Atoms | X      | Y      | Z      |
|-------|--------|--------|--------|
| C     | -6.13737800 | 4.74469500 | -1.99713700 |
| H     | -9.44578600  | -2.03021100 | 1.50071700  |
| H     | -6.21980900  | 5.07795400  | 1.88551300  |
| H     | -7.99423600  | 6.09242500  | 0.50570700  |
| H     | -7.93737200  | 5.87906200  | -1.97516000 |
| H     | -6.10618500  | 4.64763200  | -3.07901900 |
| H     | 6.20475800   | -4.33063300 | 2.96379800  |
| H     | 7.99679200   | -5.60685000 | 1.84740300  |
| H     | 7.95802400   | -5.93479100 | -0.62117100 |
| H     | 6.12578400   | -4.99175000 | -1.97599200 |
| H     | 9.47766400   | 1.64391300  | 1.10890400  |
| H     | 9.47371400   | 1.51041800  | -1.42691500 |
| C     | -7.36323000  | -2.44179000 | -2.61465300 |
| C     | -7.43872900  | -1.47644600 | 3.06535000  |
| C     | 7.42488200   | 1.72628200  | 2.72367300  |
| C     | 4.93494400   | 1.59514800  | -3.07269400 |
| C     | 1.96523400   | -2.34757800 | -2.61827000 |
| C     | 1.98300000   | -2.41704900 | -3.82304400 |
| H     | 1.99207500   | -2.46910800 | -4.88908100 |
| C     | 2.05223500   | -1.60191800 | 3.02206000  |
| C     | 2.11553700   | -1.32754500 | 4.19529400  |
| H     | 2.16647800   | -1.06627500 | 5.22949100  |
| C     | -1.96119200  | 1.90969200  | -3.10326100 |
| C     | -1.96565200  | 1.72923300  | -4.29654800 |
| H     | -1.96377800  | 1.56011400  | -5.35037800 |
| C     | -2.09258000  | 2.39047400  | 2.56528600  |
| C     | -2.16993000  | 2.36797800  | 3.76938900  |
| H     | -2.24169800  | 2.32450200  | 4.83345500  |
| N     | -2.53800900  | -1.40734400 | -1.25534900 |
| N     | -2.53909900  | -1.02394300 | 1.54591400  |
| N     | 2.53038600   | 1.19119900  | -1.54500500 |
| N     | 2.51750700   | 1.45353100  | 1.27376500  |
| N     | 6.18794400   | 1.42135200  | -3.68585200 |
| N     | 6.20255300   | 1.79592400  | 3.37576900  |
| N     | -6.23978500  | -1.18563200 | 3.69696100  |
| C     | -4.97915000  | -1.08069500 | 3.08054500  |
| C     | -4.88321400  | -2.31615200 | -2.64497500 |
| C     | 4.94430500   | 1.90628300  | 2.75646500  |
| C     | 7.41316000   | 1.42386400  | -3.03431200 |
| O     | 8.46554200   | 1.34692100  | -3.63672300 |
| O     | 3.96768200   | 1.79865800  | -3.76793700 |
| O     | 8.47947300   | 1.70750700  | 3.32711900  |
| O     | 3.98142700   | 2.16166900  | 3.44048400  |
| O     | -3.89119800  | -2.55109100 | -3.29362000 |
|   |   |   |
|---|---|---|
| O | -8.40820700 | -2.63395900 | -3.20412500 |
| O | -8.49293600 | -1.52927100 | 3.66781700 |
| O | -4.03271300 | -0.76985000 | 3.76508600 |
| C | 6.19916400 | 1.91208000 | 4.83287000 |
| H | 5.91062600 | 2.92340700 | 5.12797900 |
| H | 5.47191800 | 1.21116600 | 5.24361800 |
| H | 7.20203200 | 1.68625700 | 5.18575000 |
| C | 6.17801100 | 1.40505600 | -5.14750000 |
| H | 5.89928900 | 2.38912600 | -5.53135800 |
| H | 7.17594200 | 1.13629300 | -5.48387400 |
| H | 5.43999700 | 0.67931900 | -5.48998900 |
| C | -6.11033700 | -2.73358900 | -4.69593600 |
| H | -5.46453800 | -2.01272700 | -5.19796200 |
| H | -5.70391300 | -3.73428200 | -4.85928300 |
| H | -7.12933300 | -2.67249300 | -5.06890500 |
| C | -6.25584900 | -0.92156400 | 5.13484500 |
| H | -5.56505800 | -1.60150000 | 5.63585100 |
| H | -5.92873500 | 0.10276300 | 5.32391300 |
| H | -7.27251400 | -1.07140500 | 5.48806400 |
| N | -6.13917500 | -2.43152200 | -3.26583400 |