Supporting Information For

**Aromatic Heterobicycle-Fused Porphyrins: Impact on Aromaticity and Excited State Electron Transfer Leading to Long-Lived Charge Separation**

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General Experimental Information

Chemicals

Reagents were purchased from commercially available sources and used without further purification. Buckminsterfullerene, C_{60} (+99.95%), was obtained from SES Research, (Houston, TX). Tetra-n-butylammonium perchlorate, (n-Bu_4N)ClO_4, used in electrochemical studies was from Fluka Chemicals. Silica gel with pore size 43 – 63 μm was used when purification of compounds through column chromatography was performed. Synthesis of dialdehydebeinzoporphyrin was done using a previously published procedure.¹

Spectral measurements

NMR spectroscopy experiments were performed using a 500 MHz Varian NMR instrument. All NMR experiments were conducted using CDCl_3 passed through a pad of alumina as a solvent (δ ¹H = 7.26 ppm; δ ¹³C = 77.16 ppm). Mass spectrometry experiments were done using a Thermoscientific MALDI-LTQ-XL-Orbitrap mass spectrometer. UV/Vis data was obtained using either a CARY 5000 spectrometer or a Shimadzu Model 2550 double monochromator UV-visible spectrophotometer. The fluorescence emission was monitored by using a Horiba Yvon Nanolog coupled with time-correlated single-photon counting with nanoLED excitation sources. Degassed toluene was used as solvent for all luminescence and lifetime experiments. A right angle detection method was used. Differential pulse voltammograms were recorded on an EG&G PARSTAT electrochemical analyser using a three-electrode system. A platinum button electrode was used as the working electrode. A platinum wire served as the counter electrode and an Ag/AgCl electrode was used as the reference electrode. Ferrocene/ferrocenium redox couple was used as an internal standard. All the solutions were purged prior to electrochemical and spectral measurements using nitrogen gas.

Femtosecond Transient Absorption Spectroscopy. Femtosecond transient absorption spectroscopy experiments were performed using an Ultrafast Femtosecond Laser Source (Libra) by Coherent incorporating diode-pumped, mode locked Ti:Sapphire laser (Vitesse) and diode-pumped intra cavity doubled Nd:YLF laser (Evolution) to generate a compressed laser output of 1.45 W. For optical detection, a Helios transient absorption spectrometer coupled with femtosecond harmonics generator both provided by Ultrafast Systems LLC was used. The source for the pump and probe pulses were derived from the fundamental output of Libra (Compressed output 1.45 W, pulse width 100 fs) at a repetition rate of 1 kHz. 95% of the fundamental output of the laser was introduced into a TOPAS-Prime-OPA system with 290-2600 nm tuning range from Altos Photonics Inc., (Bozeman, MT), while the rest of the output was used for generation of white light continuum. Kinetic traces at appropriate wavelengths were assembled from the time-resolved spectral data. Data analysis was performed using Surface Xplorer software supplied by Ultrafast Systems. All measurements were conducted in degassed solutions at 298 K. The estimated error in the reported rate constants is ±10%.
Nanosecond Laser Flash Photolysis. The studied compounds were excited by an Opolette HE 355 LD pumped by a high energy Nd:YAG laser with third harmonics OPO (tuning range 410-2200 nm, pulse repetition rate 20 Hz, pulse length 7 ns) with the powers of 1.0 to 3 mJ per pulse. The transient absorption measurements were performed using a Proteus UV-Vis-NIR flash photolysis spectrometer (Ultrafast Systems, Sarasota, FL) with a fiber-optic delivered white probe light and either a fast rise Si photodiode detector covering the 200-1000 nm range or an InGaAs photodiode detector covering 900-1600 nm range. The output from the photodiodes and a photomultiplier tube was recorded with a digitizing Tektronix oscilloscope. Data analysis was performed using Surface Xplorer software supplied by Ultrafast Systems.

Synthesis

β,β'-Benzimidazole-Fused Free-Base Benzoporphyrin (AMIm-1)

Monobenzodialdehyde porphyrin (50 mg, 0.043 mmol) was combined with o-phenylenediamine (4.7 mg, 0.043 mmol), DCM (5 mL) and formic acid (1.25 mL) and stirred at room temperature for 1 hour. The reaction mixture was then quenched by addition of triethylamine (1.5 mL), filtered, and washed with methanol to yield 41.7 mg (79% yield) pure AMIm-1.

\[ \text{H NMR (500 MHz, CDCl}_3 \] δ 8.97 (d, J = 2.9 Hz, 2H), 8.93 (d, J = 1.8 Hz, 2H), 8.12 (s, 2H), 8.11 (d, J = 1.7 Hz, 1H), 8.09 (t, J = 1.6 Hz, 6H), 7.99 (t, J = 1.8 Hz, 1H), 7.87 (dd, J = 6.2, 2.8 Hz, 1H), 7.79 (t, J = 1.8 Hz, 2H), 7.61 (s, 1H), 7.45 (dd, J = 6.2, 2.7 Hz, 1H), 7.27 – 7.26 (m, 1H), 7.25 (t, J = 1.4 Hz, 1H), 6.90 (s, 1H), 4.93 (s, 2H), 1.60 (d, J = 1.0 Hz, 16H), 1.55 (s, 14H), 1.53 (s, 42H).

\[ \text{C NMR (126 MHz, CDCl}_3 \] δ 159.16, 150.95, 149.39, 149.17, 142.43, 141.72, 141.50, 141.30, 134.31, 133.41, 129.98, 128.94, 128.82, 128.35, 127.77, 122.70, 122.66, 122.62, 122.59, 122.14, 121.98, 121.44, 121.43, 121.28, 120.37, 119.31, 119.01, 118.69, 109.45, 47.40, 35.71, 35.64, 35.46, 32.20, 32.15. UV/Vis (Toluene): \( \lambda_{\text{max}} \) (log ε) = 436 (5.70), 522 (4.59), 599 (4.08), 652 (3.11), nm; HRMS (MALDI): m/z: calculated for C_{88}H_{100}N_{6}: 1240.800; found: 1240.7967

β,β'-Benzimidazole-Fused Zinc Benzoporphyrin (AMIm-2)

AMIm-1 (10 mg, 0.0081 mmol) was combined with zinc acetate (14.8 mg, 0.081 mmol) chloroform (1.5 mL) and methanol (0.5 mL) and refluxed for 1 hour. The reaction mixture was then cooled to room temperature and recrystallized with methanol to yield 9.7 mg (92% yield) pure AMIm-2.

\[ \text{H NMR (500 MHz, CDCl}_3 \] δ 9.02 (dd, J = 4.6, 3.1 Hz, 2H), 8.94 (d, J = 4.6 Hz, 1H), 8.93 (s, 2H), 8.92 (d, J = 4.6 Hz, 1H), 8.12 (s, 3H), 8.10 (t, J = 1.8 Hz, 4H), 8.09 (d, J = 1.8 Hz, 2H), 8.00 (t, J = 1.8 Hz, 1H), 7.91 – 7.89 (m, 1H), 7.83 (s, 1H), 7.79 (t, J = 1.8 Hz, 2H), 7.49 – 7.47 (m, 1H), 7.28 (dd, J = 5.6, 3.4 Hz, 2H), 7.10 (s, 1H), 4.99 (s, 2H), 1.60 (s, 16H), 1.55 (s, 14H), 1.53 (s, 42H).

\[ \text{C NMR (126 MHz, CDCl}_3 \] δ 158.83,
β,β'-Benzimidazole-Fused Nickel Benzoporphyrin (AMIm-5)

Nickel acetate tetrahydrate (110 mg, 0.44 mmol) was added with benzonitrile (45 mL) and heated at 110 °C for 1 hour. 1 (55 mg, 0.044 mmol) was then added to the reaction mixture, the system was purged with argon, and the reaction was heated at 175 °C overnight. The reaction was then cooled, and the solvent removed through rotary evaporation. A short silica column was then performed using 1:1 DCM:Hexanes as the eluent. The desired band was collected and recrystallized from DCM and MeOH to yield 50 mg (87% yield) of pure AMIm-5.

β,β'-Platinum-Benzimidazole-Fused Platinum Benzoporphyrin (AMIm-6)

PtCl₂ (12.5 mg, 0.0470 mmol) was added with benzonitrile (3 mL) and heated at 110 °C for 1 hour. 1 (10 mg, 0.0081 mmol) was then added to the reaction mixture, the system was purged with argon, and the reaction was heated at 175 °C overnight. The reaction was then cooled, and the solvent removed through rotary evaporation. A short silica plug was then run using 2:1 DCM:Hexanes as the eluent. The desired band was collected and recrystallized from DCM and MeOH to yield 7.5 mg (54% yield) pure AMIm-6.
$^1$H NMR (500 MHz, CDCl$_3$) δ 9.48 (s, 1H), 8.81 – 8.75 (m, 5H), 8.69 (d, J = 5.1 Hz, 1H), 8.22 (d, J = 5.1 Hz, 1H), 8.20 (d, J = 1.7 Hz, 2H), 8.03 (dd, J = 6.7, 1.8 Hz, 4H), 8.00 (d, J = 1.8 Hz, 2H), 7.99 – 7.96 (m, 2H), 7.96 (s, 1H), 7.90 (s, 1H), 7.83 (t, J = 7.7 Hz, 1H), 7.77 (d, J = 1.7 Hz, 1H), 7.75 (d, J = 1.7 Hz, 1H), 7.67 (t, J = 7.9 Hz, 2H), 7.44 (t, J = 7.8 Hz, 2H), 7.39 – 7.36 (m, 1H), 7.11 (s, 1H), 5.06 (s, 2H), 1.57 (s, 18H), 1.52 (s, 18H), 1.51 (s, 18H), 1.49 (s, 18H).

$^{13}$C NMR (126 MHz, CDCl$_3$) δ 157.01, 151.07, 150.17, 149.08, 149.03, 145.55, 144.78, 142.89, 141.43, 141.29, 140.57, 140.37, 140.33, 140.27, 139.83, 139.55, 139.43, 136.50, 135.41, 134.80, 133.89, 131.26, 131.07, 130.95, 130.67, 130.26, 130.16, 129.70, 129.52, 128.96, 128.83, 127.98, 124.96, 124.94, 123.89, 123.85, 122.35, 121.86, 121.83, 121.43, 121.34, 121.33, 120.12, 119.99, 117.15, 110.95, 109.66, 47.60, 35.54, 35.41, 35.20, 32.03, 31.96, 31.87.

UV/Vis (Toluene): $\lambda_{\text{max}}$ (log ε) = 426 (5.39), 526 (4.48), 559 (4.38) nm; HRMS (MALDI): m/z: calculated for C$_{95}$H$_{103}$Cl$_2$N$_7$Pt$_2$: 1802.7020; found: 1802.7033.

β,β'-Platinum-Benzimidazolyl-Fused Nickel Benzoporphyrin (AMIm-7)

PtCl$_2$ (24.0 mg, 0.09 mmol) was added with benzonitrile (6 mL) and heated at 110 °C for 1 hour. 3 (20 mg, 0.015 mmol) was then added to the reaction mixture, the system was purged with argon, and the reaction was heated at 175 °C overnight. The reaction was then cooled, and the solvent removed through rotary evaporation. A short silica plug was then run using 2:1 DCM:Hexanes as the eluent. The desired band was collected and recrystallized from DCM and MeOH to yield 14 mg (55% yield) of pure AMIm-7.

$^1$H NMR (500 MHz, CDCl$_3$) δ 9.30 (s, 1H), 8.82 (d, J = 5.0 Hz, 1H), 8.75 (d, J = 5.0 Hz, 1H) 8.72 – 8.66 (m, 5H), 8.34 (d, J = 5.0 Hz, 1H), 7.93 (d, J = 1.7 Hz, 2H), 7.91-7.90 (b, 2H), 7.86 (t, J = 1.8 Hz, 1H), 7.84 (d, J = 1.8 Hz, 2H), 7.81 (t, J = 1.6 Hz, 4H), 7.78-7.77 (m, 2H), 7.69 (t, J = 1.8 Hz, 1H), 7.67 (t, J = 1.8 Hz, 1H), 7.66 - 7.62 (b, 2H), 7.42 – 7.39 (m, 2H), 7.36-7.33 (m, 1H) 7.02 (s, 1H), 5.03 (s, 2H), 1.48 (s, 18H), 1.47 (s, 18H), 1.46 (s, 18H), 1.45 (s, 18H). $^{13}$C NMR (126 MHz, CDCl$_3$) δ 156.84, 150.83, 150.04, 149.06, 145.26, 145.01, 143.03, 142.68, 141.74, 141.38, 140.85, 140.62, 139.45, 139.23, 136.73, 135.74, 134.64, 133.71, 132.65, 132.12, 131.65, 131.33, 130.57, 129.51, 128.39, 128.35, 128.31, 127.61, 124.74, 123.67, 123.02, 122.03, 121.55, 121.20, 121.11, 121.08, 118.82, 117.34, 116.77, 115.84, 110.69, 109.51, 77.28, 77.02, 76.77, 35.25, 35.16, 34.98, 34.96, 31.82, 31.74, 31.66. UV/Vis (Toluene): $\lambda_{\text{max}}$ (log ε) = 444 (5.33), 548 (4.37), 589 (4.06) nm; HRMS (ESI): m/z: calculated for C$_{95}$H$_{103}$N$_7$NiPt: 1665.6726; found: 1665.6693.
### Crystal Structures and Crystallography Data

#### Table S1 Crystallographic refinement data for AMIm-4

| Compound | AMIm-4 |
|----------|--------|
| **Empirical formula** | C104 H141 I N6 O4 Zn |
| **Formula weight** | 1731.52 |
| **Temperature** | 220.0(8) K |
| **Wavelength** | 1.54184 Å |
| **Crystal system** | Triclinic |
| **Space group** | P-1 |
| **Unit cell dimensions** |  
| a = 9.3273(4) Å  | a = 90.976(3)°. |
| b = 15.4601(6) Å  | b = 92.533(3)°. |
| c = 34.2082(10) Å | g = 95.704(3)°. |
| **Volume** | 4902.5(3) Å³ |
| **Z** | 2 |
| **Density (calculated)** | 1.197 Mg/m³ |
| **Absorption coefficient** | 3.235 mm⁻¹ |
| **F(000)** | 1884 |
| **Crystal size** | 0.07 x 0.045 x 0.01 mm³ |
| **Theta range for data collection** | 4.770 to 66.600°. |
| **Index ranges** | -11<=h<=11, -18<=k<=12, -40<=l<=40 |
| **Reflections collected** | 59348 |
| **Independent reflections** | 17099 [R(int) = 0.0763] |
| **Completeness to theta = 66.600°** | 98.7 % |
| **Absorption correction** | Semi-empirical from equivalents |
| **Max. and min. transmission** | 1.00000 and 0.88344 |
| **Refinement method** | Full-matrix least-squares on F² |
| **Data / restraints / parameters** | 17099 / 67 / 993 |
| **Goodness-of-fit on F²** | 1.042 |
| **Final R indices [I>2sigma(I)]** | R₁ = 0.1157, wR₂ = 0.3237 |
| **R indices (all data)** | R₁ = 0.1373, wR₂ = 0.3407 |
| **Extinction coefficient** | n/a |
| **Largest diff. peak and hole** | 1.340 and -1.829 e.Å⁻³ |
Table S2. Crystallographic refinement data for AMIm-6

| Compound      | AMIm-6                                      |
|---------------|---------------------------------------------|
| Formula       | C_{133.5}H_{147}Cl_2N_7Pt_2                 |
| D_{calc.} g cm\(^{-3}\) | 1.278                                      |
| m/mm\(^{-1}\) | 5.081                                      |
| Formula Weight| 2310.65                                    |
| Colour        | metallic dark red                          |
| Shape         | block                                      |
| Size/mm\(^3\) | 0.05×0.04×0.03                             |
| T/K           | 220.1(8)                                   |
| Crystal System| triclinic                                  |
| Space Group   | P-1                                        |
| a/Å           | 10.41830(10)                               |
| b/Å           | 17.4812(2)                                 |
| c/Å           | 34.5651(2)                                 |
| \(a'\)       | 85.0250(10)                                |
| \(b'\)       | 89.3060(10)                                |
| \(c'\)       | 73.2960(10)                                |
| V/Å\(^3\)     | 6006.25(10)                                |
| Z             | 2                                          |
| Z'            | 1                                          |
| Wavelength/Å  | 1.54184                                    |
| Radiation type| Cu K\(_{\alpha}\)                          |
| Q_{min}/°     | 2.842                                      |
| Q_{max}/°     | 79.252                                     |
| Measured Refl.| 74162                                      |
| Independent Refl.| 25221                                   |
| Reflections with I > 2(I) | 22137                                     |
| R_{int}       | 0.0295                                     |
| Parameters    | 1033                                       |
| Restraints    | 96                                         |
| Largest Peak  | 1.824                                      |
| Deepest Hole  | -1.011                                     |
| GooF          | 1.096                                      |
| wR\(_2\) (all data) | 0.1547                                    |
| wR\(_2\)      | 0.1484                                     |
| R\(_1\) (all data) | 0.0637                                    |
| R\(_1\)       | 0.0559                                     |
Table S3. Crystallographic refinement data for AMIm-7

| Compound | AMIm-7 |
|----------|--------|
| Formula  | C\textsubscript{112.50}H\textsubscript{23}Cl\textsubscript{2}N\textsubscript{2}NiPt |
| \(D_{\text{calc.}} \ g \text{ cm}^{-3}\) | 1.287 |
| \(m/\text{mm}^{-1}\) | 3.758 |
| Formula Weight | 1897.9619 |
| Colour | metallic dark red |
| Shape | block |
| Size/mm\(^3\) | 0.05×0.035×0.025 |
| \(T/K\) | 99.9(3) |
| Crystal System | triclinic |
| Space Group | \(P-1\) |
| \(a/\text{Å}\) | 15.4224(2) |
| \(b/\text{Å}\) | 18.4372(2) |
| \(c/\text{Å}\) | 18.7956(3) |
| \(\alpha/°\) | 68.6230(10) |
| \(\beta/°\) | 81.3910(10) |
| \(\gamma/°\) | 81.8510(10) |
| \(V/\text{Å}^3\) | 4898.58(12) |
| \(Z\) | 2 |
| \(Z'\) | 1 |
| Wavelength/Å | 1.54184 |
| Radiation type | Cu K\(_\alpha\) |
| \(Q_{\text{min/f}}\) | 2.539 |
| \(Q_{\text{max/f}}\) | 80.618 |
| Measured Refl. | 209129 |
| Independent Refl. | 21185 |
| \(R_{\text{int}}\) | 0.0633 |
| Parameters | 1001 |
| Restraints | 32 |
| Largest Peak | 1.721 |
| Deepest Hole | -2.495 |
| Goof | 1.059 |
| \(wR_2\) (all data) | 0.3046 |
| \(wR_2\) | 0.3035 |
| \(R_1\) (all data) | 0.1309 |
| \(R_1\) | 0.1288 |
Figure S1. NMR Spectra
Figure S1. Proton NMR of product mixture resulting from reaction of AMIm-2, PtCl₂, and benzonitrile. Overlay with pure AMIm-6 proton NMR indicates AMIm-6 is a major product of the reaction.
Figure S2. Fourier Transform Infrared Spectra

IR Spectrum of AMIm-1

IR Spectrum of AMIm-2
Figure S2. FT-IR spectra of the indicated compounds.
Figure S3. Crystal structure of AMIm-4

Crystal structure of AMIm-7
Acid Titration Date for AMIm-2

Figure S4. UV-Vis monitored acid titration of AMIm-2 with TFA in DCM. Concentration of AMIm-2: 4.0x10^{-6} M. Concentration of TFA: 2.5 x 10^{-3} M. Titration stopped upon appearance of absorbance band at ~700nm corresponding to demetallated and protonated porphyrin.

Figure S5. Fluorescence monitored titration of AMIm-2 with TFA. Concentration of AMIm-2: 1.5x10^{-7} M. Concentration of TFA: 2.5 x 10^{-3} M. Sample was excited at 439
nm for the entirety of the titration and stopped upon appearance of absorbance band at \(\sim 700\) nm corresponding to demetallated and protonated porphyrin.

**Optimized Structures**

![Optimized Structures](image)

**Figure S6** Optimized using B3LYP/6-31G(d,p) for all atoms besides platinum, and LANL2DZ for platinum atoms in AMIm-6. All structures did not possess negative frequencies from frequency calculation.

**Energy Level Diagram**

![Energy Level Diagram](image)
**Figure S7.** Energy values obtained from Opt/Freq calculation using B3LYP/6-31G(d,p) for all atoms besides platinum, and LANL2DZ for platinum atoms in AMIm-6.

**TD-DFT Graphs** (Optimized structures above were used and TD-DFT calculations were run using B3LYP/6-31G(d,p) for all atoms besides platinum, LANL2DZ for platinum atoms in AMIm-6, and toluene PCM to account for solvent.)

**Figure S8.** Experimental UV-Vis and TD-DFT oscillator strengths overlayed for AMIm-1 and AM-Im1’
**Figure S9.** Experimental UV-Vis and TD-DFT oscillator strengths overlayed for AMIm-2

**Figure S10.** Experimental UV-Vis and TD-DFT oscillator strengths overlayed for AMIm-6
Figure S11. B3LYP/6-31G* optimized structures and frontier orbitals of AMIm-2:ImC_{60}
Figure S12. Phosphorescence spectrum of AMIm-2 in the presence of C$_{60}$Im at liquid nitrogen temperature
Figure S13. (a) Fs-TA ($\lambda_{\text{exc}}=420$ nm) and (b) ns-TA ($\lambda_{\text{exc}}=420$ nm) spectra of AMIm-2:ImC$_{60}$ at indicated delay times in DCB.
## TD-DFT Oscillator Tables

### Table S4 TD-DFT oscillator strength table for AMIm-1

| AMIm-1 | Transition energy (eV) | Wavelength (nm) | Oscillator Strength, f | Orbital Transition | % Probability |
|--------|------------------------|-----------------|------------------------|-------------------|---------------|
| Singlet A 2.1138 | 586 | 0.0265 | HOMO | LUMO | 63.6 |
| | | | HOMO-1 | LUMO+1 | 31.2 |
| | | | HOMO-1 | LUMO | 2.2 |
| Singlet A 2.2401 | 553 | 0.0143 | HOMO-1 | LUMO | 52.1 |
| | | | HOMO | LUMO+1 | 43.2 |
| | | | HOMO | LUMO | 2.9 |
| Singlet A 2.8233 | 439 | 2.3241 | HOMO-1 | LUMO+1 | 59 |
| | | | HOMO | LUMO | 26.2 |
| | | | HOMO-2 | LUMO | 3.9 |
| | | | HOMO-2 | LUMO+1 | 3.3 |
| | | | HOMO-5 | LUMO | 2.1 |
| Singlet A 2.9169 | 425 | 1.2342 | HOMO | LUMO+1 | 47 |
| | | | HOMO-1 | LUMO | 40 |
| | | | HOMO-2 | LUMO | 6.7 |
| | | | HOMO-1 | LUMO+1 | 2.4 |
| Singlet A 3.1104 | 399 | 0.2862 | HOMO-2 | LUMO | 73.6 |
| | | | HOMO-4 | LUMO | 11.3 |
| | | | HOMO | LUMO+1 | 5.3 |
| | | | HOMO-1 | LUMO | 3.1 |
| | | | HOMO-1 | LUMO+2 | 2.1 |
| Singlet A 3.2158 | 386 | 0.0036 | HOMO-4 | LUMO | 45.9 |
| | | | HOMO-2 | LUMO+1 | 41.7 |
| | | | HOMO-2 | LUMO | 4.0 |
| | | | HOMO | LUMO+2 | 2.4 |
| Singlet A 3.2471 | 382 | 0.0042 | HOMO-2 | LUMO+1 | 44.9 |
| | | | HOMO-4 | LUMO | 27.9 |
| | | | HOMO-5 | LUMO | 10.6 |
| | | | HOMO-2 | LUMO | 8.4 |
| Singlet A 3.3559 | 369 | 0.384 | HOMO-5 | LUMO | 65.6 |
| | | | HOMO | LUMO+2 | 15.8 |
| | | | HOMO-4 | LUMO | 3.2 |
| | | | HOMO-9 | LUMO | 2.4 |
| Singlet A 3.3922 | 365 | 0.0006 | HOMO-3 | LUMO+1 | 95.3 |
| | | | HOMO-4 | LUMO+1 | 2.6 |
| Singlet A 3.4421 | 360 | 0.1153 | HOMO | LUMO+2 | 70.2 |
| | | | HOMO-5 | LUMO | 12.0 |
| | | | HOMO-2 | LUMO+1 | 4.7 |
| | | | HOMO-4 | LUMO+1 | 2.9 |
| AMIm-1’  | Transition energy (eV) | Wavelength (nm) | Oscillator Strength, f | Orbital Transition | % Probability |
|---------|------------------------|-----------------|------------------------|--------------------|---------------|
| Singlet A 2.1016 | 590 | 0.012 | HOMO | LUMO+1 | 55.7 |
|         |                      |                 | HOMO-1 | LUMO | 37.7 |
|         |                      |                 | HOMO | LUMO | 3.3 |
|         |                      |                 | HOMO-1 | LUMO+1 | 2.1 |
| Singlet A 2.2378 | 554 | 0.0076 | HOMO | LUMO | 54.8 |
|         |                      |                 | HOMO-1 | LUMO+1 | 38.9 |
|         |                      |                 | HOMO | LUMO+1 | 2.9 |
|         |                      |                 | HOMO-1 | LUMO | 2.4 |
| Singlet A 2.7891 | 445 | 1.7087 | HOMO-1 | LUMO+1 | 25.6 |
|         |                      |                 | HOMO-2 | LUMO+1 | 20.1 |
|         |                      |                 | HOMO-1 | LUMO | 19.0 |
|         |                      |                 | HOMO | LUMO | 15.3 |
|         |                      |                 | HOMO | LUMO+2 | 10.7 |
|         |                      |                 | HOMO-2 | LUMO | 7.1 |
| Singlet A 2.8690 | 432 | 1.0725 | HOMO-1 | LUMO | 28.9 |
|         |                      |                 | HOMO-1 | LUMO+1 | 20.8 |
|         |                      |                 | HOMO | LUMO+1 | 16.2 |
|         |                      |                 | HOMO-2 | LUMO | 13.8 |
|         |                      |                 | HOMO | LUMO | 13.2 |
|         |                      |                 | HOMO-2 | LUMO+1 | 4.2 |
| Singlet A 3.0176 | 411 | 0.6353 | HOMO-2 | LUMO | 45.4 |
|         |                      |                 | HOMO-2 | LUMO+1 | 34.1 |
|         |                      |                 | HOMO-1 | LUMO+1 | 6.1 |
|         |                      |                 | HOMO | LUMO | 5.4 |
|         |                      |                 | HOMO | LUMO+1 | 3.4 |
|         |                      |                 | HOMO-1 | LUMO | 2.4 |
| Singlet A 3.0648 | 405 | 0.6889 | HOMO-2 | LUMO+1 | 38.2 |
|         |                      |                 | HOMO-2 | LUMO | 30.8 |
|         |                      |                 | HOMO | LUMO+1 | 8.3 |
|         |                      |                 | HOMO-1 | LUMO | 6.7 |
|         |                      |                 | HOMO | LUMO | 5.9 |
|         |                      |                 | HOMO-1 | LUMO+1 | 4.6 |
| Singlet A 3.3798 | 367 | 0.0041 | HOMO-3 | LUMO+1 | 63.6 |
|         |                      |                 | HOMO-3 | LUMO | 35.0 |
| Singlet A 3.3975 | 365 | 0.1045 | HOMO-4 | LUMO+1 | 49.1 |
|         |                      |                 | HOMO-3 | LUMO | 14.8 |
|         |                      |                 | HOMO | LUMO+2 | 13.2 |
|         |                      |                 | HOMO-5 | LUMO+1 | 5.4 |
|         |                      |                 | HOMO-3 | LUMO+1 | 4.6 |
|         |                      |                 | HOMO-4 | LUMO | 2.1 |
| Singlet A 3.4021 | 364 | 0.0143 | HOMO-3 | LUMO | 48.8 |
|         |                      |                 | HOMO-3 | LUMO+1 | 31.0 |
|         |                      |                 | HOMO-4 | LUMO+1 | 13.1 |
|         |                      |                 | HOMO-5 | LUMO+1 | 2.1 |
### Table S6: TD-DFT oscillator strength table for AMIm-2

| AMIm-2 | Transition energy (eV) | Wavelength (nm) | Oscillator Strength, f | Orbital Transition | % Probability |
|--------|------------------------|-----------------|------------------------|--------------------|--------------|
| Singlet A 3.4718 | 357 | 0.0395 | HOMO-4 | LUMO | 89.9 | HOMO | LUMO+2 | 4.3 |
| Singlet A 2.2347 | 555 | 0.0064 | HOMO | HOMO-2 | 32.2 |
| | | | HOMO-1 | LUMO+1 | 19.7 |
| | | | LUMO | 22.5 |
| Singlet A 2.2555 | 550 | 0.0006 | HOMO-1 | LUMO+1 | 30.8 |
| | | | HOMO | 26 |
| | | | HOMO-1 | LUMO | 23 |
| | | | HOMO+1 | 19.1 |
| Singlet A 2.8592 | 434 | 2.3236 | HOMO-1 | LUMO+1 | 45.7 |
| | | | HOMO | 35.7 |
| | | | HOMO-1 | LUMO+1 | 6.6 |
| | | | LUMO | 4.6 |
| | | | LUMO+1 | 2.4 |
| Singlet A 2.9390 | 422 | 1.2778 | HOMO-1 | LUMO+1 | 47.7 |
| | | | HOMO | 41.5 |
| | | | HOMO-1 | 4.6 |
| Singlet A 3.1395 | 395 | 0.2045 | HOMO-2 | LUMO | 78.6 |
| | | | HOMO-2 | LUMO+1 | 11.8 |
| | | | HOMO-1 | LUMO+2 | 2.6 |
| | | | HOMO+1 | 2.4 |
| Singlet A 3.1952 | 388 | 0.1317 | HOMO-2 | LUMO+1 | 76.7 |
| | | | HOMO-2 | LUMO | 8.9 |
| | | | HOMO-1 | LUMO+1 | 4.2 |
| | | | HOMO | 4.2 |
| Singlet A 3.3022 | 375 | 0.0814 | HOMO-7 | LUMO | 50 |
| | | | HOMO-6 | LUMO | 33.7 |
| | | | HOMO-5 | LUMO | 6.9 |
| | | | HOMO-8 | LUMO | 3.8 |
| Singlet A | 3.4141 | 363 | 0.0246 | HOMO-7 | LUMO+1 | 49.9 |
|          |       |     |        | HOMO-6 | LUMO+1 | 35.5 |
|          |       |     |        | HOMO-5 | LUMO+1 |  6.7 |
|          |       |     |        | HOMO-8 | LUMO+1 |  3.6 |
| Singlet A | 3.4779 | 356 | 0.0003 | HOMO-3 | LUMO   | 86.9 |
|          |       |     |        | HOMO-4 | LUMO   |  7.2 |
| Singlet A | 3.513  | 353 | 0.0434 | HOMO-2 | LUMO+2 | 70.9 |
|          |       |     |        | HOMO-3 | LUMO+2 | 17.1 |
|          |       |     |        | HOMO-4 | LUMO+1 |  2.8 |
|          |       |     |        |       | LUMO+1 |  2.4 |

**Table S7 TD-DFT oscillator strength table for AMIm-6**

| AMIm-6 | Transition energy (eV) | Wavelength (nm) | Oscillator Strength, f | Orbital Transition | % Probability |
|--------|------------------------|-----------------|------------------------|--------------------|---------------|
| Singlet A | 2.3902 | 519 | 0.0346 | HOMO | LUMO | 63.4 |
|          |       |     |        | HOMO-1 | LUMO+1 | 35.5 |
| Singlet A | 2.4066 | 515 | 0.0151 | HOMO | LUMO+1 | 52.9 |
|          |       |     |        | HOMO-1 | LUMO   | 45.7 |
| Singlet A | 2.7108 | 457 | 0.0009 | HOMO-2 | LUMO+1 | 82.0 |
|          |       |     |        | HOMO-2 | LUMO+1 | 11.5 |
|          |       |     |        | HOMO-3 | LUMO   |  4.9 |
| Singlet A | 2.8987 | 428 | 0.8325 | HOMO-2 | LUMO+1 |  36 |
|          |       |     |        | HOMO-1 | LUMO   |  13 |
|          |       |     |        | HOMO   | LUMO+1 | 11.9 |
|          |       |     |        | HOMO-3 | LUMO   |  9.4 |
|          |       |     |        | HOMO-1 | LUMO+1 |  9.2 |
|          |       |     |        | HOMO   | LUMO   |  5.1 |
|          |       |     |        | HOMO-3 | LUMO+1 |  4.8 |
|          |       |     |        | HOMO   | LUMO+4 |  2.1 |
|          |       |     |        | HOMO-2 | LUMO   |  2.1 |
| Singlet A | 2.9431 | 421 | 0.6971 | HOMO-3 | LUMO   | 36.7 |
|          |       |     |        | HOMO-3 | LUMO+1 | 19 |
|          |       |     |        | HOMO-2 | LUMO+1 | 13.4 |
|          |       |     |        | HOMO-1 | LUMO+1 |  6.7 |
|          |       |     |        | HOMO-1 | LUMO   |  6.2 |
|          |       |     |        | HOMO   | LUMO+1 |  5.6 |
|          |       |     |        | HOMO   | LUMO   |  4.3 |
| Singlet A | 2.9804 | 416 | 0.4976 | HOMO-3 | LUMO+1 | 44.2 |
|          |       |     |        | HOMO-1 | LUMO   | 12.2 |
|          |       |     |        | HOMO-2 | LUMO+1 |  11 |
|          |       |     |        | HOMO   | LUMO+1 |  9.9 |
| Singlet | A  | 2.9976 | 414 | 0 | HOMO-4 | LUMO+1 | 3.5 |
|---------|----|--------|-----|---|--------|--------|-----|
|         |    |        |     |   | HOMO-4 | LUMO+3 | 55.2|
|         |    |        |     |   | HOMO-4 | LUMO+4 | 26.0|
|         |    |        |     |   | HOMO-4 | LUMO+2 | 11.7|
|         |    |        |     |   | HOMO-3 | LUMO+3 | 2.6 |

| Singlet | A  | 3.0173 | 411 | 1.0542 | HOMO-1 | LUMO+1 | 37.5 |
|---------|----|--------|-----|--------|--------|--------|-----|
|         |    |        |     |        | HOMO-3 | LUMO+1 | 15.5|
|         |    |        |     |        | HOMO-1 | LUMO+4 | 2.8 |

| Singlet | A  | 3.0878 | 402 | 0.0039 | HOMO   | LUMO+2 | 98.2 |
|---------|----|--------|-----|--------|--------|--------|-----|
|         |    |        |     |        | HOMO-4 | LUMO+1 | 89.8|
|         |    |        |     |        | HOMO-1 | LUMO+1 | 2.0 |

| Singlet | A  | 3.1866 | 389 | 0.0137 | HOMO-3 | LUMO   | 37.3 |
|---------|----|--------|-----|--------|--------|--------|-----|
|         |    |        |     |        | HOMO-2 | LUMO+1 | 22.4|
|         |    |        |     |        | HOMO-3 | LUMO+1 | 16.8|
|         |    |        |     |        | HOMO-2 | LUMO   | 9.8 |
|         |    |        |     |        | HOMO-1 | LUMO+2 | 8.6 |

| Singlet | A  | 3.1882 | 389 | 0.0039 | HOMO-1 | LUMO+2 | 89.8 |
|---------|----|--------|-----|--------|--------|--------|-----|
|         |    |        |     |        | HOMO-3 | LUMO   | 3.8 |
|         |    |        |     |        | HOMO-2 | LUMO+1 | 2.0 |

| Singlet | A  | 3.2147 | 386 | 0.0001 | HOMO-4 | LUMO   | 73.9 |
|---------|----|--------|-----|--------|--------|--------|-----|
|         |    |        |     |        | HOMO-4 | LUMO+1 | 18.4|
|         |    |        |     |        | HOMO-3 | LUMO+1 | 2.7 |
|         |    |        |     |        | HOMO-4 | LUMO+4 | 2.5 |

| Singlet | A  | 3.2356 | 383 | 0.0003 | HOMO-5 | LUMO+3 | 31.6 |
|---------|----|--------|-----|--------|--------|--------|-----|
|         |    |        |     |        | HOMO-5 | LUMO+4 | 15.0|
|         |    |        |     |        | HOMO-6 | LUMO+3 | 5.9 |
|         |    |        |     |        | HOMO-5 | LUMO+2 | 4.6 |
|         |    |        |     |        | HOMO-12| LUMO+3 | 4.5 |
|         |    |        |     |        | HOMO   | LUMO+3 | 4.4 |
|         |    |        |     |        | HOMO-3 | LUMO+3 | 3.7 |
|         |    |        |     |        | HOMO-8 | LUMO+3 | 3.5 |
|         |    |        |     |        | HOMO-6 | LUMO+4 | 2.8 |
|         |    |        |     |        | HOMO-12| LUMO+4 | 2.1 |
|         |    |        |     |        | HOMO   | LUMO+4 | 2.1 |

| Singlet | A  | 3.2683 | 379 | 0.0001 | HOMO-9 | LUMO   | 92.5 |
|---------|----|--------|-----|--------|--------|--------|-----|
|         |    |        |     |        | HOMO-9 | LUMO+1 | 6.3 |

| Singlet | A  | 3.3272 | 373 | 0.0002 | HOMO-4 | LUMO+1 | 72.7 |
|---------|----|--------|-----|--------|--------|--------|-----|
|         |    |        |     |        | HOMO-4 | LUMO   | 21.0|
|         |    |        |     |        | HOMO-3 | LUMO+1 | 3.2 |

| Singlet | A  | 3.3322 | 372 | 0.0004 | HOMO-14| LUMO+3 | 29.9 |
|---------|----|--------|-----|--------|--------|--------|-----|
|         |    |        |     |        | HOMO-14| LUMO+4 | 14.5|
|         |    |        |     |        | HOMO-7 | LUMO+3 | 12.0|
|         |    |        |     |        | HOMO-12| LUMO+3 | 10.4|
|         |    |        |     |        | HOMO-8 | LUMO+3 | 6.9 |
|         |    |        |     |        | HOMO-7 | LUMO+4 | 5.7 |
| Singlet | A | 3.3757 | 367 | 0.0013 | HOMO-12 | LUMO+4 | 4.5 |
|---------|---|--------|-----|--------|---------|--------|-----|
|         |   |        |     |        | HOMO-14 | LUMO+2 | 4.2 |
|         |   |        |     |        | HOMO-8  | LUMO+4 | 3.3 |
| Singlet | A | 3.3872 | 366 | 0.1474 | HOMO-4  | LUMO+4 | 54.6|
|         |   |        |     |        | HOMO-4  | LUMO+3 | 29.6|
|         |   |        |     |        | HOMO-4  | LUMO+2 | 2.5 |
| Singlet | A | 3.3945 | 365 | 0.0018 | HOMO-9  | LUMO+1 | 90.5|
|         |   |        |     |        | HOMO-1  | LUMO+1 | 6.0 |
| Singlet | A | 3.4323 | 361 | 0.0007 | HOMO    | LUMO+3 | 59.0|
|         |   |        |     |        | HOMO    | LUMO+4 | 31.7|

**Table S8. Atom coordinates for optimized structures using B3LYP 6-31G(d,p) (and LANL2DZ for platinum atoms) in vacuuo**

Atom coordinates for optimized **AMIm-1**:

|   | X              | Y              | Z              |
|---|----------------|----------------|----------------|
| C | -5.3804190     | -1.1184020     | -0.2445630     |
| C | -5.5093750     | 0.2484020      | -0.2707910     |
| C | -3.9963460     | -1.4286100     | -0.0683780     |
| C | -4.2086730     | 0.8185360      | -0.1088900     |
| N | -3.3283640     | -0.2304130     | 0.0003680      |
| C | -3.8762740     | 2.1874690      | -0.0716570     |
| C | -2.5706010     | 2.6988650      | 0.0210340      |
| N | -1.4035640     | 1.9699270      | 0.0128150      |
| C | -0.4055310     | 2.8881590      | 0.1082900      |
| C | -2.2911980     | 4.1230520      | 0.1527540      |
| C | -0.9446930     | 4.2431030      | 0.2057970      |
| C | 0.9953000      | 2.6447660      | 0.1005560      |
| C | 1.6223550      | 1.3973730      | 0.0437650      |
| N | 0.9749750      | 0.1792100      | 0.0414560      |
| C | 1.8373020      | -0.8965200     | 0.0252380      |
| C | 3.1814160      | -0.3269190     | -0.0246010     |
| C | 3.0472130      | 1.0912430      | -0.0061910     |
| C | 1.4593120      | -2.2399200     | 0.0805390      |
| C | 0.1289360      | -2.7410130     | 0.1220520      |
| N | -1.0254690     | -2.0287610     | 0.0377350      |
| C   | -2.0338460 | -2.9640410 | 0.0898500 |
| C   | -0.1423650 | -4.1707080 | 0.2593880 |
| C   | -1.4880870 | -4.3068510 | 0.2437440 |
| C   | -3.4130580 | -2.7095130 | 0.0088840 |
| H   | -6.1627780 | -1.8537130 | -0.3502360 |
| H   | -6.4152020 | 0.8197020  | -0.4014750 |
| H   | -3.0310000 | 4.9071530  | 0.2096540 |
| H   | -0.3649480 | 5.1476600  | 0.3084740 |
| H   | 0.6014230  | -4.9456080 | 0.3649220 |
| H   | -2.0658110 | -5.2138860 | 0.3384080 |
| C   | -5.0205560 | 3.1531170  | -0.1389370 |
| C   | -5.9531840 | 3.2248600  | 0.9095420 |
| C   | -5.1758020 | 3.9912390  | -1.2450200 |
| C   | -7.0246540 | 4.1192320  | 0.8660460 |
| C   | -6.2399450 | 4.9039140  | -1.3299310 |
| C   | -7.1443940 | 4.9471650  | -0.2653600 |
| H   | -7.9724970 | 5.6439430  | -0.3075720 |
| H   | -5.8131350 | 2.5715500  | 1.7619550 |
| H   | -4.4525170 | 3.9200010  | -2.0507230 |
| C   | 1.8598470  | 3.8735370  | 0.1632770 |
| C   | 2.3114080  | 4.3539410  | 1.3977540 |
| C   | 3.1033920  | 5.5065460  | 1.4809900 |
| C   | 2.9874130  | 5.7147330  | -0.9726260 |
| C   | 3.4281400  | 6.1595690  | 0.2826770 |
| H   | 2.0338250  | 3.8079150  | 2.2912360 |
| H   | 4.0407220  | 7.0543720  | 0.3298020 |
| C   | 2.1928410  | 4.5613660  | -1.0092810 |
| H   | 1.8234650  | 4.1732260  | -1.9507670 |
| C   | 2.5441830  | -3.2804840 | 0.0984410 |
| C   | 2.9183490  | -3.9165460 | -1.0907540 |
| C   | 3.1807520  | -3.6228900 | 1.2968750 |
| C   | 3.9325690  | -4.8825840 | -1.1066460 |
| C   | 4.2070890  | -4.5757760 | 1.3232560 |
| C   | 4.5555900  | -5.1891130 | 0.1112730 |
| H   | 5.3492970  | -5.9292110 | 0.1155000 |
| H   | 2.4085610  | -3.6349160 | -2.0042430 |
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| H       | 2.8747910    | -3.1144550   | 2.2034300    |
| C       | -4.3581440   | -3.8726790   | -0.0061800   |
| C       | -5.2426720   | -4.0792840   | 1.0608440    |
| C       | -4.3695330   | -4.7614100   | -1.0894620   |
| C       | -6.1328060   | -5.1599120   | 1.0676330    |
| C       | -5.2462110   | -5.8524240   | -1.1238830   |
| C       | -6.1128710   | -6.0253410   | -0.0352570   |
| C       | -6.7982950   | -6.8669970   | -0.0467310   |
| H       | -3.6820010   | -4.5785810   | -1.9060830   |
| H       | -5.2125040   | -3.3846890   | 1.8914290    |
| C       | 4.4514350    | -0.9273430   | -0.0872780   |
| C       | 5.5552370    | -0.0915710   | -0.1094010   |
| C       | 4.1866800    | 1.9238900    | -0.0466570   |
| C       | 5.4249070    | 1.3199350    | -0.0927260   |
| C       | 6.9769660    | -0.3968750   | -0.1433060   |
| C       | 6.8003730    | 1.9746860    | -0.1317620   |
| N       | 7.6658640    | 0.8033010    | -0.1614310   |
| H       | 6.9962480    | 2.5937070    | 0.7525750    |
| H       | 6.9422510    | 2.6007490    | -1.0214810   |
| N       | 7.7454950    | -1.4605020   | -0.1443410   |
| C       | 9.0081700    | 0.4949410    | -0.1742160   |
| C       | 9.0328040    | -0.9335550   | -0.1651230   |
| C       | 10.2649890   | -1.5982950   | -0.1756960   |
| C       | 11.4278450   | -0.8343300   | -0.1939580   |
| C       | 11.3829790   | 0.5737580    | -0.2021700   |
| C       | 10.1728690   | 1.2639440    | -0.1928240   |
| H       | 10.1423440   | 2.3490990    | -0.1997820   |
| H       | 10.2960000   | -2.6829420   | -0.1692770   |
| H       | 12.3934340   | -1.3310520   | -0.2022490   |
| H       | 12.3126800   | 1.1346990    | -0.2164090   |
| H       | 4.5894950    | 1.9963790    | -0.1164520   |
| H       | 4.0997050    | 3.0001870    | -0.0416310   |
| H       | -2.3200560   | -0.1343780   | 0.0759560    |
| H       | -0.0382000   | 0.0846510    | 0.0512410    |
| C       | -8.0618060   | 4.2289370    | 2.0010300    |
| C       | -6.3711040   | 5.8018330    | -2.5757810   |
| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| H    | 3.405220 | 7.9196650 | 3.9700080 |
| C    | 3.3818500 | 6.4931340 | -2.2431110 |
| C    | 2.8510140 | 7.9430980 | -2.1463080 |
| H    | 1.7595140 | 7.9550650 | -2.0618870 |
| H    | 3.1284010 | 8.5109460 | -3.0414330 |
| H    | 3.2583750 | 8.4705790 | -1.2788430 |
| C    | 4.9233430 | 6.5199560 | -2.3730720 |
| H    | 5.3982670 | 7.0020480 | -1.5134850 |
| H    | 5.2211030 | 7.0728260 | -3.2710170 |
| H    | 5.3260420 | 5.5045500 | -2.4528440 |
| C    | 2.8049960 | 5.8571160 | -3.5221530 |
| H    | 4.9617600 | -4.9532740 | 2.6121650 |
| C    | 4.5134050 | -4.1080540 | 3.8193550 |
| H    | 4.6916590 | -3.0403720 | 3.6554710 |
| H    | 5.0806430 | -4.4057420 | 4.7070570 |
| H    | 3.4515040 | -4.2478610 | 4.0462960 |
| C    | 6.4791700 | -4.7279360 | 2.4029240 |
| H    | 6.6919750 | -3.6985540 | 2.0979950 |
| H    | 6.8858690 | -5.3871660 | 1.6305300 |
| H    | 7.0236390 | -4.9339130 | 3.3314230 |
| C    | 4.7027900 | -6.4426020 | 2.9403130 |
| H    | 3.6372500 | -6.6267280 | 3.1134310 |
| H    | 5.2492840 | -6.7359410 | 3.8438970 |
| H    | 5.0267530 | -7.0986970 | 2.1268050 |
| C    | 4.3843310 | -5.5943580 | -2.3966520 |
| C    | 3.6022780 | -5.1148290 | -3.6339690 |
| H    | 2.5287660 | -5.3079260 | -3.5389700 |
| H    | 3.9558650 | -5.6487210 | -4.5219280 |
| H    | 3.7429310 | -4.0444750 | -3.8154360 |
| C    | 4.1623820 | -7.1183040 | -2.2487130 |
| H    | 3.1029160 | -7.3468340 | -2.0925180 |
| H    | 4.7211280 | -7.5312870 | -1.4037430 |
| H    | 4.4927640 | -7.6405500 | -3.1537320 |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 5.3569440 | 1.0825470 | -0.5961650 |
| C    | 5.4775890 | -0.2673970 | -0.6033340 |
| C    | 3.9609730 | 1.3673940 | -0.2876850 |
C  4.1543510  -0.7987960  -0.2998990
N  3.2477020   0.2110300  -0.1405250
C  3.8823540  -2.1797980  -0.1778970
C  2.6068250  -2.7344670   0.0151870
N  1.4049450  -2.0578000   0.0102220
C  0.3560380  -2.9238420   0.2121600
C  2.2950980  -4.1107350   0.2588610
C  0.9365580  -4.2254080   0.3826660
C  -1.0210800 -2.6289560   0.2121850
C  -1.5966050 -1.3450210   0.0856600
N  -0.8961530 -0.1747060   0.1565730
C  -1.7881780  0.8566190   0.1189450
C  -3.1572350  0.3405280  -0.0835430
C  -3.0325710 -1.0701960  -0.1115840
C  -1.4499000  2.2193270   0.2697130
C  -0.1503350  2.7586040   0.2640060
N  1.0387350  2.1013310   0.0543490
C  2.0937760  2.9890290   0.0510750
C  0.1788800  4.1460620   0.4277580
C  1.5341420  4.2849110   0.2952010
C  3.4474730  2.6767360  -0.1509450
H  6.1212500  1.8190200  -0.7943230
H  6.3605750  -0.8541220  -0.8081210
H  3.0292730  -4.8969840   0.3401170
H  0.3725610  -5.1235680   0.5783670
H  -0.5436750  4.9234010   0.6204470
H  2.1102050  5.1943030   0.3664800
C  5.0318180  -3.1381500  -0.2386220
C  6.0332900  -3.1040400   0.7470730
C  5.1252800  -4.0775540  -1.2681570
C  7.1138160  -3.9873070   0.7133830
C  6.1956570  -4.9841920  -1.3401260
C  7.1709510  -4.9168380  -0.3414720
H  8.0063100  -5.6052570  -0.3751620
H  5.9393930  -2.3749540   1.5422080
H  4.3510290  -4.0881040  -2.0284820
C -1.917555  -3.816578  0.410405
C -2.578003  -3.987896  1.633256
C -3.425526  -5.079691  1.853709
C -2.936934  -5.869075 -0.429781
C -3.588987  -5.997403  0.805372
H -2.419898  -3.245319  2.405687
H -4.245311  -6.848436  0.959017
C -2.094359  -4.763543 -0.606627
H -1.571262  -4.611495 -1.542953
C -2.547982  3.220242  0.490387
C -2.982727  4.053457 -0.547574
C -3.155706  3.307496  1.748154
C -4.044735  4.948060 -0.359524
C -4.202706  4.206020  1.985450
C -4.626995  5.005571  0.914910
H -5.451274  5.692330  1.076680
H -2.500558  3.963312 -1.513669
H -2.801175  2.651928  2.534197
C  4.405026  3.826849 -0.207381
C  5.396001  3.961940  0.773558
C  4.320157  4.773326 -1.237833
C  6.301338  5.036198  0.742967
C  5.206582  5.854899 -1.306286
C  6.182672  5.959991 -0.305231
H  6.878013  6.792747 -0.343589
H  3.554275  4.639780 -1.992071
H  5.438912  3.231314  1.565108
C -4.392360  0.959895 -0.317029
C -5.480870  0.138011 -0.580242
C -4.144570 -1.889677 -0.381267
C -5.360479 -1.270375 -0.610444
C -6.863734  0.465828 -0.890115
C -6.706916 -1.905364 -0.937054
N -7.545231 -0.722884 -1.084556
H -7.071375 -2.556396 -0.132428
H -6.681240 -2.494192 -1.862539
| Atom | X      | Y      | Z     |
|------|--------|--------|-------|
| H    | -6.9038720 | 4.6698380 | 2.4978900 |
| H    | -6.9163470 | 4.0600780 | 4.1576100 |
| C    | -4.7551990 | 5.7703600 | 3.8849880 |
| H    | -3.7006900 | 6.0325040 | 4.0207190 |
| H    | -5.2577220 | 5.8731580 | 4.8533340 |
| H    | -5.1961650 | 6.5030680 | 3.2028610 |
| C    | -4.6001670 | 5.8322130 | -1.4924260 |
| C    | -3.8905600 | 5.5737280 | -2.8348740 |
| H    | -2.8189090 | 5.7922130 | -2.7805530 |
| H    | -4.3187630 | 6.2206280 | -3.6072500 |
| H    | -4.0134570 | 4.5377460 | -3.1663600 |
| C    | -4.4091380 | 7.3224390 | -1.1240440 |
| H    | -3.3476430 | 7.5659090 | -1.0078160 |
| H    | -4.9141880 | 7.5769250 | -0.1874760 |
| H    | -4.8205190 | 7.9656390 | -1.9101490 |
| C    | -6.1086290 | 5.5366100 | -1.6788160 |
| H    | -6.2880370 | 4.4748240 | -1.8749710 |
| H    | -6.5055900 | 6.1162880 | -2.5199750 |
| H    | -6.6881690 | 5.8063030 | -0.7910860 |
| C    | 5.1474990  | 6.9083440 | -2.4298690 |
| C    | 6.4843240  | 6.9073490 | -3.2087360 |
| H    | 7.3341350  | 7.1414910 | -2.5609950 |
| H    | 6.4597100  | 7.6556310 | -4.0088960 |
| H    | 6.6710240  | 5.9292020 | -3.6636930 |
| C    | 4.0101340  | 6.6328130 | -3.4319620 |
| H    | 4.0059950  | 7.4071300 | -4.2057900 |
| H    | 3.0280530  | 6.6444900 | -2.9482790 |
| H    | 4.1326380  | 5.6671250 | -3.9328140 |
| C    | 4.9159020  | 8.3081860 | -1.8131990 |
| H    | 5.7124280  | 8.5843680 | -1.1160770 |
| H    | 3.9676220  | 8.3437190 | -1.2668780 |
| H    | 4.8831900  | 9.0704810 | -2.5997380 |
| C    | 7.4009960  | 5.2211720 | 1.8069530  |
| C    | 7.3711840  | 4.1139880 | 2.8776700  |
| H    | 6.4221330  | 4.093150  | 3.4231810  |
| H    | 8.1683130  | 4.2863160 | 3.6080660  |
Atom coordinates for optimized $\text{AMIm-2}$:

|   | X        | Y        | Z        |
|---|----------|----------|----------|
| C | -5.30334 | -1.10389 | -0.48140 |
| C | -5.43328 | 0.25224  | -0.47304 |
| C | -3.91096 | -1.39343 | -0.23946 |
| C | -4.12076 | 0.79804  | -0.22639 |
| N | -3.20477 | -0.22085 | -0.11041 |
| C | -3.82809 | 2.17044  | -0.11453 |
| C | -2.53657 | 2.69563  | 0.04984  |
| N | -1.35274 | 1.97888  | 0.03847  |
| C | -0.33994 | 2.89490  | 0.19477  |
| C | -2.25133 | 4.09309  | 0.25898  |
| C | -0.89976 | 4.21708  | 0.35063  |
| C | 1.04629  | 2.63345  | 0.17675  |
| C | 1.63660  | 1.36436  | 0.06531  |
| N | 0.94235  | 0.17412  | 0.10310  |
| C | 1.84550  | -0.86503 | 0.09338  |
| C | 3.20308  | -0.32512 | -0.04119 |
| C | 3.06854  | 1.08579  | -0.07110 |
| C | 1.50448  | -2.22188 | 0.20879  |
| C | 0.19356  | -2.73990 | 0.20080  |
| N | -0.97265 | -2.03098 | 0.03931  |
| C | -1.99777 | -2.96031 | 0.02365  |
| C | -0.10396 | -4.14784 | 0.32262  |
C  -1.4527680  -4.2822920  0.2118120  
C  -3.3640840  -2.6872490  -0.1427520 
H  -6.0732090  -1.8422960  -0.6468430  
H  -6.3299820   0.8323710  -0.6301980  
H  -2.9935960   4.8727430   0.3364470  
H  -0.3305100   5.1192350   0.5124580  
H   0.6285510  -4.9258600   0.4725520  
H  -2.0333430  -5.1908800   0.2602860  
C  -4.9751600   3.1328500  -0.1683160  
C  -5.9455690   3.1353210   0.8480890  
C  -5.0980430   4.0362680  -1.2261110  
C  -7.0242540   4.0213030   0.8181390  
C  -6.1673700   4.9443580  -1.2954120  
C  -7.1114000   4.9147360  -0.2653220  
H  -7.9454580   5.6048780  -0.2965250  
H  -5.8299770   2.4324460  1.6638840  
H  -4.3458300   4.0195590  -2.0081340  
C   1.9260050   3.8418820   0.3245770  
C   2.5184530   4.1258090  1.5606200  
C   3.3348210   5.2503560  1.7322520  
C   2.9540200   5.8382890  -0.6309830  
C   3.5375190   6.0822280   0.6210530  
H   2.3328370   3.4467090  2.3838050  
H   4.1681710   6.9580600   0.7378460  
C   2.1401030   4.7048630  -0.7572200  
H   1.6651840   4.4678360  -1.7016100  
C   2.5972520  -3.2383480   0.3860200  
C   3.1001780  -3.9512060  -0.7085960  
C   3.1183340  -3.4731850  1.6630830  
C   4.1461670  -4.8705500  -0.5532430  
C   4.1446630  -4.4040400  1.8668580  
C   4.6390790  -5.0803220   0.7429010  
H   5.4467680  -5.7916100   0.8800980  
H   2.6833070  -3.7484760  -1.6878650  
H   2.7105400  -2.9093270  2.4933090  
C  -4.3081420  -3.8489390  -0.2117120
| Element | X      | Y      | Z      |
|---------|--------|--------|--------|
| C       | -5.2463610 | -4.0576240 | 0.8079370 |
| C       | -4.2634220 | -4.7367060 | -1.2948910 |
| C       | -6.1357780 | -5.1379660 | 0.7674100 |
| C       | -5.1373280 | -5.8275910 | -1.3764410 |
| C       | -6.0581870 | -6.0025900 | -0.3337000 |
| H       | -6.7408240 | -6.8453910 | -0.3806870 |
| H       | -3.5356990 | -4.5527450 | -2.0758870 |
| H       | -5.2599010 | -3.3623840 | 1.6384420 |
| C       | 4.4596010  | -0.9327030 | -0.1978510 |
| C       | 5.5515400  | -0.1023620 | -0.3980140 |
| C       | 4.1914220  | 1.9153140  | -0.2731910 |
| C       | 5.4203550  | 1.3071830  | -0.4343290 |
| C       | 6.9526440  | -0.4163970 | -0.6308240 |
| C       | 6.7775250  | 1.9542200  | -0.6835920 |
| N       | 7.6329040  | 0.7790140  | -0.7838660 |
| H       | 7.0895650  | 2.6078190  | 0.1406570 |
| H       | 6.7992180  | 2.5432740  | -1.6089860 |
| N       | 7.7065980  | -1.4845110 | -0.7469820 |
| C       | 8.9518770  | 0.4625220  | -1.0236250 |
| C       | 8.9737720  | -0.9657220 | -0.9935490 |
| C       | 10.1841610 | -1.6371720 | -1.2033020 |
| C       | 11.3286890 | -0.8802520 | -1.4358320 |
| C       | 11.2866750 | 0.5274870  | -1.4622700 |
| C       | 10.0978670 | 1.2243200  | -1.2563010 |
| H       | 10.0691660 | 2.3093820  | -1.2769520 |
| H       | 10.2132300 | -2.7217470 | -1.1828350 |
| H       | 12.2770810 | -1.3827040 | -1.6011910 |
| H       | 12.2013150 | 1.0829260  | -1.6471370 |
| H       | 4.5980310  | -2.0021620 | -0.1877440 |
| H       | 4.1014440  | 2.9908060  | -0.3229660 |
| C       | -8.1053950 | 4.0523360  | 1.9162920 |
| C       | -6.2589490 | 5.9187470  | -2.4864230 |
| C       | -9.4846470 | 3.7408760  | 1.2882060 |
| H       | -9.7545500 | 4.4664970  | 0.5152350 |
| H       | -10.2671460 | 3.7646680  | 2.0551210 |
| H       | -9.4896630 | 2.7467840  | 0.8292170 |
| Atoms | X-Position | Y-Position | Z-Position |
|-------|------------|------------|------------|
| C     | -7.8421210 | 3.0196530  | 3.0283620  |
| H     | -8.6349790 | 3.0799840  | 3.7808240  |
| H     | -6.8899060 | 3.2014990  | 3.5370150  |
| H     | -7.8322440 | 1.9957300  | 2.6411600  |
| C     | -8.1443450 | 5.4561370  | 2.5657980  |
| H     | -8.3740040 | 6.2382370  | 1.8362340  |
| H     | -7.1815260 | 5.7010200  | 3.0259550  |
| H     | -8.9129500 | 5.4934050  | 3.3460620  |
| C     | -7.4825630 | 6.8494870  | -2.3946700 |
| H     | -8.4231010 | 6.2889540  | -2.3951600 |
| H     | -7.4551430 | 7.4724670  | -1.4946380 |
| H     | -7.4994160 | 7.5207240  | -3.2592650 |
| C     | -4.9880360 | 6.8001730  | -2.5280620 |
| H     | -5.0331030 | 7.4947320  | -3.3745420 |
| H     | -4.0792230 | 6.2014380  | -2.6374490 |
| H     | -4.8913190 | 7.3902740  | -1.6106490 |
| C     | -6.3657680 | 5.1125070  | -3.8026310 |
| H     | -7.2632990 | 4.4854390  | -3.8053220 |
| H     | -5.5018210 | 4.4584030  | -3.9512840 |
| H     | -6.4224950 | 5.7904550  | -4.6617830 |
| C     | 3.9996140  | 5.5981840  | 3.0788410  |
| C     | 3.6773000  | 4.5654010  | 4.1751750  |
| H     | 2.6028690  | 4.5047700  | 4.3755190  |
| H     | 4.1706130  | 4.8540750  | 5.1088000  |
| H     | 4.0327030  | 3.5644190  | 3.9102630  |
| C     | 5.5358710  | 5.6448400  | 2.9011370  |
| H     | 5.9211190  | 4.6738270  | 2.5724100  |
| H     | 6.0211330  | 5.8971800  | 3.8505730  |
| H     | 5.8404600  | 6.3934030  | 2.1637700  |
| C     | 3.4985730  | 6.9814100  | 3.5578840  |
| H     | 2.4131690  | 6.9764200  | 3.7006950  |
| H     | 3.7374040  | 7.7724440  | 2.8409940  |
| H     | 3.9657280  | 7.2451440  | 4.5132090  |
| C     | 3.2188080  | 6.8066640  | -1.8007710 |
| C     | 2.7123300  | 8.2191900  | -1.4238030 |
| H     | 1.6361550  | 8.2073800  | -1.2229340 |
Atom coordinates for optimized AMIm-6:

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -6.6865270| 1.5475170 | -0.0069010|
| C    | -6.0424530| 2.7441650 | 0.0088790 |
| C    | -5.6776500| 0.5200800 | -0.0282600|
| C    | -4.6291620| 2.4683060 | -0.0040810|
| N    | -4.4273170| 1.1041280 | -0.0220160|
| C    | -3.6358400| 3.4539110 | 0.0298120 |
C  -2.2672070  3.1843830  0.0498540
N  -1.6750010  1.9366790  0.0313590
C  -0.3184300  2.1319140  0.0527100
C  -1.2402300  4.1943920  0.0803300
C  -0.0449640  3.5526320  0.0918190
C  -4.0715000  4.8892770  0.0502600
C  -4.5836880  5.4866280 -1.1081980
C  -3.9685900  5.6407060  1.2274880
C  -4.9948100  6.8256730 -1.1106390
C  -4.3689510  6.9824690  1.2675280
C  -4.8764140  7.5451110  0.0874640
C  -5.5563640  7.5190340 -2.3677350
C  -4.2698320  7.8400670  2.5444380
C  -5.6211760  6.5711620 -3.5806420
H  -4.6312100  6.1964760 -3.8602950
H  -6.0263930  7.1077110 -4.4447630
H  -6.2715780  5.7106460 -3.3923930
C  -6.9890430  8.0278050 -2.0803200
H  -7.6546250  7.1976750 -1.8214500
H  -7.3999190  8.5291220 -2.9640720
H  -7.0102960  8.7432510 -1.2530670
C  -4.6520970  8.7175320 -2.7421060
H  -3.6319790  8.3845290 -2.9596340
H  -4.5979230  9.4546980 -1.9355990
H  -5.0411870  9.2243830 -3.6321940
C  -3.3510020  9.0561830  2.2777980
H  -2.3422170  8.7314790  2.0021390
H  -3.2731330  9.6792070  3.1760880
H  -3.7310470  9.6866680  1.4683490
C  -3.6879920  7.0536630  3.7347170
H  -2.6755090  6.6912470  3.5291200
H  -4.3110380  6.1933090  4.0001600
H  -3.6330250  7.7041240  4.6136990
C  -5.6791940  8.3400400  2.9418890
H  -6.1361330  8.9436740  2.1521010
H  -5.6230540  8.9594470  3.8442550
|     |        |        |        |        |        |
|-----|--------|--------|--------|--------|--------|
| H   | -6.3486590 | 7.4986020 | 3.1487750 |        |        |
| H   | -5.1914230 | 8.5839940 | 0.1016640 |        |        |
| H   | -4.6490350 | 4.8866950 | -2.0079930 |        |        |
| H   | -3.5728460 | 5.1557720 | 2.1118540 |        |        |
| C   | -5.9543570 | -0.8517180 | -0.0162630 |        |        |
| C   | -4.9741210 | -1.8443810 | 0.0098700 |        |        |
| N   | -3.6077820 | -1.6462270 | 0.0056840 |        |        |
| C   | -3.0219780 | -2.8848280 | 0.0397310 |        |        |
| C   | -5.2477530 | -3.2590390 | 0.0422660 |        |        |
| C   | -4.0511420 | -3.8992940 | 0.0755510 |        |        |
| C   | -1.6478500 | -3.1638660 | 0.0204510 |        |        |
| C   | -0.6245380 | -2.2085810 | -0.0411590 |        |        |
| N   | -0.7870970 | -0.8363850 | -0.0104860 |        |        |
| C   | 0.4613980 | -0.2318640 | -0.0261780 |        |        |
| C   | 1.4954800 | -1.2733810 | -0.1059150 |        |        |
| C   | 0.7995490 | -2.5068840 | -0.1348970 |        |        |
| C   | 0.6849810 | 1.1455990 | 0.0241730 |        |        |
| C   | 2.0696020 | 1.7277940 | 0.0643150 |        |        |
| C   | 2.6533560 | 2.2118290 | -1.1127060 |        |        |
| C   | 2.6775920 | 1.9836440 | 1.2938630 |        |        |
| C   | 3.8570830 | 2.7385900 | 1.3764900 |        |        |
| C   | 3.8222220 | 2.9803790 | -1.0787190 |        |        |
| C   | 4.4012830 | 3.2266220 | 0.1797450 |        |        |
| C   | 4.3617540 | 3.6506070 | -2.3600960 |        |        |
| C   | 3.7304240 | 5.0621300 | -2.4539110 |        |        |
| H   | 2.6376240 | 5.0030220 | -2.4947860 |        |        |
| H   | 4.0765150 | 5.5791560 | -3.3568290 |        |        |
| H   | 4.0007800 | 5.6749130 | -1.5870230 |        |        |
| C   | 3.9914940 | 2.8486040 | -3.6264270 |        |        |
| H   | 2.9122000 | 2.8257630 | -3.8047910 |        |        |
| H   | 4.3598070 | 1.8206210 | -3.5614230 |        |        |
| H   | 4.4486850 | 3.3179160 | -4.5042070 |        |        |
| C   | 5.8984560 | 3.7914820 | -2.3398490 |        |        |
| H   | 6.2497050 | 4.4129250 | -1.5100540 |        |        |
| H   | 6.2293220 | 4.2771540 | -3.2651190 |        |        |
| H   | 6.3762230 | 2.8097900 | -2.2804650 |        |        |
|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| H | -11.2482990 | 0.4813570 | -1.9192570 |
| H | -12.2054010 | -0.9023920 | -1.3758870 |
| H | -12.2163720 | -0.4417170 | -3.0828370 |
| C | -11.1876950 | -1.8301180 | 2.8219310  |
| H | -10.8412390 | -0.8139670 | 3.0370490  |
| H | -11.6872730 | -2.2156970 | 3.7178920  |
| H | -11.9347820 | -1.7666580 | 2.0252680  |
| C | -10.5308470 | -4.1727800 | 2.1475830  |
| H | -11.2583140 | -4.1852240 | 1.3306880  |
| H | -9.7114190  | -4.8463530 | 1.8756250  |
| C | -9.0404280  | -2.8221750 | 3.6303770  |
| H | -8.6525650  | -1.8363990 | 3.9068580  |
| H | -8.1886040  | -3.4803410 | 3.4298940  |
| H | -9.5694390  | -3.2237680 | 4.5008090  |
| C | -1.3107620  | -4.6256630 | 0.1125000  |
| C | -0.9746840  | -5.1816940 | 1.3522910  |
| C | -1.3669010  | -5.4444430 | -1.0218830 |
| C | -0.6654090  | -6.5421050 | 1.4759530  |
| C | -1.0678960  | -6.8115610 | -0.9422020 |
| C | -0.7150720  | -7.3274560 | 0.3142200  |
| H | -1.6400750  | -4.9913280 | -1.9674660 |
| H | -0.9493830  | -4.5275800 | 2.2155720  |
| H | -0.4787380  | -8.3840880 | 0.3927670  |
| C | -0.2831540  | -7.1885860 | 2.8217650  |
| C | -1.3068380  | -8.2954290 | 3.1700420  |
| H | -2.3157540  | -7.8797550 | 3.2599000  |
| H | -1.0480480  | -8.7674180 | 4.1245230  |
| H | -1.3351030  | -9.0796660 | 2.4076130  |
| C | -0.2663360  | -6.1695180 | 3.9773100  |
| H | -1.2491390  | -5.7131360 | 4.1331000  |
| H | 0.4591880   | -5.3676260 | 3.8060480  |
| H | 0.0138850   | -6.6735840 | 4.9078940  |
| C | 1.1281760   | -7.8134350 | 2.7110210  |
| H | 1.1753930   | -8.5824770 | 1.9340880  |
| H | 1.4138950   | -8.2809270 | 3.6598260  |
| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| H    | 1.8762060 | -7.0491830 | 2.4736060 |
| C    | -1.1169560 | -7.7458420 | -2.1672850 |
| C    | -1.5317720 | -7.0049770 | -3.4527310 |
| H    | -2.5294540 | -6.5628940 | -3.3651840 |
| H    | -1.5555740 | -7.7084980 | -4.2911720 |
| H    | -0.8266130 | -6.2084490 | -3.715260 |
| C    | 0.2806390  | -8.3678270 | -2.4001650 |
| H    | 1.0256190  | -7.5911280 | -2.6040040 |
| H    | 0.2571170  | -9.0464110 | -3.2602430 |
| H    | 0.6228410  | -8.9418360 | -1.5337790 |
| C    | -2.1425940 | -8.8761400 | -1.9117450 |
| H    | -3.1438640 | -8.4655300 | -1.7454460 |
| H    | -1.8794410 | -9.4781760 | -1.0369320 |
| H    | -2.1905640 | -9.5484210 | -2.7757230 |
| H    | -7.7496850 | 1.3623370  | 0.0066810  |
| H    | -6.4732240 | 3.7332730  | 0.0374090  |
| H    | -1.4247500 | 5.2576440  | 0.0911500  |
| H    | 0.9387560  | 3.9924910  | 0.1170040  |
| H    | -6.2359670 | -3.6928300 | 0.0421140  |
| H    | -3.8704140 | -4.9620130 | 0.1100530  |
| Pt   | -2.6199290 | 0.1375840  | 0.0009840  |
| C    | 2.9052760  | -1.2332140 | -0.1728780 |
| C    | 3.5808850  | -2.4501580 | -0.2798830 |
| C    | 1.4908100  | -3.7219270 | -0.2738930 |
| C    | 2.8628990  | -3.6743760 | -0.3419920 |
| H    | 3.4564780  | -0.3033920 | -0.1509430 |
| H    | 0.9804320  | -4.6697380 | -0.3363380 |
| C    | 4.9963070  | -2.8168070 | -0.3603660 |
| C    | 3.7988890  | -4.8536610 | -0.4851560 |
| N    | 5.0841400  | -4.1801300 | -0.4811810 |
| H    | 3.6464750  | -5.4064210 | -1.4202440 |
| H    | 3.7235870  | -5.5617060 | 0.3490940  |
| N    | 6.2111050  | -2.2760080 | -0.3402970 |
| C    | 7.1226460  | -3.3322100 | -0.4517100 |
| C    | 6.4089140  | -4.5481950 | -0.5418860 |
| C    | 8.5202780  | -3.3324840 | -0.4786240 |
| Element | X  | Y  | Z  |
|---------|----|----|----|
| C       |  9.1610210 | -4.5614480 | -0.5981560 |
| C       |  8.4388280 | -5.7678310 | -0.6887740 |
| C       |  7.0476210 | -5.7837720 | -0.6618480 |
| H       |  6.4876160 | -6.7106200 | -0.7308840 |
| H       |  9.0713400 | -2.4028320 | -0.4024090 |
| H       | 10.2458150 | -4.5925170 | -0.6206450 |
| H       |  8.9788270 | -6.7052030 | -0.7808810 |
| Pt      |  6.8728060 | -0.3706300 | -0.2128060 |
| Cl      |  7.2226320 | -0.6670720 | 2.1338550 |
| Cl      |  6.5455760 | -0.1313390 | -2.5665670 |
| N       |  7.7217280 | 1.4058340  | -0.1012030 |
| C       |  8.3597750 | 2.3696280  | -0.0219770 |
| C       |  9.1510660 | 3.5523200  | 0.0865640  |
| C       |  9.6184420 | 3.9595910  | 1.3496950  |
| C       |  9.4646960 | 4.2941550  | -1.0669470 |
| C       | 10.3952660 | 5.1099200  | 1.4498730  |
| C       | 10.2429530 | 5.4418650  | -0.9477160 |
| C       | 10.7070190 | 5.8498710  | 0.3058720  |
| H       | 10.4876150 | 6.0183610  | -1.8341730 |
| H       | 11.3137230 | 6.7463600  | 0.3914820  |
| H       |  9.3698610 | 3.3746580  | 2.2285420  |
| H       | 10.7582350 | 5.4289140  | 2.4217230  |
| H       |  9.0969320 | 3.9661890  | -2.0329500 |

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