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 dialdehydebenzoporphyrin was done using a previously published procedure.[1]

Spectral measurements

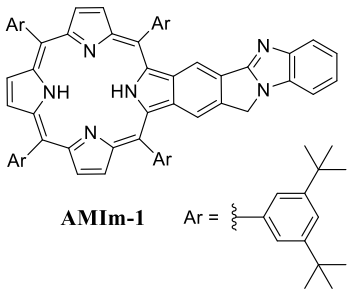
NMR spectroscopy experiments were performed using a 500 MHz Varian NMR instrument. All NMR experiments were conducted using $CDCl_3$ passed through a pad of alumina as a solvent (δ ^{1}H = 7.26 ppm; δ ^{13}C = 77.16 ppm). Mass spectrometry experiments were done using a Thermoscientific MALDI-LTQ-XL-Orbitrap 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 $\pm$10%.

Nanosecond Laser Flash Photolysis. The studied compounds were excited by a 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

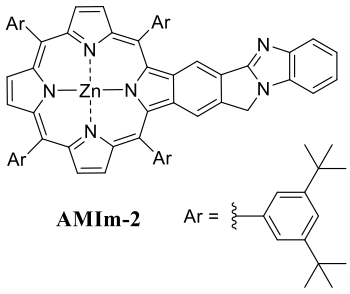
β,β'-Benzimidazole-Fused Free-Base Benzoporphyrin (AMIm-1)



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**.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.97 (d, J = 2.9 Hz, 2H), 8.93 (d, J = 4.8 Hz, 2H), 8.78 (s, 2H), 8.12 (d, J = 1.8 Hz, 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), -2.58 (s, 2H). ^{13}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): λ_{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)



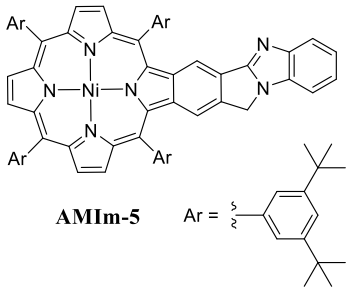
AMIm-1 (10 mg, 0.0081 mmol) was combined with zinc acetate (14.8 mg, 0.081 mmol) chloroform (1.5 mL) and methanol (0.5 mL) and refluxed for 1 hour. The reaction mixture was then cooled to room temperature and recrystallized with methanol to yield 9.7 mg (92% yield) pure **AMIm-2**.

^{1}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). ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.83,

152.09, 151.63, 150.59, 150.56, 150.14, 150.07, 149.35, 149.19, 149.08, 148.69, 145.85, 145.24, 142.80, 142.07, 141.84, 141.82, 141.20, 140.98, 140.74, 133.19, 132.32, 132.26, 131.76, 131.38, 129.57, 128.26, 128.23, 127.54, 124.09, 124.06, 122.41, 122.25, 121.88, 121.53, 121.13, 120.97, 120.33, 119.60, 119.06, 109.25, 47.17, 35.44, 35.38, 35.20, 31.96, 31.91. UV/Vis (Toluene): λ_{max} (log ε) = 442 (5.78), 563 (4.58), 601 (3.85), nm; HRMS (MALDI): m/z: calculated for $C_{88}H_{98}N_6Zn$: 1302.713; found: 1302.7129

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**.

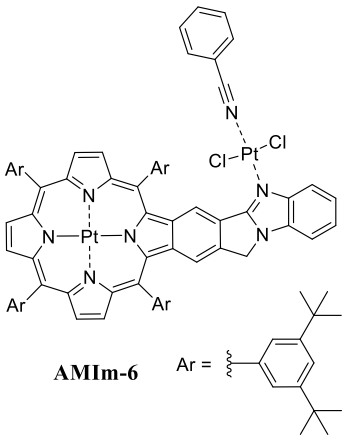


AMIm-5

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.81 (d, J = 4.9 Hz, 1H), 8.77 – 8.71 (m, 6H), 7.96 (t, J = 1.7 Hz ,1H), 7.87 (t, 2H), 7.84 (t, 4H), 7.83 (d, J = 1.9 Hz ,2H), 7.82 (d, J = 1.9 Hz, 2H), 7.78 (s, 1H), 7.70 (m, 2H), 7.45 – 7.43 (m, 1H), 7.28 (m, 1H), 6.97 (s, 1H), 4.95 (s, 2H), 1.48 (s, 16H), 1.47 (s, 53H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.46, 150.73, 450.69,149.05, 139.32, 132.83, 131.78, 131.73, 131.65, 128.39, 127.55, 127.48, 121.19, 120.81, 119.24, 109.10, 77.27, 77.02, 76.77, 46.96, 35.20, 35.15, 34.98, 31.71, 31.66, 29.73. UV/Vis (Toluene): λ_{max} (log ε) = 437 (5.48), 547 (4.39), 584 (4.14) nm; MS (ESI): m/z: calculated for $C_{88}H_{98}N_6Ni$: 1297.7279; found: 1297.7257.

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

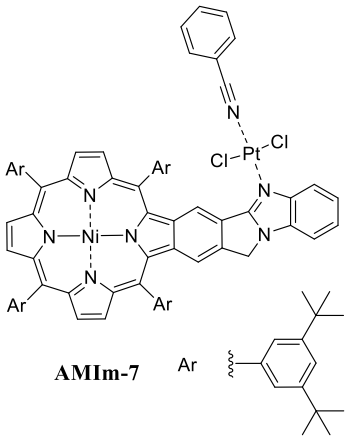
$PtCl_2$ (12.5 mg, 0.0470 mmol) was added with benzonitrile (3 mL) and heated at 110 ˚C for 1 hour. **1** (10 mg, 0.0081 mmol) was then added to the reaction mixture, the system was purged with argon, and the reaction was heated at 175 ˚C overnight. The reaction was then cooled, and the solvent removed 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): λ_{max} (log ε) = 426 (5.39), 526 (4.48), 559 (4.38) nm; HRMS (MALDI): m/z: calculated for $C_{95}H_{103}Cl_2N_7Pt_2$: 1802.7020; found: 1802.7033

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

$PtCl_2$ (24.0mg, 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): λ_{max} (log ε) = 444 (5.33), 548 (4.37), 589 (4.06) nm; HRMS (ESI): m/z: calculated for $C_{95}H_{103}N_7NiPt$: 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) $Å^3$	
Z	2	
Density (calculated)	1.197 Mg/m^3	
Absorption coefficient	3.235 mm^{-1}	
F(000)	1884	
Crystal size	0.07 x 0.045 x 0.01 mm^3	
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 F^2	
Data / restraints / parameters	17099 / 67 / 993	
Goodness-of-fit on F^2	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 $e.Å^{-3}$	

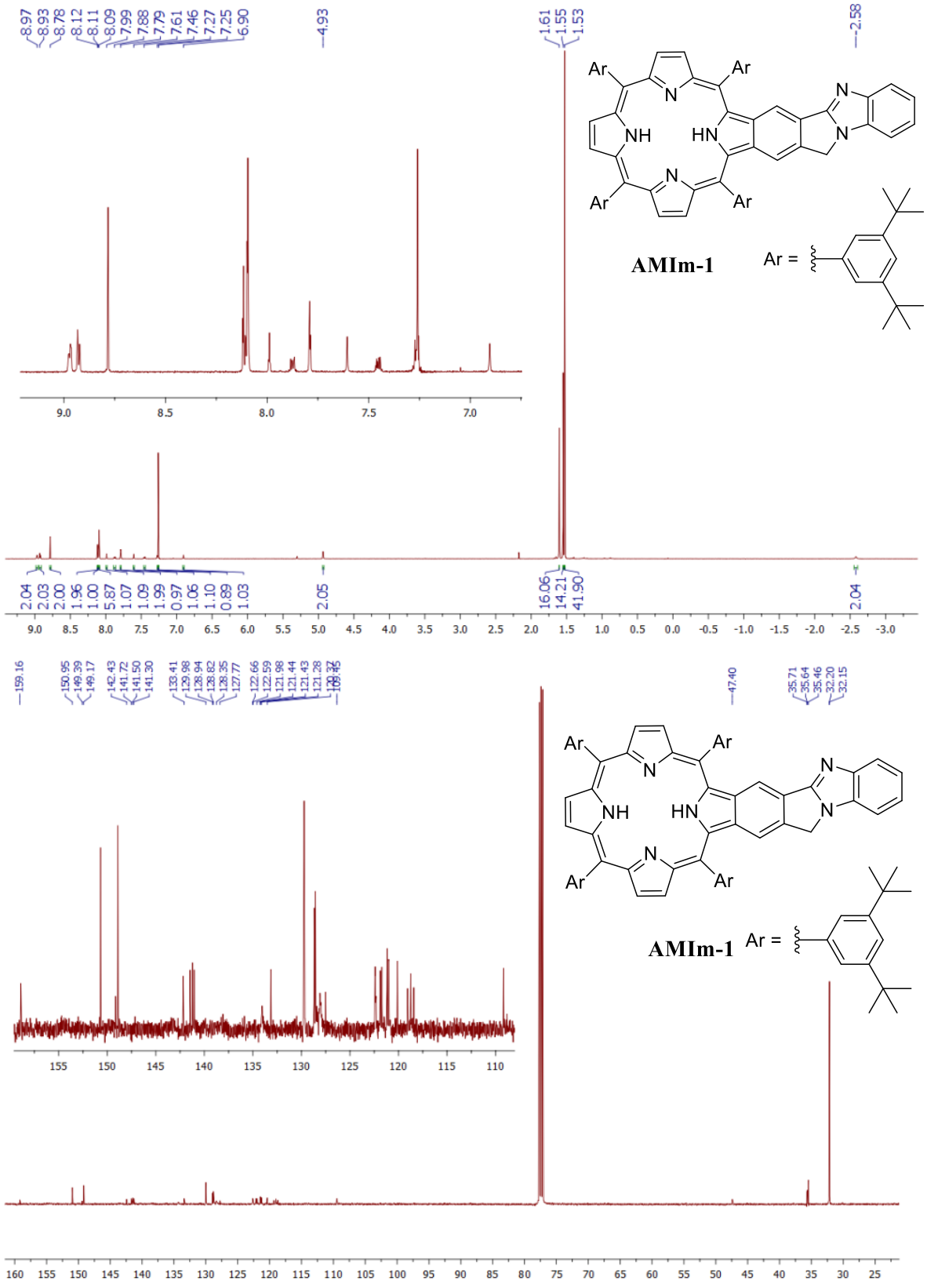
Table S2. Crystallographic refinement data for **AMIm-6**

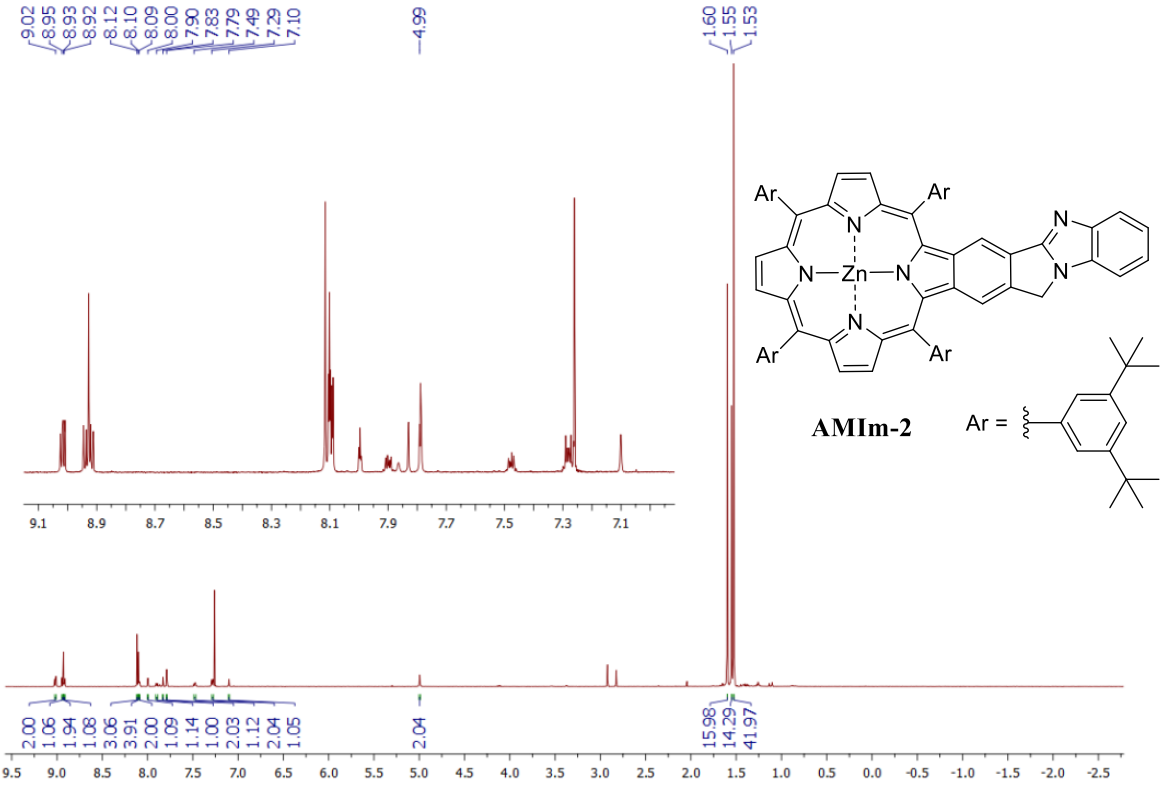
Compound	**AMIm-6**
Formula	$C_{133.5}H_{147}Cl_2N_7Pt_2$
$D_{calc.}$/ g cm^{-3}	1.278
m/mm^{-1}	5.081
Formula Weight	2310.65
Colour	metallic dark red
Shape	block
Size/mm^3	0.05×0.04×0.03
T/K	220.1(8)
Crystal System	triclinic
Space Group	P-1
a/Å	10.41830(10)
b/Å	17.4812(2)
c/Å	34.5651(2)
a/°	85.0250(10)
b/°	89.3060(10)
g/°	73.2960(10)
V/Å^3	6006.25(10)
Z	2
Z'	1
Wavelength/Å	1.54184
Radiation type	Cu K_a
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	$C_{112.50}H_{123}Cl_2N_7NiPt$
$D_{calc.}$/ g cm^{-3}	1.287
m/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/Å	15.4224(2)
b/Å	18.4372(2)
c/Å	18.7956(3)
a/°	68.6230(10)
b/°	81.3910(10)
g/°	81.8510(10)
V/Å^3	4898.58(12)
Z	2
Z'	1
Wavelength/Å	1.54184
Radiation type	Cu K_a
Q_{min}/°	2.539
Q_{max}/°	80.618
Measured Refl.	209129
Independent Refl.	21185
R_{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

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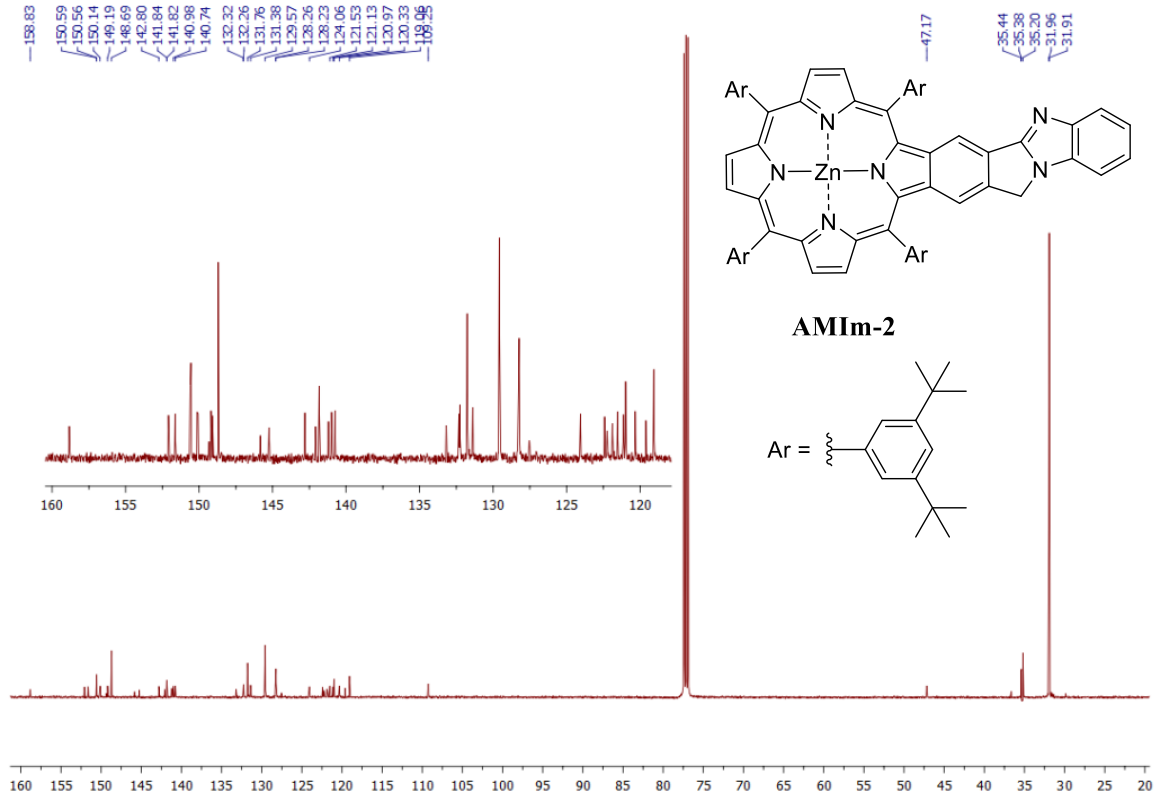
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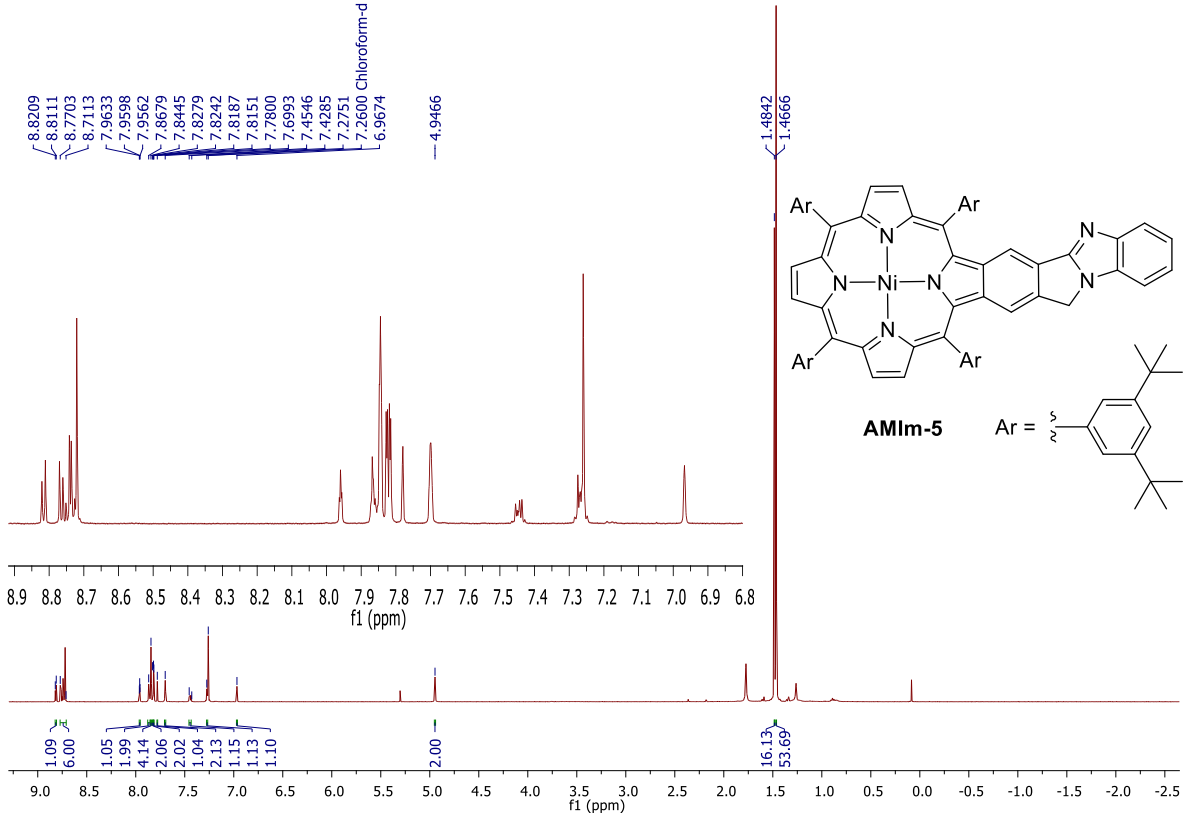
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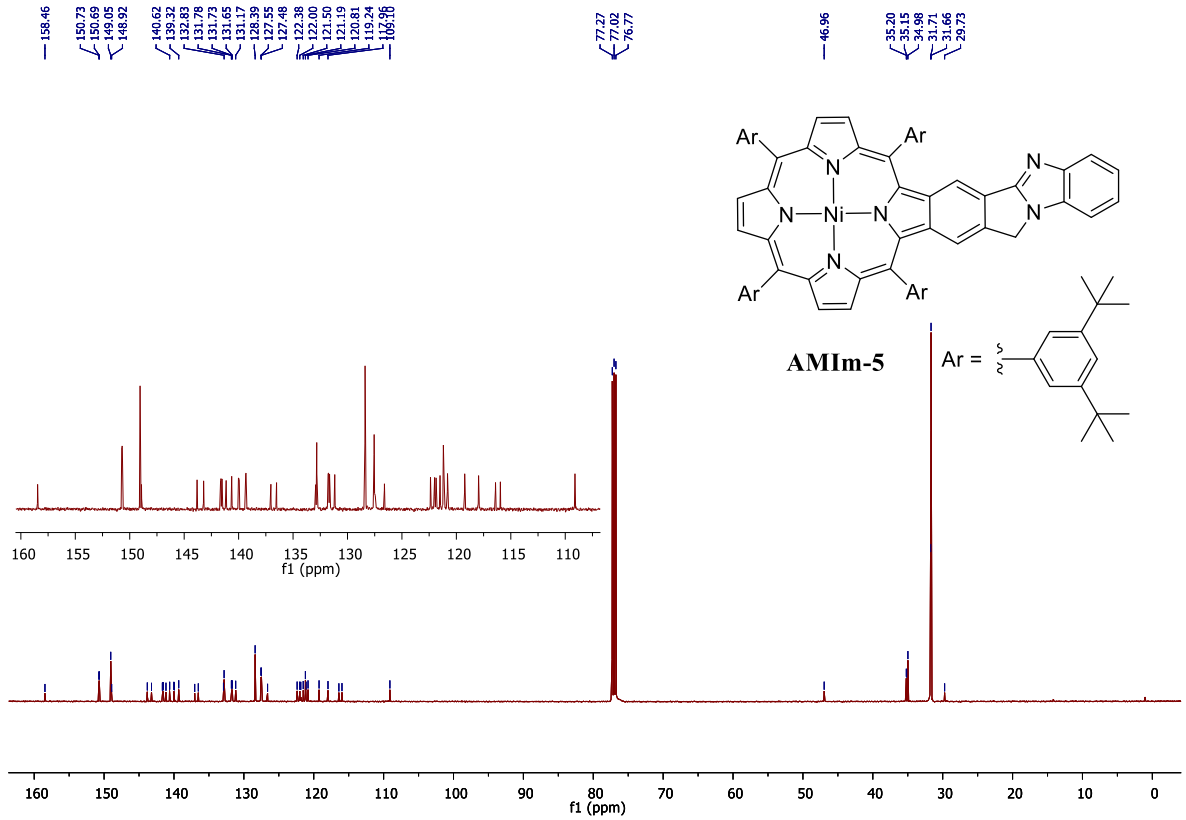
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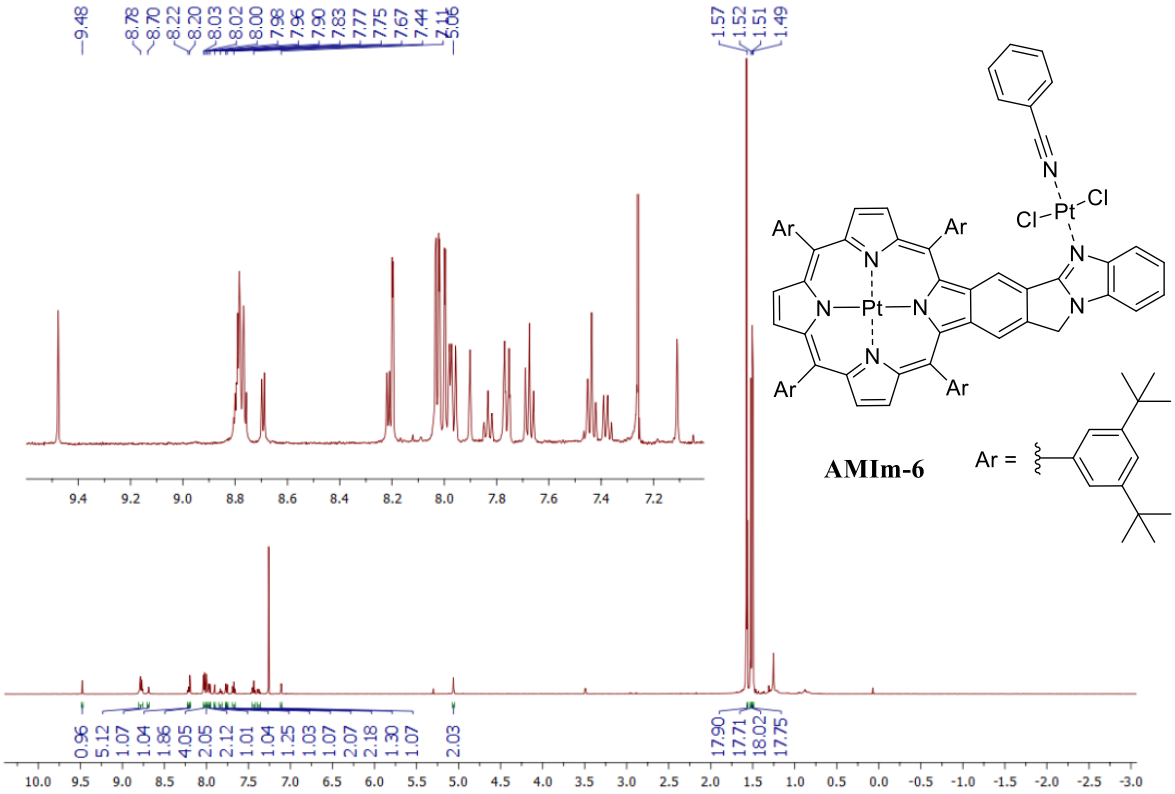
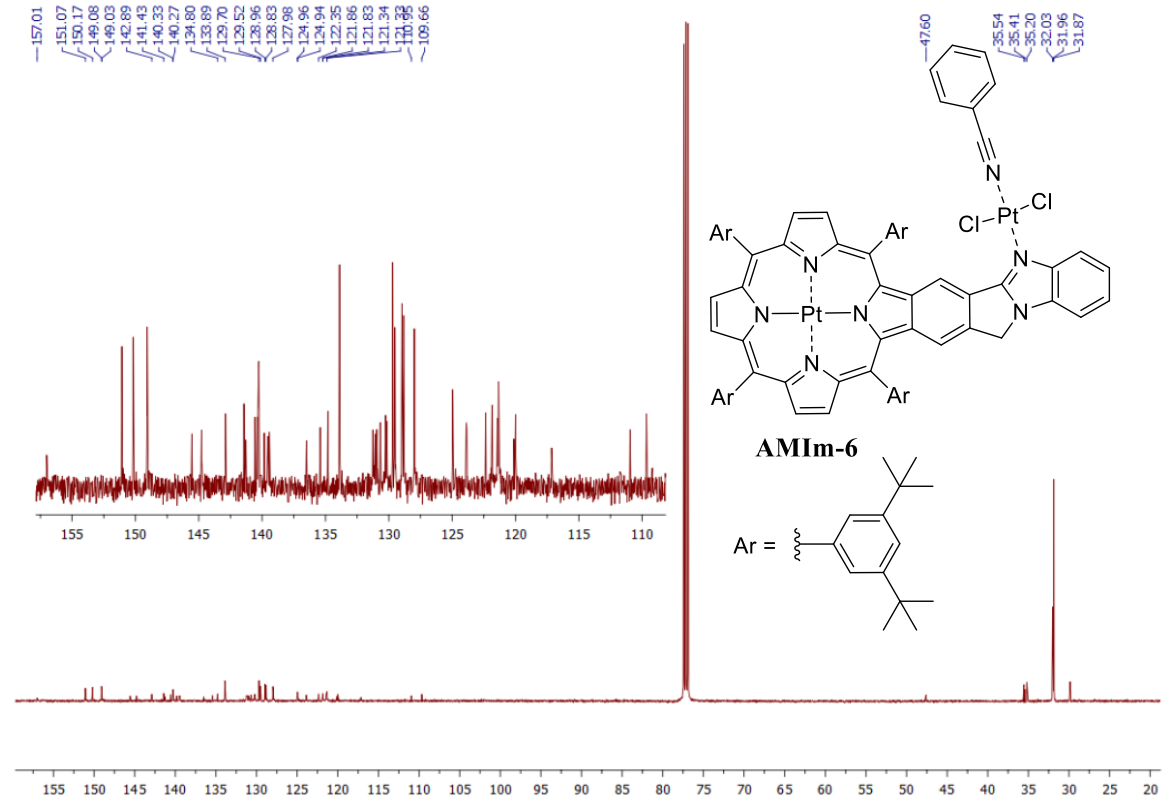
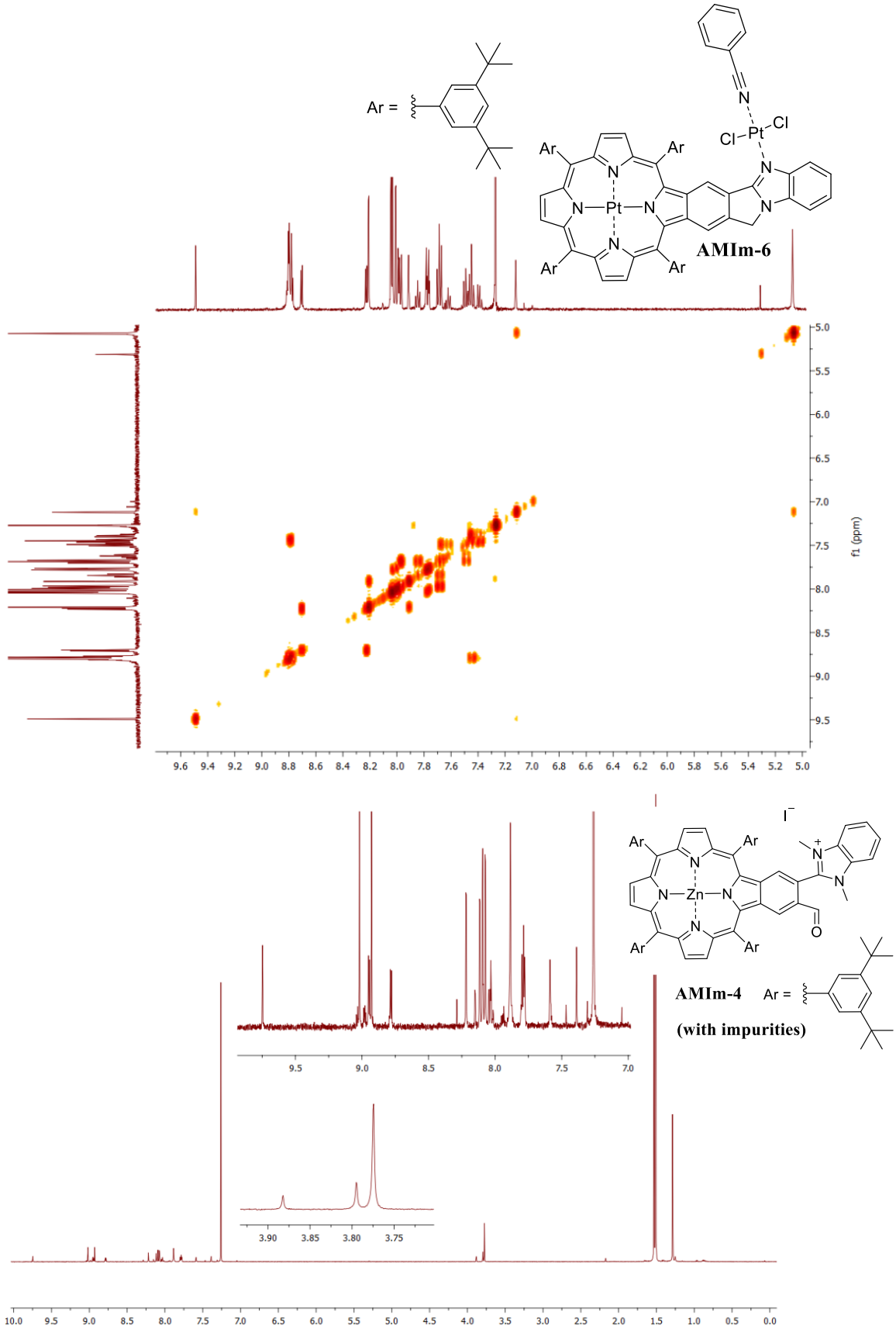

AMIm-6
Ar =


AMIm-6
Ar =


Ar =
AMIm-6
f1 (ppm)
AMIm-4
Ar =
(with impurities)

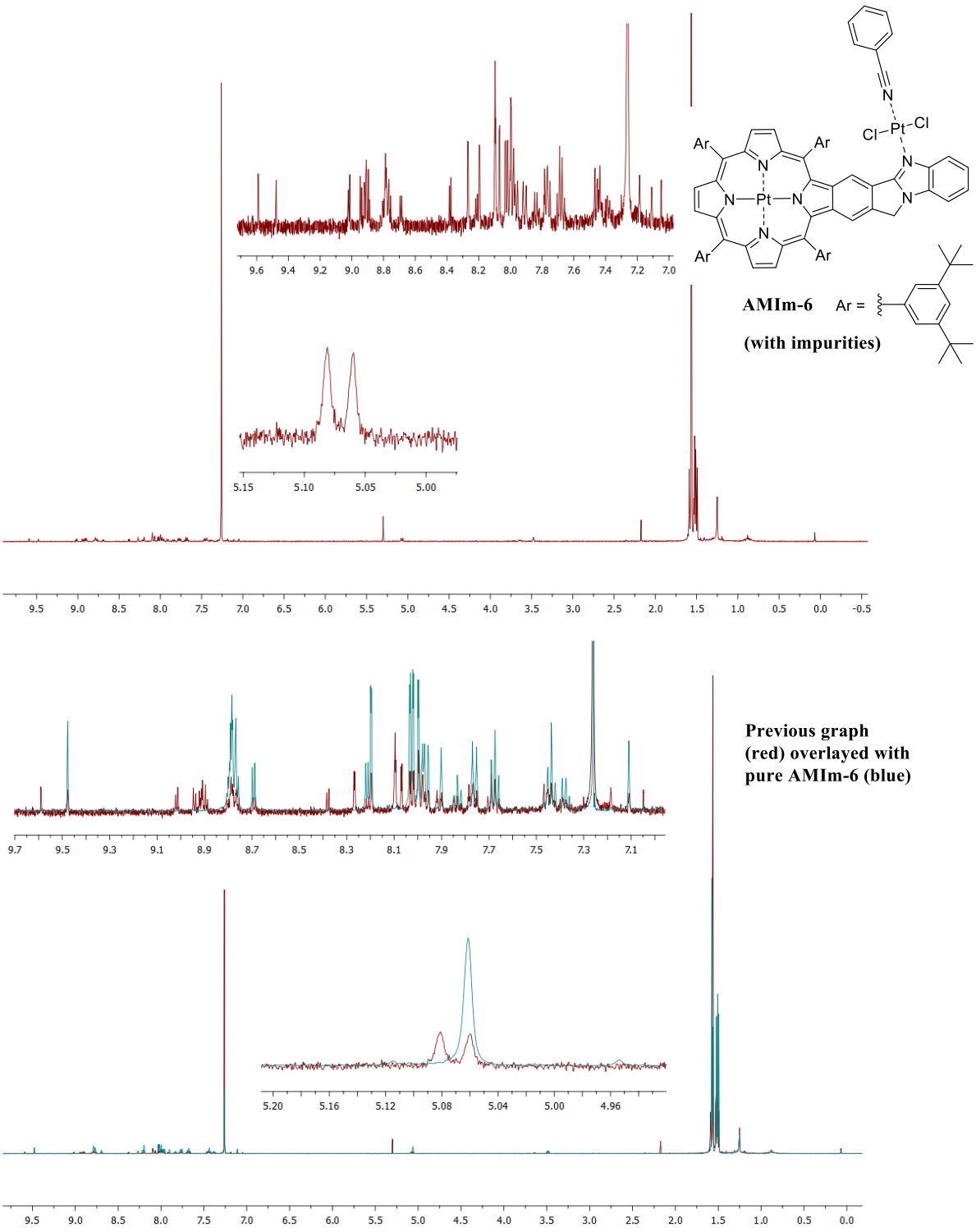
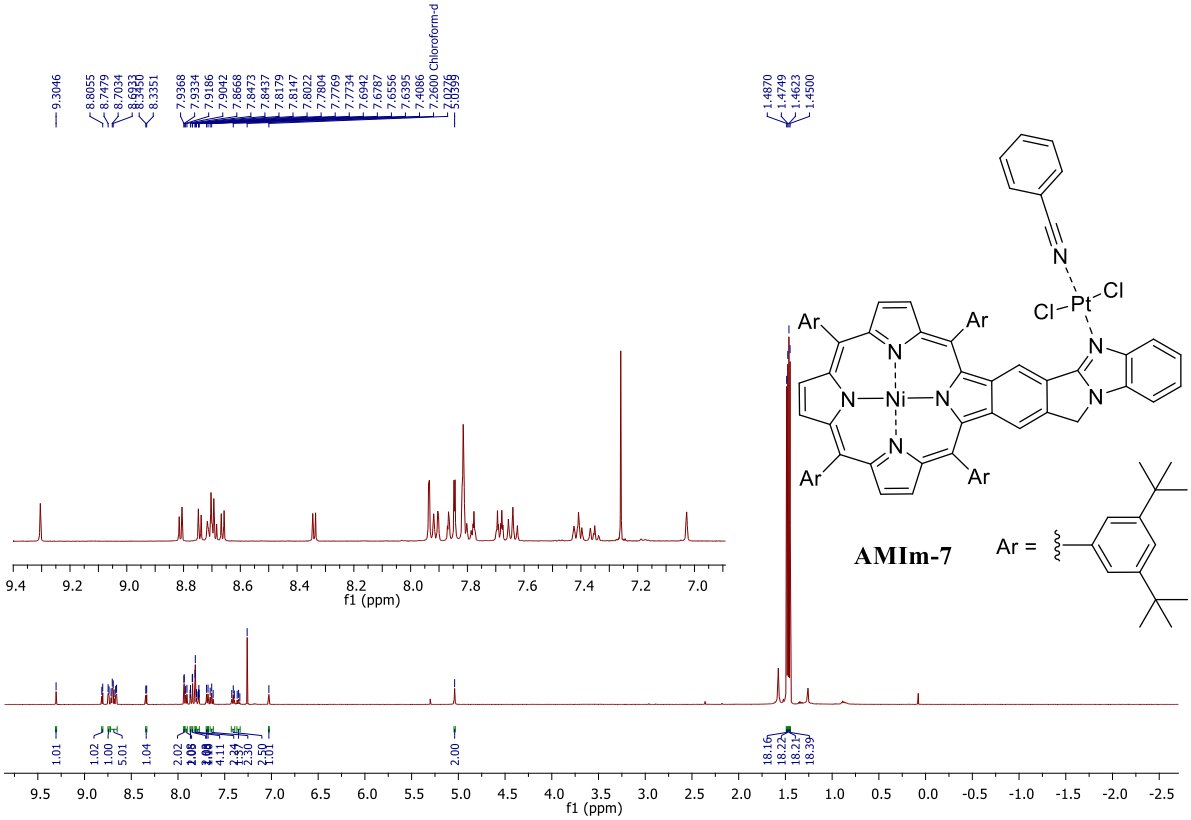


Figure S1. Proton NMR of product mixture resulting from reaction of **AMIm-2**, $PtCl_2$, and benzonitrile. Overlay with pure **AMIm-6** proton NMR indicates **AMIm-6** is a major product of the reaction.


AMIm-7
Ar =
f1 (ppm)

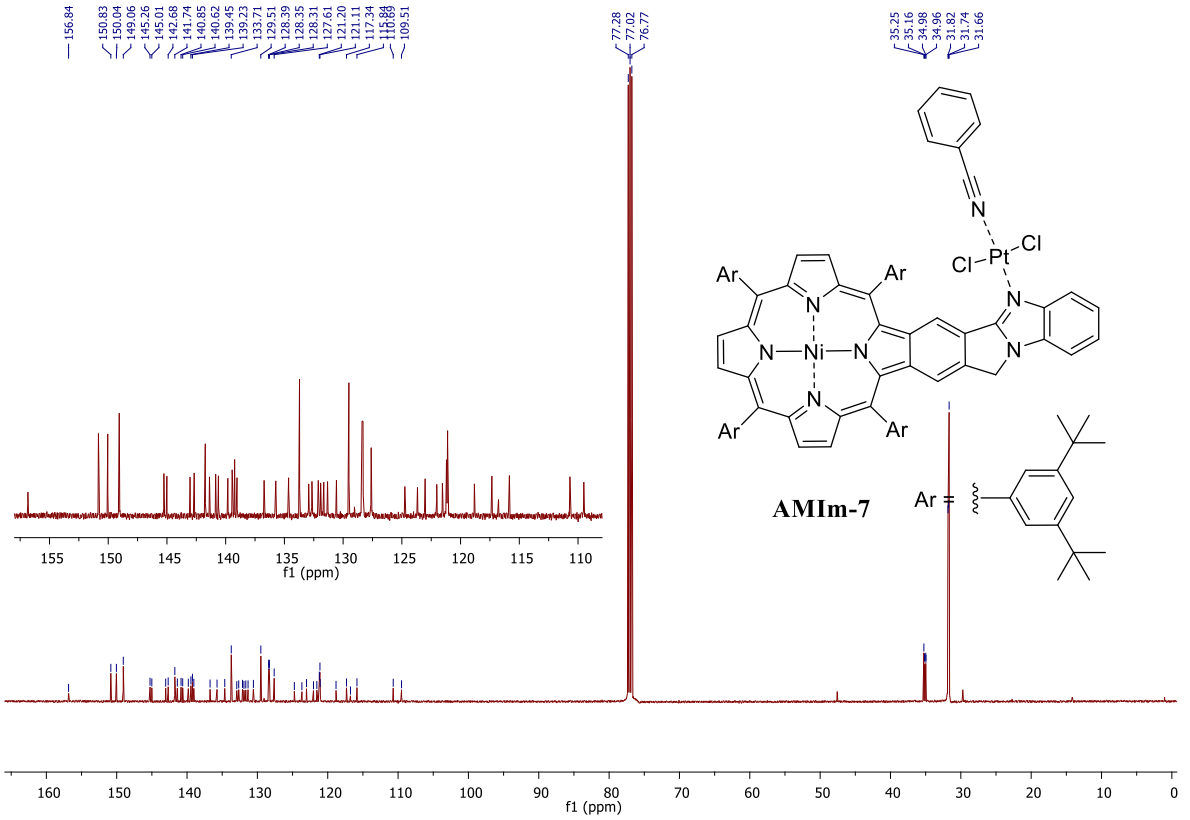
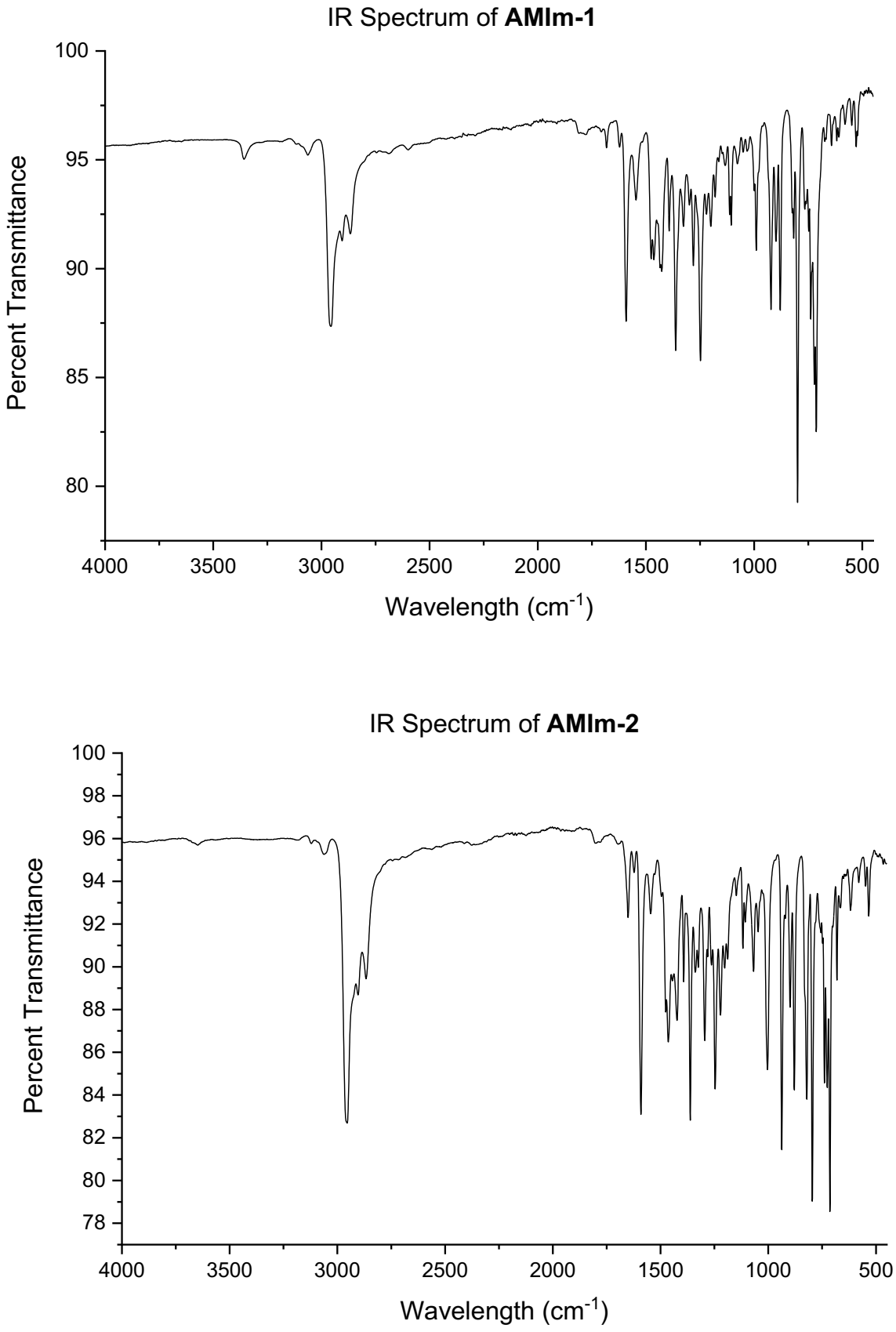

AMIm-7
Ar =
f1 (ppm)

Figure S2. Fourier Transform Infrared Spectra



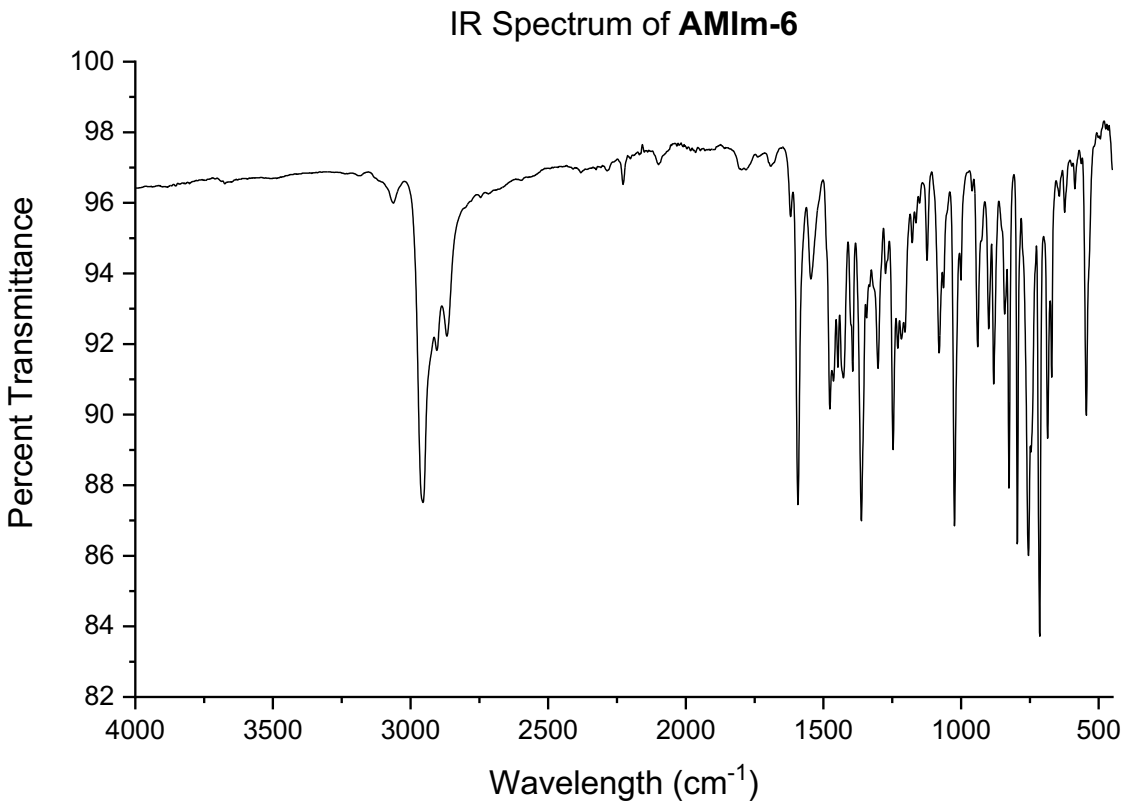


Figure S2. FT-IR spectra of the indicated compounds.

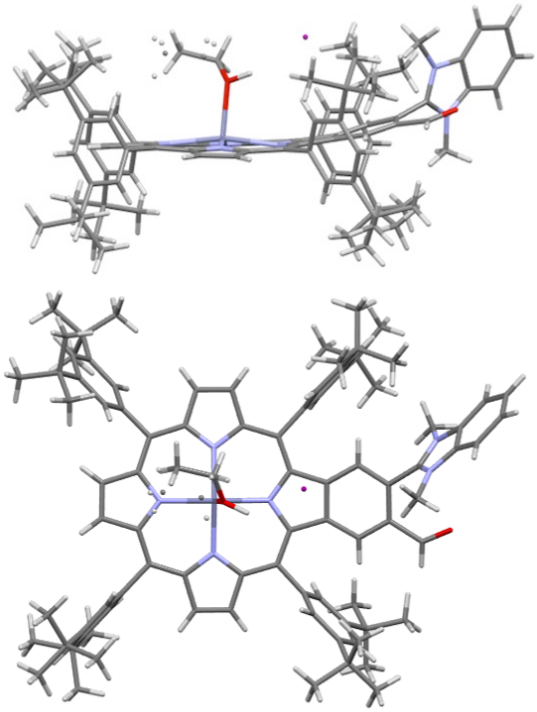
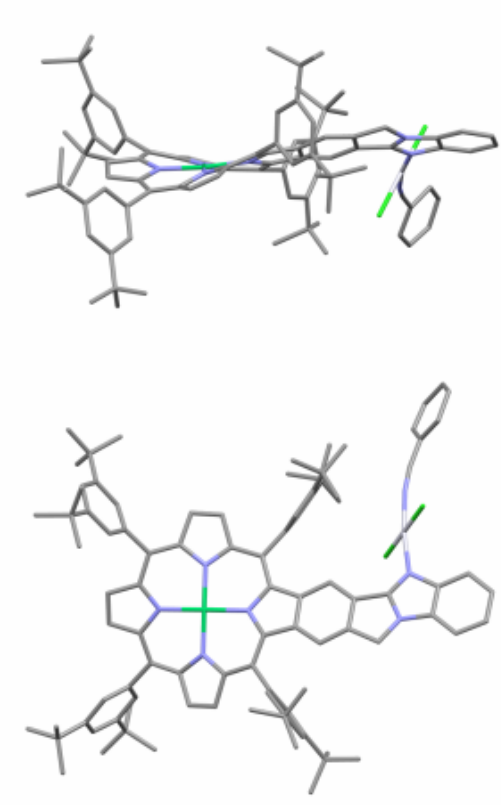


Figure S3. Crystal structure of **AMIm-4**



Crystal structure of **AMIm-7**

Acid Titration Date for AMIm-2

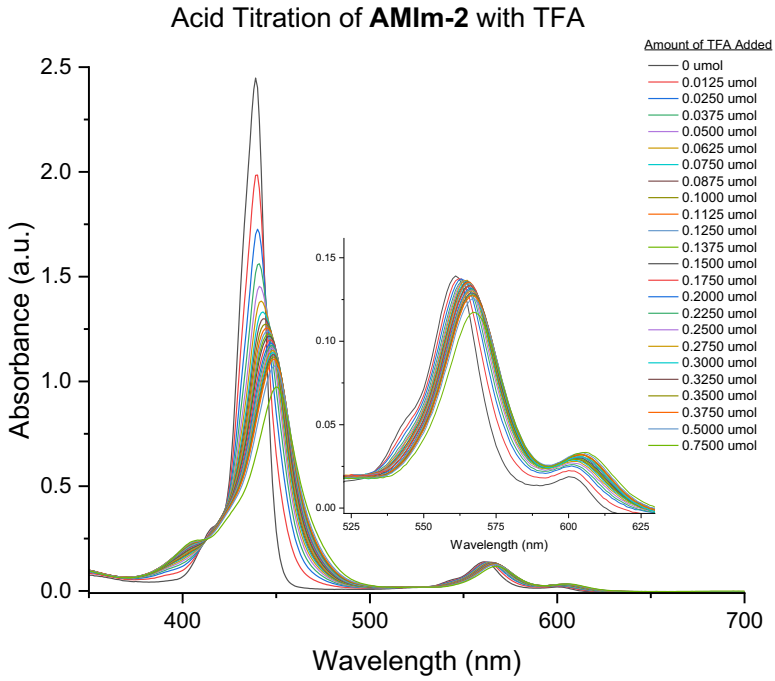


Figure S4. UV-Vis monitored acid titration of **AMIm-2** with TFA in DCM. Concentration of AMIm-2: 4.0×10^{-6} M. Concentration of TFA: 2.5×10^{-3} M. Titration stopped upon appearance of absorbance band at ~700nm corresponding to demetallated and protonated porphyrin.

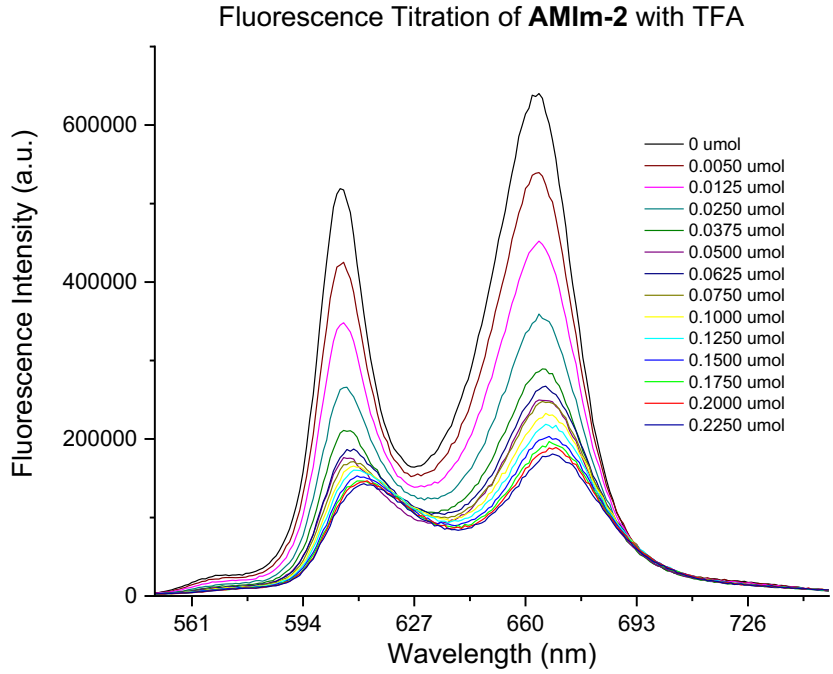


Figure S5. Fluorescence monitored titration of **AMIm-2** with TFA. Concentration of **AMIm-2**: 1.5×10^{-7} M. Concentration of TFA: 2.5×10^{-3} M. Sample was excited at 439

nm for the entirety of the titration and stopped upon appearance of absorbance band at ~700nm corresponding to demetallated and protonated porphyrin.

Optimized Structures

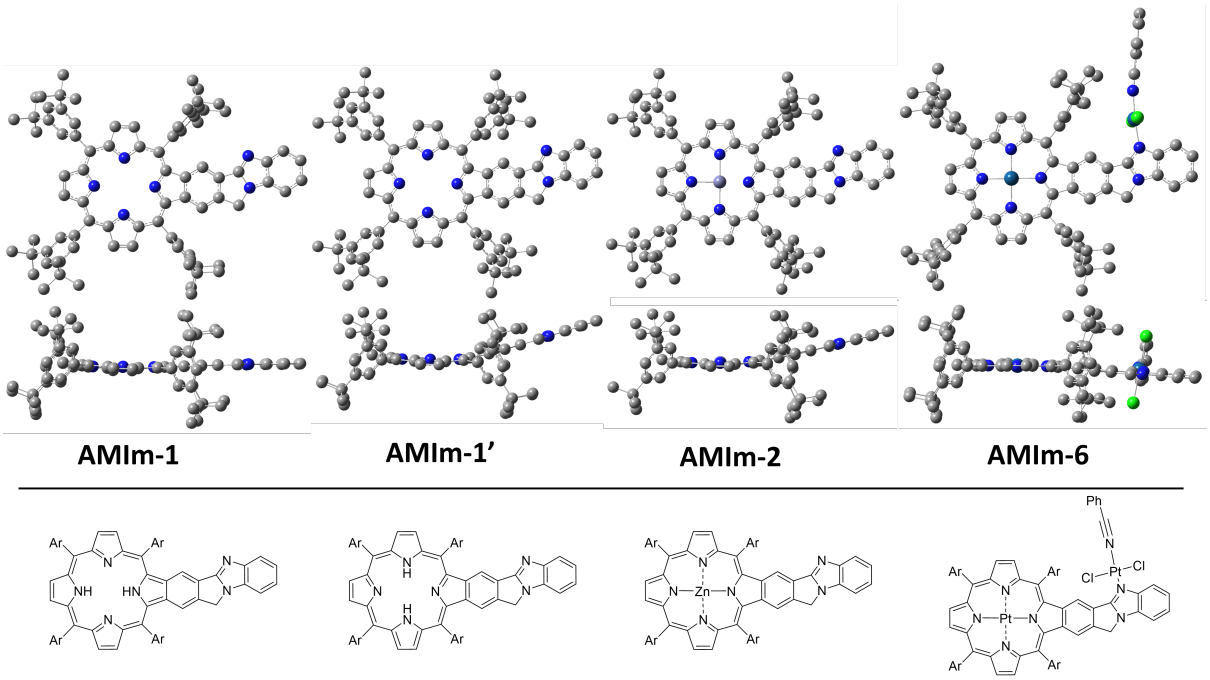


Figure S6 Optimized using B3LYP/6-31G(d,p) for all atoms besides platinum, and LANL2DZ for platinum atoms in **AMIm-6**. All structures did not possess negative frequencies from frequency calculation.

Energy Level Diagram

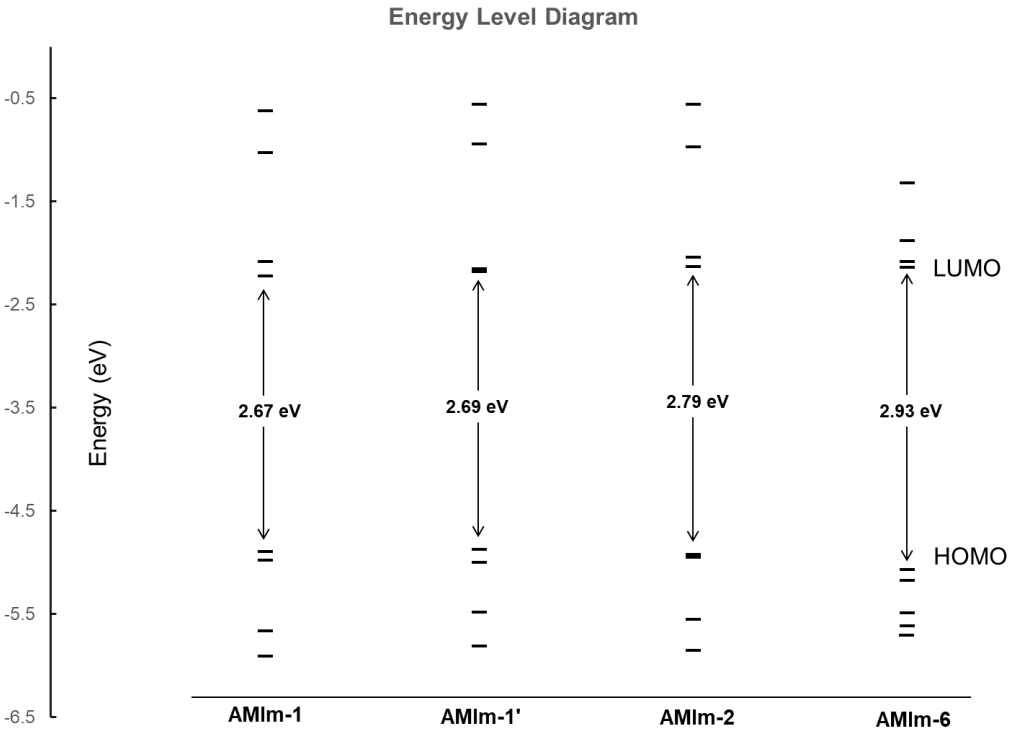


Figure S7. Energy values obtained from Opt/Freq calculation using B3LYP/6-31G(d,p) for all atoms besides platinum, and LANL2DZ for platinum atoms in **AMIm-6**.

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.)

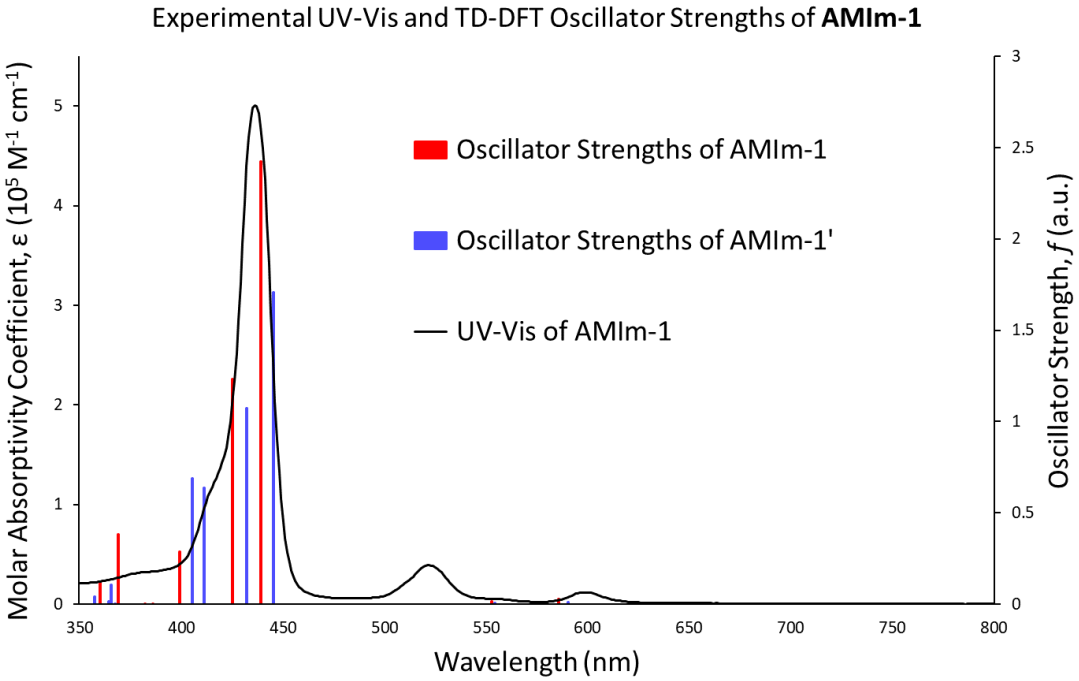


Figure S8. Experimental UV-Vis and TD-DFT oscillator strengths overlayed for **AMIm-1** and **AM-Im1'**

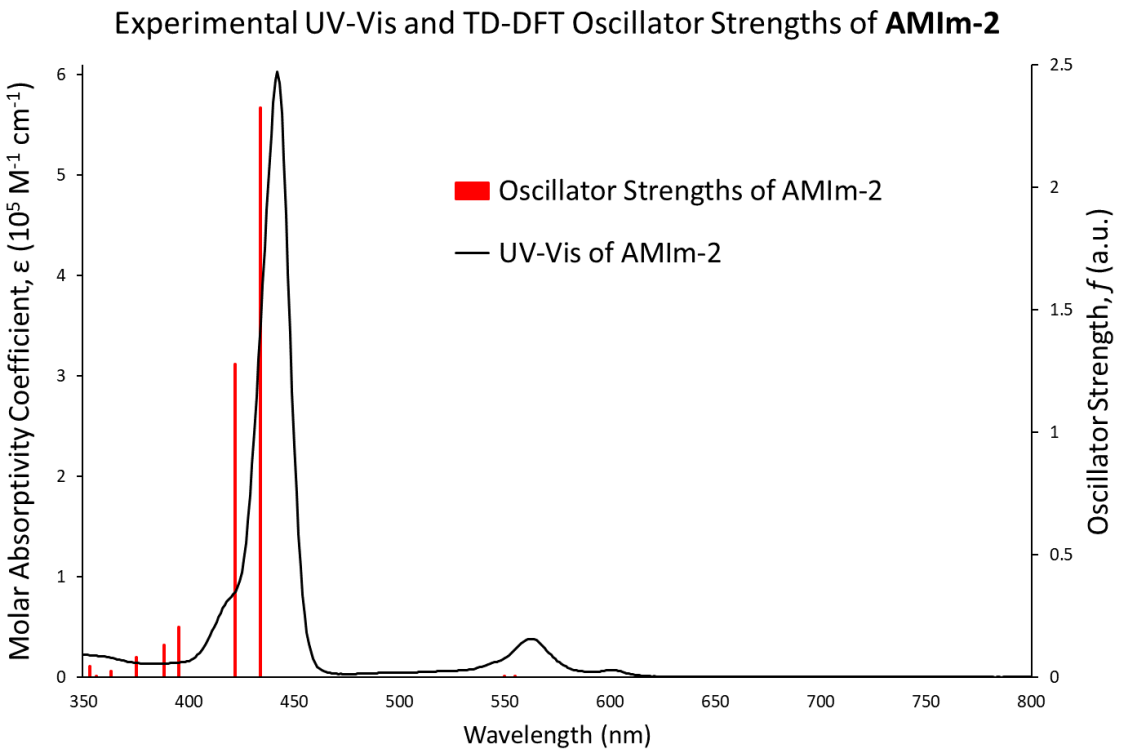


Figure S9. Experimental UV-Vis and TD-DFT oscillator strengths overlayed for **AMIm-2**

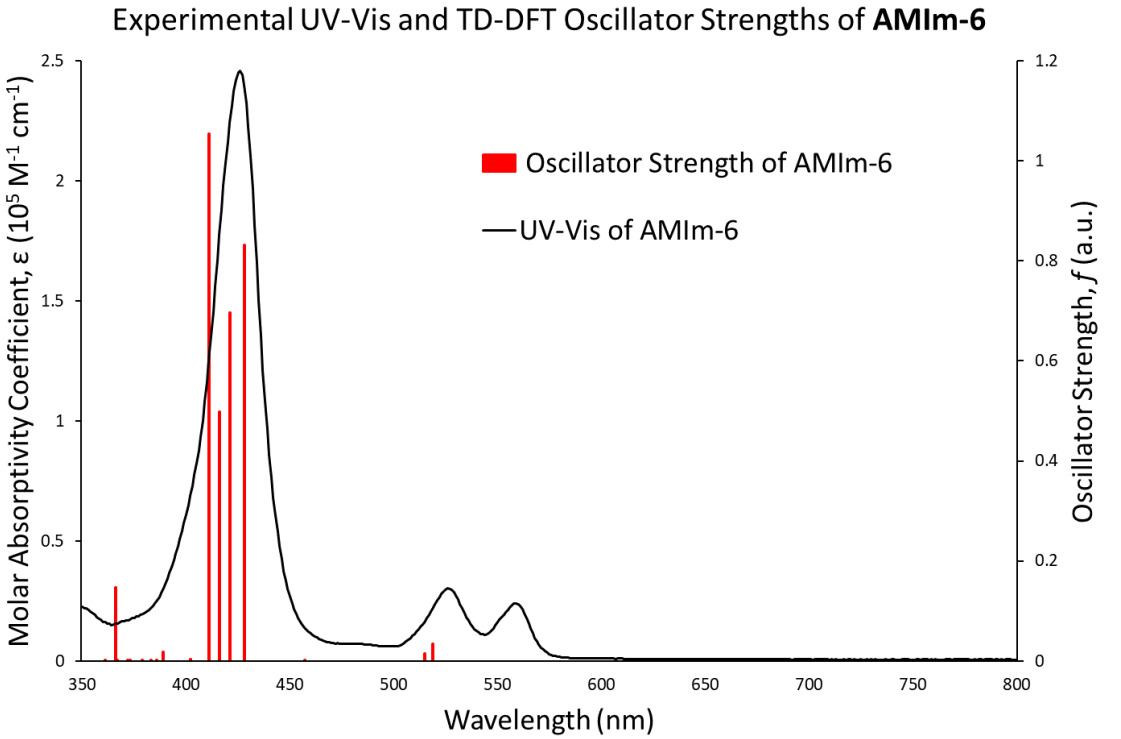


Figure S10. Experimental UV-Vis and TD-DFT oscillator strengths overlayed for **AMIm-6**

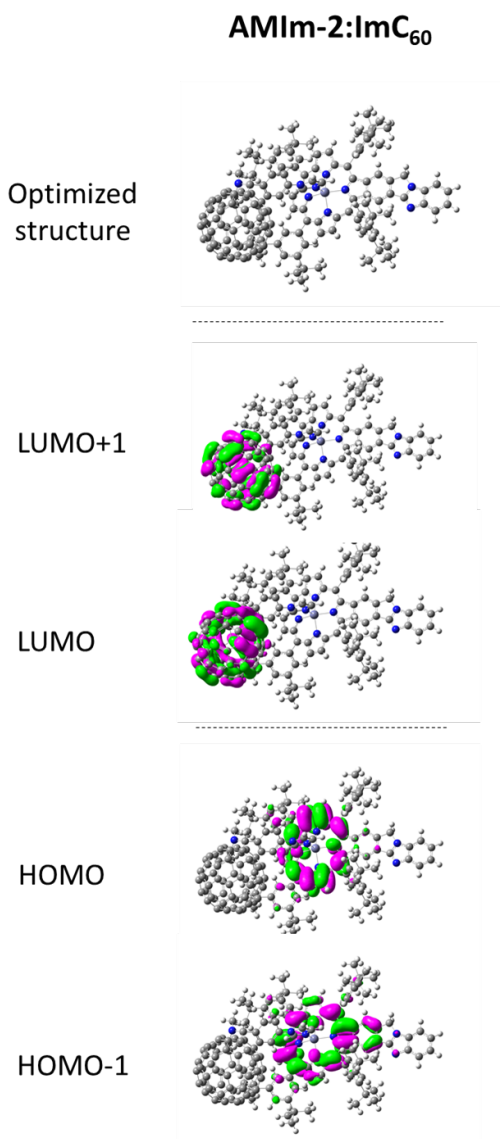


Figure S11. B3LYP/6-31G* optimized structures and frontier orbitals of **AMIm-2:ImC$_{60}$**

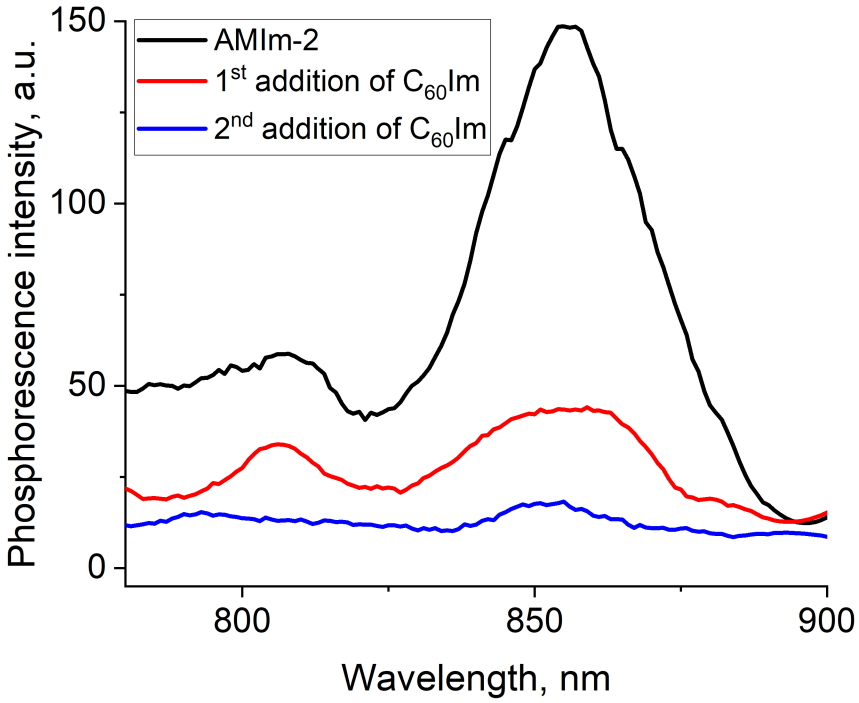


Figure S12. Phosphorescence spectrum of **AMIm-2** in the presence of C_{60}Im at liquid nitrogen temperature

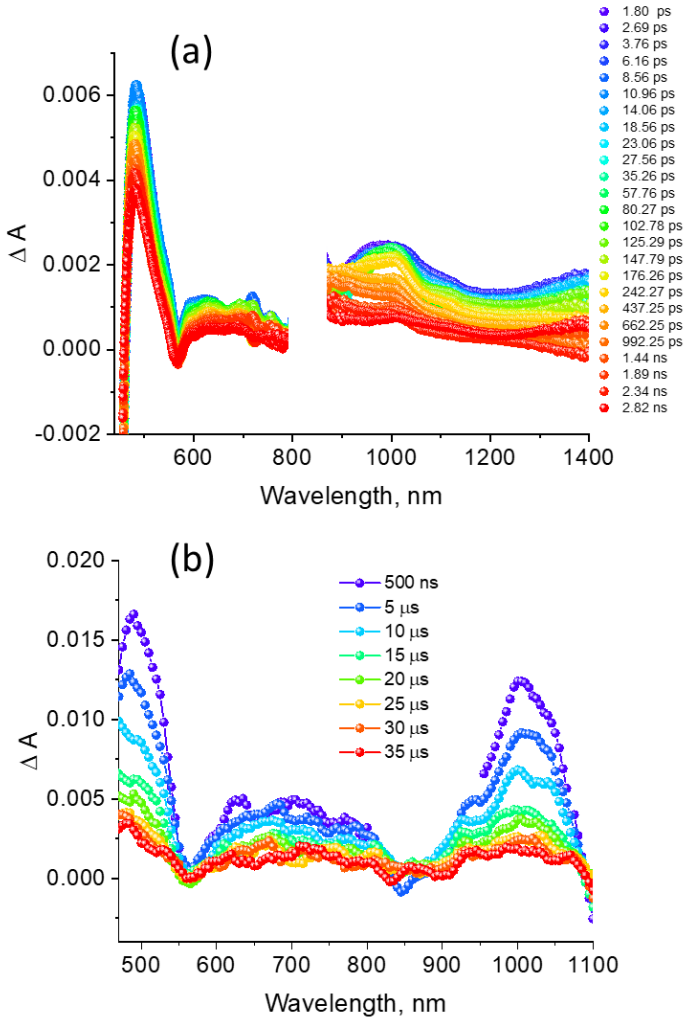


Figure S13. (a) Fs-TA (λ_{exc}=420 nm) and (b) ns-TA (λ_{exc}=420 nm) spectra of **AMIm-2:ImC$_{60}$** at indicated delay times in DCB

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

Table S5 TD-DFT oscillator strength table for **AMIm-1'**

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

Singlet	A	3.4718	357	0.0395	HOMO-4 HOMO	LUMO LUMO+2	89.9 4.3

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	2.2347	555	0.0064	HOMO	LUMO	32.2
					HOMO-1	LUMO+1	24.9
					HOMO-1	LUMO	22.5
					HOMO	LUMO+1	19.7
Singlet	A	2.2555	550	0.0006	HOMO-1	LUMO	30.8
					HOMO	LUMO+1	26
					HOMO	LUMO	23
					HOMO-1	LUMO+1	19.1
Singlet	A	2.8592	434	2.3236	HOMO-1	LUMO+1	45.7
					HOMO	LUMO	35.7
					HOMO-2	LUMO+1	6.6
					HOMO-2	LUMO	4.6
					HOMO	LUMO+1	2.4
Singlet	A	2.9390	422	1.2778	HOMO	LUMO+1	47.7
					HOMO-1	LUMO	41.5
					HOMO-2	LUMO	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	LUMO+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	LUMO	3.7
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	LUMO+2	70.9
					HOMO-2	LUMO+2	17.1
					HOMO-3	LUMO+1	2.8
					HOMO-4	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	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

					HOMO-1	LUMO+1	3.5
					HOMO-2	LUMO	3.5
					HOMO-5	LUMO+1	3
					HOMO-4	LUMO+1	2.1
Singlet	A	2.9976	414	0	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	LUMO	20.9
					HOMO-1	LUMO	17.3
					HOMO	LUMO+1	15.5
					HOMO-1	LUMO+4	2.8
Singlet	A	3.0878	402	0.0039	HOMO	LUMO+2	98.2
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

					HOMO-12	LUMO+4	4.5
					HOMO-14	LUMO+2	4.2
					HOMO-8	LUMO+4	3.3
Singlet	A	3.3757	367	0.0013	HOMO-4	LUMO+2	82.6
					HOMO-4	LUMO+3	8.2
					HOMO-3	LUMO+2	3.4
					HOMO-4	LUMO+4	3.3
Singlet	A	3.3872	366	0.1474	HOMO	LUMO+4	54.6
					HOMO	LUMO+3	29.6
					HOMO-1	LUMO+1	2.5
Singlet	A	3.3945	365	0.0018	HOMO-9	LUMO+1	90.5
					HOMO-9	LUMO	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

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
H	-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	4.1866680	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

C	-9.4709180	3.9172490	1.4430330
H	-9.7592640	4.6116450	0.6484490
H	-10.2211520	3.9918620	2.2383010
H	-9.5127710	2.9033410	1.0316870
C	-7.7770850	3.2470130	3.1530460
H	-8.5402840	3.3602640	3.9296870
H	-6.8035400	3.4335630	3.6176390
H	-7.8008520	2.2052980	2.8169970
C	-8.0457470	5.6641060	2.5786280
H	-8.2892190	6.4126290	1.8189570
H	-7.0600280	5.9106820	2.9863690
H	-8.7805030	5.7583650	3.3862480
C	-7.5812950	6.7510900	-2.4952480
H	-8.5265590	6.2034030	-2.4215780
H	-7.5115710	7.4308310	-1.6395800
H	-7.6271710	7.3652840	-3.4002790
C	-5.0952850	6.6640700	-2.7264860
H	-5.1682400	7.2997590	-3.6161320
H	-4.1963760	6.0497210	-2.8298560
H	-4.9571680	7.3140720	-1.8560540
C	-6.5394920	4.9138060	-3.8316170
H	-7.4405700	4.2964000	-3.7561870
H	-5.6869550	4.2435300	-3.9739640
H	-6.6281610	5.5358970	-4.7294620
C	3.6104020	6.0714920	2.8226590
C	3.1668270	5.2145440	4.0234600
H	2.0766680	5.1654240	4.1088750
H	3.5505160	5.6529930	4.9502690
H	3.5507470	4.1912980	3.9589560
C	5.1567220	6.1208930	2.8132860
H	5.5791210	5.1186780	2.6846190
H	5.5306580	6.5260830	3.7600770
H	5.5420630	6.7523250	2.0072770
C	3.0541330	7.5015770	3.0198590
H	1.9595160	7.4962220	3.0350500
H	3.3732700	8.1771140	2.2207890

H	3.4050220	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	1.7106790	5.8341070	-3.5080950
H	3.1664910	4.8342730	-3.6691650
H	3.1111570	6.4432610	-4.3945840
C	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

C	5.8870300	-5.3154300	-2.6381060
H	6.0779150	-4.2417640	-2.7311260
H	6.2207750	-5.8043100	-3.5604470
H	6.5081890	-5.6902910	-1.8198410
C	-5.2847980	-6.8507030	-2.2976650
C	-6.6992630	-6.8596330	-2.9242350
H	-7.4655420	-7.1501610	-2.1995110
H	-6.7428460	-7.5706640	-3.7569820
H	-6.9630360	-5.8694020	-3.3097450
C	-4.2739410	-6.4934530	-3.4037010
H	-4.3393550	-7.2281000	-4.2126720
H	-3.2436810	-6.5009040	-3.0336710
H	-4.4740470	-5.5077620	-3.8359820
C	-4.9463710	-8.2676870	-1.7767740
H	-5.6581160	-8.6042160	-1.0172670
H	-3.9465800	-8.2915490	-1.3311310
H	-4.9691200	-8.9920510	-2.5987760
C	-7.1087990	-5.4229490	2.2314020
C	-6.9791980	-4.3747060	3.3528760
H	-5.9770540	-4.3699830	3.7933620
H	-7.6902540	-4.6024370	4.1535690
H	-7.1992940	-3.3639400	2.9943610
C	-8.5628900	-5.3849670	1.7045320
H	-8.7994210	-4.4048680	1.2773530
H	-9.2687610	-5.5787110	2.5200860
H	-8.7360790	-6.1369560	0.9292410
C	-6.8218280	-6.8157270	2.8410190
H	-5.7993760	-6.8696260	3.2286610
H	-6.9421390	-7.6166010	2.1055690
H	-7.5103700	-7.0184850	3.6690520

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

	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	-1.9175550	-3.8165780	0.4104050
C	-2.5780030	-3.9878960	1.6332560
C	-3.4255260	-5.0796910	1.8537090
C	-2.9369340	-5.8690750	-0.4297810
C	-3.5889870	-5.9974030	0.8053720
H	-2.4198980	-3.2453190	2.4056870
H	-4.2453110	-6.8484360	0.9590170
C	-2.0943590	-4.7635430	-0.6066270
H	-1.5712620	-4.6114950	-1.5429530
C	-2.5479820	3.2202420	0.4903870
C	-2.9827270	4.0534570	-0.5475740
C	-3.1557060	3.3074960	1.7481540
C	-4.0447350	4.9480600	-0.3595240
C	-4.2027060	4.2060200	1.9854500
C	-4.6269950	5.0055710	0.9149100
H	-5.4512740	5.6923300	1.0766680
H	-2.5005580	3.9633120	-1.5136690
H	-2.8011750	2.6519280	2.5341970
C	4.4050260	3.8268490	-0.2073810
C	5.3960010	3.9691940	0.7735580
C	4.3201570	4.7733260	-1.2378330
C	6.3013380	5.0361980	0.7429670
C	5.2065820	5.8548990	-1.3062860
C	6.1826720	5.9599910	-0.3052310
H	6.8780130	6.7927470	-0.3435890
H	3.5542750	4.6397800	-1.9920710
H	5.4389120	3.2313140	1.5651080
C	-4.3923600	0.9598950	-0.3170290
C	-5.4808700	0.1380110	-0.5802420
C	-4.1445700	-1.8896770	-0.3812670
C	-5.3604790	-1.2703750	-0.6104440
C	-6.8637340	0.4658280	-0.8901150
C	-6.7069160	-1.9053640	-0.9370540
N	-7.5452310	-0.7228840	-1.0845560
H	-7.0713750	-2.5563960	-0.1324280
H	-6.6812400	-2.4941920	-1.8625390

N	-7.6009090	1.5412460	-1.0418300
C	-8.8468420	-0.3936990	-1.3928200
C	-8.8575910	1.0346430	-1.3583110
C	-10.0490200	1.7176010	-1.6297580
C	-11.1864290	0.9719820	-1.9259800
C	-11.1555960	-0.4358310	-1.9555610
C	-9.9855030	-1.1440900	-1.6891670
H	-9.9653890	-2.2293140	-1.7124650
H	-10.0694460	2.8023470	-1.6066120
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H	-12.0639470	-0.9824200	-2.1910270
H	-4.5209440	2.0313640	-0.3189600
H	-4.0591580	-2.9663060	-0.4303900
C	8.2262380	-3.9808600	1.7804710
C	6.2532470	-5.9994940	-2.4988250
C	9.5878420	-3.6968690	1.1028170
H	9.8341820	-4.4506890	0.3492760
H	10.3913970	-3.6961560	1.8479730
H	9.5827320	-2.7198900	0.6084930
C	7.9961950	-2.9073030	2.8607090
H	8.8108130	-2.9405920	3.5913090
H	7.0595130	-3.0693110	3.4036840
H	7.9745920	-1.8986600	2.4358250
C	8.2800900	-5.3603160	2.4790920
H	8.4864660	-6.1691210	1.7720550
H	7.3300680	-5.5844060	2.9750450
H	9.0704850	-5.3722730	3.2380500
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H	7.4991170	-7.5072480	-1.4969710
H	7.4798620	-7.6179510	-3.2591760
C	4.9897920	-6.8919100	-2.4617240
H	5.0099220	-7.6158830	-3.2841140
H	4.0721960	-6.3043540	-2.5586370
H	4.9328090	-7.4495120	-1.5209290
C	6.3046460	-5.2409260	-3.8462260

H	7.1950920	-4.6064740	-3.9039580
H	5.4294920	-4.6003150	-3.9877620
H	6.3376490	-5.9494130	-4.6816530
C	-4.1717130	-5.2975820	3.1845300
C	-3.8682180	-4.1919840	4.2131960
H	-2.8036010	-4.1497740	4.4643860
H	-4.4178110	-4.3900750	5.1389780
H	-4.1740030	-3.2045840	3.8528430
C	-5.6966190	-5.3045950	2.9225720
H	-6.0221910	-4.3517450	2.4919800
H	-6.2443420	-5.4573450	3.8591610
H	-5.9891500	-6.1015250	2.2324380
C	-3.7499800	-6.6545380	3.7961310
H	-2.6744400	-6.6738800	3.9998940
H	-3.9781270	-7.4915770	3.1296470
H	-4.2773090	-6.8281060	4.7409190
C	-3.1669800	-6.9238830	-1.5301280
C	-2.7331480	-8.3153050	-1.0104720
H	-1.6702610	-8.3212340	-0.7476540
H	-2.8960220	-9.0772750	-1.7808640
H	-3.2974500	-8.6147100	-0.1225750
C	-4.6685370	-6.9619830	-1.9012180
H	-5.2963090	-7.2098860	-1.0402570
H	-4.8518970	-7.7156580	-2.6751490
H	-4.9994770	-5.9925960	-2.2886350
C	-2.3652270	-6.6199420	-2.8099480
H	-1.2867950	-6.6068720	-2.6222470
H	-2.6473170	-5.6578970	-3.2495510
H	-2.5601280	-7.3940940	-3.5589340
C	-4.9028360	4.3250440	3.3531450
C	-4.3062320	3.3666470	4.4013340
H	-4.4130930	2.3187720	4.1031310
H	-4.8298600	3.4928690	5.3544430
H	-3.2443490	3.5655670	4.5793160
C	-6.4041120	3.9876460	3.1913550
H	-6.5388970	2.9713170	2.8082550

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	4.0993150	3.4231810
H	8.1683130	4.2863160	3.6080660

H	7.5301900	3.1215450	2.4437280
C	8.7880590	5.1904300	1.1221390
H	8.9524060	4.2339940	0.6151200
H	9.5835010	5.3224890	1.8642310
H	8.8931990	5.9846680	0.3772560
C	7.2103110	6.5822780	2.5170980
H	6.2373130	6.6300690	3.0168100
H	7.2665030	7.4199450	1.8156900
H	7.9885670	6.7298340	3.2743560
H	1.3227250	-1.0528190	-0.0767730
H	1.1475820	1.0986270	-0.0307440

Atom coordinates for optimized **AMIm-2**:

	X	Y	Z
C	-5.3033430	-1.1038990	-0.4814020
C	-5.4332830	0.2522420	-0.4730340
C	-3.9109660	-1.3934360	-0.2394620
C	-4.1207670	0.7980390	-0.2263900
N	-3.2047710	-0.2208510	-0.1104120
C	-3.8280950	2.1704490	-0.1145330
C	-2.5365730	2.6956310	0.0498410
N	-1.3527480	1.9788820	0.0384790
C	-0.3399480	2.8949060	0.1947760
C	-2.2513320	4.0930940	0.2589880
C	-0.8997690	4.2170880	0.3506300
C	1.0462930	2.6334550	0.1767530
C	1.6366050	1.3643680	0.0653170
N	0.9423580	0.1741250	0.1031030
C	1.8455020	-0.8650350	0.0933850
C	3.2030800	-0.3251220	-0.0411960
C	3.0685400	1.0857920	-0.0711000
C	1.5044820	-2.2218820	0.2087940
C	0.1935560	-2.7399060	0.2000800
N	-0.9726540	-2.0309820	0.0393160
C	-1.9977670	-2.9603120	0.0236540
C	-0.1039560	-4.1478360	0.3226200

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	0.3860020
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

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

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	7.2454140	4.5132090
C	3.2188080	6.8066640	-1.8007710
C	2.7123300	8.2191900	-1.4238030
H	1.6361550	8.2073800	-1.2229340

H	2.8969600	8.9221410	-2.2438660
H	3.2138400	8.6083790	-0.5328890
C	4.7377000	6.8679520	-2.0880560
H	5.3043800	7.2162540	-1.2195920
H	4.9418020	7.5562020	-2.9158460
H	5.1232990	5.8813240	-2.3658950
C	2.5048110	6.3721880	-3.0948580
H	1.4175390	6.3420930	-2.9713430
H	2.8370430	5.3857370	-3.4342110
H	2.7255740	7.0870640	-3.8939570
C	4.7412910	-4.6926730	3.2580630
C	4.0803370	-3.8483510	4.3640770
H	4.2160200	-2.7755150	4.1935460
H	4.5341520	-4.0886000	5.3309350
H	3.0069250	-4.0487400	4.4447060
C	6.2549210	-4.3717690	3.2468070
H	6.4311640	-3.3203810	2.9991350
H	6.7961900	-4.9779510	2.5148740
H	6.6925950	-4.5694110	4.2318970
C	4.5358600	-6.1861770	3.6057430
H	3.4710170	-6.4401460	3.6297110
H	4.9607910	-6.4095750	4.5908890
H	5.0198020	-6.8443720	2.8781310
C	4.7732650	-5.6273590	-1.7395070
C	4.1773320	-5.1900410	-3.0909950
H	3.1023230	-5.3895670	-3.1506390
H	4.6597800	-5.7457470	-3.9013970
H	4.3391590	-4.1238600	-3.2795360
C	4.5265560	-7.1451030	-1.5693450
H	3.4548530	-7.3708140	-1.5617410
H	4.9539110	-7.5228990	-0.6355430
H	4.9844700	-7.7014630	-2.3951320
C	6.2971250	-5.3544540	-1.7742930
H	6.5128680	-4.2824280	-1.8216500
H	6.7465600	-5.8378100	-2.6492490
H	6.8007270	-5.7494950	-0.8870820

C	-5.1167290	-6.8221160	-2.5537680
C	-6.4976650	-6.8276790	-3.2513610
H	-7.2999560	-7.1180370	-2.5667850
H	-6.5001000	-7.5373070	-4.0863650
H	-6.7399990	-5.8362420	-3.6476860
C	-4.0510100	-6.4614360	-3.6062170
H	-4.0752870	-7.1929770	-4.4202980
H	-3.0407650	-6.4708800	-3.1845560
H	-4.2287280	-5.4740550	-4.0443970
C	-4.8061820	-8.2413450	-2.0219800
H	-5.5526480	-8.5776750	-1.2964690
H	-3.8277600	-8.2695650	-1.5313400
H	-4.7935790	-8.9634680	-2.8461700
C	-7.1715220	-5.4022200	1.8779500
C	-7.1053120	-4.3506980	3.0018780
H	-6.1282650	-4.3421340	3.4955670
H	-7.8575880	-4.5781770	3.7640510
H	-7.3078240	-3.3414670	2.6290910
C	-8.5952920	-5.3704360	1.2734400
H	-8.8101930	-4.3930580	0.8290640
H	-9.3439760	-5.5620460	2.0504030
H	-8.7247800	-6.1266270	0.4937030
C	-6.9125360	-6.7927630	2.5046970
H	-5.9128820	-6.8414700	2.9484990
H	-6.9879760	-7.5947520	1.7644620
H	-7.6449790	-6.9980890	3.2935250
Zn	-1.1531420	-0.0257910	0.0172530

Atom coordinates for optimized **AMIm-6**:

	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	9.2248380	-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

C	4.4375090	3.0829540	2.7631120
C	5.8368320	3.7204450	2.6731360
H	6.5433330	3.0459190	2.1809360
H	6.2122110	3.9202010	3.6823410
H	5.8271650	4.6745330	2.1353820
C	3.4853780	4.0909690	3.4529720
H	3.3963510	5.0130260	2.8678340
H	3.8626760	4.3543890	4.4480720
H	2.4804810	3.6746680	3.5744300
C	4.5557740	1.8109810	3.6340710
H	5.2203420	1.0743830	3.1731690
H	3.5846520	1.3369100	3.8040320
H	4.9647620	2.0712630	4.6172480
H	5.2969270	3.8315150	0.2265690
H	2.1932960	1.6241350	2.1958930
H	2.1489270	2.0158760	-2.0514870
C	-7.3924270	-1.2786670	-0.0188540
C	-8.1578990	-1.1679410	-1.1863000
C	-7.9796310	-1.7873370	1.1464290
C	-9.3214880	-2.1888560	1.1649350
C	-9.5029770	-1.5583020	-1.2102070
C	-10.0547260	-2.0636050	-0.0240300
H	-7.6810950	-0.7742840	-2.0760250
H	-11.0960210	-2.3709150	-0.0258950
H	-7.3693290	-1.8576100	2.0388260
C	-10.0035900	-2.7458780	2.4302150
C	-10.3759260	-1.4509270	-2.4760180
C	-9.6007420	-0.8718020	-3.6749730
H	-9.2285500	0.1376130	-3.4716260
H	-10.2619560	-0.8101100	-4.5454510
H	-8.7482670	-1.5001990	-3.9528730
C	-10.8900410	-2.8561460	-2.8699980
H	-10.0556830	-3.5306730	-3.0887570
H	-11.5204110	-2.7940760	-3.7643570
H	-11.4866670	-3.3107110	-2.0735600
C	-11.5827330	-0.5249180	-2.1925360

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	-11.0236750	-4.5801760	3.0376820
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
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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

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	-3.7115260
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
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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
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C	6.4089140	-4.5481950	-0.5418860
C	8.5202780	-3.3324840	-0.4786240

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
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Cl	7.2226320	-0.6670720	2.1338550
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C	10.7070190	5.8498710	0.3058720
H	10.4876150	6.0183610	-1.8341730
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H	10.7582350	5.4289140	2.4217230
H	9.0969320	3.9661890	-2.0329500

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