Supporting Information

Highly shape-selective guest encapsulation in the precisely defined cavity of calix[4]arene-capped metalloporphyrin

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General Information

The ^{1}H and ^{13}C NMR spectra at high field were recorded with a Varian System 700, a JEOL-ECA 600, a JEOL-Lambda 500 and a Varian-Mercury 300 NMR spectrometer at 700, 600, 500 and 300 MHz (^{1}H NMR) and with a JEOL-ECA 600 and a Varian-Mercury 300 NMR spectrometer at 150 and 75 MHz (^{13}C NMR). ^{1}H NMR chemical shifts (δ) are given in ppm using the residual solvent as internal standard. ^{13}C NMR chemical shifts (δ) are given in ppm from internal chloroform-*d* (δ = 77.0). All melting points were determined with a micro melting apparatus (Yanagimoto) and are uncorrected. IR spectra were measured using a JASCO FT/IR-420 infrared spectrophotometer. The mass spectra were taken with a JEOL JMS-SX 102A high-resolution double-focusing mass spectrometer at the Instrument Center for Chemical Analysis, Hiroshima University. Elemental analyses were performed on a Perkin Elmer 2400CHN elemental analyzer at the Instrument Center for Chemical Analysis, Hiroshima University. UV spectra were measured on a JASCO V-560 spectrometer.

All reactions were carried out under an argon atmosphere unless otherwise noted. Dichloromethane was freshly distilled over CaH_2. Column chromatography was performed using Merck silica gel (70–230 mesh). All reagents were of commercial grade and were used without further purification.

Density functional theory (DFT) calculation was performed with Gaussian 09. Initial geometries were determined by molecular mechanics methods, using the MMFF force field of the Macromodel V6.5 software package on a SGI O2. The initial geometries were then subjected to geometry optimization by m06-x2 and b3lyp, using the lanl2dz basis set.

Determination of the association constants for guests was carried out by means of a UV-Vis titration technique in chloroform. Stock solutions of hosts and guests were prepared in $CHCl_3$. The host (or guest) solution was added to the guest (or host) solution, and continuous changes of absorbance in UV spectra were recorded each time. Plots of the observed absorbance changes versus the concentration of the added host or guest were performed by non-linear least square regression analysis to determine the binding constants. The binding curves were fitted to the following equation:

$$\Delta A_{obs} = \frac{b\Delta\varepsilon_{11}}{2K_{11}}\left\{1 + K_{11}[H]_0 + K_{11}[G]_0 - \sqrt{(1 + K_{11}[H]_0 + K_{11}[G]_0)^2 - 4K_{11}^2[H]_0[G]_0}\right\}$$

where ΔA_{obs} is the observed absorbance change at the concentration, b is light path length, $\Delta\varepsilon_{11} = \varepsilon_{11} - \varepsilon_H - \varepsilon_G$, ε_{11}, ε_H, and ε_G are molar absorptivities of 1:1 host-guest complex, host, and guest, K_{11}

is binding constant (L mol^{-1}), and $[H]_0$ and $[G]_0$ are the total concentrations of host and guest molecules (mol L^{-1}).

Experimental Sections

Synthesis of 2-(di-1*H*-pyrrol-2-ylmethyl)benzoic acid methyl ester (3)

To a solution of methyl 2-formylbenzoate (**2**) (4.0 g, 24.4 mmol) and pyrrole (60.0 mL, 854 mmol), catalytic amounts of trifluoroacetic acid was added at 0 °C under Ar. After being stirred for 30 min, the reaction mixture was concentrated *in vacuo*. The crude product was purified by column chromatography on silica gel with 50% CH_2Cl_2 in hexane to yield **3** (2.8 g, 9.9 mmol, 40%). M.p. 88 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.46 (br s, 2H), 7.77 (d, *J* = 7.8 Hz, 1H), 7.45-7.24 (m, 3H), 6.68 (m, 2H), 6.31 (s, 1H), 6.13 (dd, *J* = 6.0, 3.0 Hz, 2H), 5.91 (m, 2H), 3.81 ppm (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 168.9, 143.7, 132.6, 132.0, 130.4, 129.9, 129.6, 126.6, 117.0, 108.2, 106.7, 52.3, 40.3 ppm; IR (KBr): 1/λ = 3383, 2950, 1713, 1444, 1262, 776, 733 cm^{-1}; FAB-HRMS calcd for $C_{17}H_{16}N_2O_2$: 280.1212 [M^+]; found 280.1221.

Synthesis of 2,2'-(10,20-diphenyl-21*H*,23*H*-porphine-5,15-diyl)bisbenzoic acid dimethyl ester stereoisomer (4)

To a solution of 2-(di-1*H*-pyrrol-2-ylmethyl)benzoic acid methyl ester (**3**) (4.2 g, 15.0 mmol) and benzaldehyde (1.6 mL, 16.0 mmol) in CH_2Cl_2 (1.5 L), trifluoroacetic acid (2.1 mL, 27.0 mmol) was added at room temperature under an argon atmosphere. The reaction mixture was stirred for 1 h, and 2,3-dichloro-5,6-dicyano-*p*-benzoquinone (3.4 g, 15.0 mmol) was added. After being stirred for another 1 h, the reaction mixture was concentrated *in vacuo*. The crude product was purified by column chromatography on silica gel with 50% CH_2Cl_2 in hexane to yield 2,2'-(10,20-diphenyl-21*H*,23*H*-porphine-5,15-diyl)bisbenzoic acid dimethyl ester (**4**) (940 mg, 1.3 mmol, 17%) as stereoisomer. M.p. >300 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.82-8.76 (m, 4H), 8.67-8.59 (m, 4H), 8.42-8.38 (m, 2H), 8.26 (d, *J* = 6.7 Hz, 1H), 8.20 (dd, *J* = 6.1, 1.8 Hz, 1H), 8.15-8.11 (m, 4H), 7.88 (td, *J* = 8.0, 1.6 Hz, 2H), 7.83 (td, *J* = 7.3, 1.5 Hz, 2H), 7.78-7.68 (m, 6H), 2.87, 2.76 (s, 6H), –2.60 ppm (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 167.9, 167.8, 142.8, 142.6, 142.5, 142.2, 142.1, 136.0, 134.6, 134.5, 134.4, 134.1, 134.0, 129.7, 129.6, 128.3, 127.6, 126.6, 120.0, 119.0, 51.7, 41.4 ppm; IR (KBr): 1/λ = 3317, 3057, 3024, 2949, 1730, 1560, 1471, 1256, 730, 703 cm^{-1}; FAB-HRMS calcd for $C_{48}H_{34}N_4O_4$: 730.2580 [M^+]; found 730.2576; elemental analysis calcd (%) for $C_{48}H_{34}N_4O_4$•H_2O: C 76.99, H 4.85, N 7.48; found: C 77.37, H 4.65, N 7.24.

Synthesis of 2,2'-(10,20-diphenyl-21H,23H-porphine-5,15-diyl)bisbenzoic acid stereoisomer

To a solution of 2,2'-(10,20-diphenyl-21*H*,23*H*-porphine-5,15-diyl)bisbenzoic acid dimethyl ester (**4**) (260 mg, 0.36 mmol) in THF (100 mL), 40 mL of saturated aqueous LiOH was added. After being stirred for 5 days at 90 °C, the reaction mixture was poured into aqueous NH_4Cl and acidified

with 6M HCl. The aqueous layer was extracted with $CHCl_3$. The organic layer was dried over Na_2SO_4 and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel with 5% MeOH in $CHCl_3$ to yield 2,2'-(10,20-diphenyl-21*H*,23*H*-porphine-5,15-diyl)bisbenzoic acid (230 mg, 0.33 mmol, 92%) as stereoisomer. M.p. >300 °C; ^{1}H NMR (600 MHz, aceton-*d*6): δ = 8.87-8.82 (m, 4H), 8.78-8.73 (m, 4H), 8.54-8.50 (m, 2H), 8.36-8.30 (m, 4H), 8.25-8.20 (m 2H), 8.08-8.01 (m, 4H), 7.90-7.82 ppm (m, 6H); IR (KBr): 1/λ = 3420, 3033, 1713, 1486, 1442, 756, 711 cm^{-1}; FAB-HRMS calcd for $C_{46}H_{30}N_4O_4$: 702.2267 [M^+]; found 702.2252.

Synthesis of capped porphyrin $1H_2$

To a solution of stereoisomeric mixture of 2,2'-(10,20-diphenyl-21*H*,23*H*-porphine-5,15-diyl)bisbenzoic acid (80 mg, 0.11 mmol) in CH_2Cl_2 (3 mL), catalytic amounts of DMF and oxalyl dichloride (0.5 mL, 5.8 mmol) was added under an argon atmosphere. After the reaction mixture was stirred for 2 h at room temperature, compound 2,2'-(10,20-diphenyl-21*H*,23*H*-porphine-5,15-diyl)bisbenzoic acid dichloride (**5**) was obtained by concentration *in vacuo* and used for the next step without further purification.

A solution of **5** in CH_2Cl_2 (15 mL) and a solution of diaminocalix[4]arene **6** (74 mg, 0.11 mmol) in CH_2Cl_2 (15 mL) were mixed dropwise in 20 ml of CH_2Cl_2 and Et_3N (0.1 mL, 0.72 mmol) at 40 °C under an argon atmosphere. After being stirred for 8 h, the reaction mixture was quenched with saturated aqueous NH_4Cl, and extracted with CH_2Cl_2. The organic layer was washed with saturated $NaHCO_3$, brine, and then dried over anhydrous Na_2SO_4. After removing Na_2SO_4 by filtration, the solvent was concentrated *in vacuo*. The crude product was purified by column chromatography on silica gel with 10% ethyl acetate in CH_2Cl_2 to yield **$1H_2$** (32 mg, 0.025 mmol, 22%). M.p. >300 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.93 (d, *J* = 4.8 Hz, 4H), 8.76 (d, *J* = 4.8 Hz, 4H), 8.67 (d, *J* = 6.9 Hz, 2H), 8.41 (d, *J* = 7.6 Hz, 2H), 8.20 (d, *J* = 7.6 Hz, 2H), 7.93-7.79 (m, 10H), 7.71 (t, *J* = 6.8 Hz, 2H), 6.48 (d, *J* = 7.6 Hz, 4H), 6.35 (t, *J* = 7.6 Hz, 4H), 5.66 (s, 4H), 5.63 (s, 2H), 4.00 (d, *J* = 12.0 Hz, 4H), 3.67 (t, *J* = 8.2 Hz, 4H), 3.34 (t, *J* = 7.6 Hz, 4H), 2.76 (d, *J* = 12.0 Hz, 4H), 1.84 (tq, *J* = 7.6, 7.6 Hz, 4H), 1.62 (tq, *J* = 7.6, 7.6 Hz, 4H), 0.82 (t, *J* = 7.6 Hz, 6H), 0.76 (t, *J* = 7.6 Hz, 6H), –2.57 ppm (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ = 167.1, 156.0 152.1 141.6, 140.1, 138.7, 136.3, 136.1, 135.1, 134.7, 132.7, 130.6, 129.4, 128.9, 128.3, 128.1, 127.9, 127.1, 127.0, 122.4, 121.6, 120.9, 116.4, 77.9, 75.8, 30.6, 23.1, 22.6, 10.3, 9.8 ppm; IR (KBr): 1/λ = 3396, 3313, 3060, 2959, 2929, 2873, 1682, 1560, 1466, 1217, 799, 752 cm^{-1}; FAB-HRMS calcd for $C_{86}H_{76}N_6O_6$: 1288.5826 [M^+]; found 1288.5833; elemental analysis calcd (%) for $C_{86}H_{76}N_6O_6$: C 80.10, H 5.94, N 6.52; found: C 79.94, H 6.14, N 6.16.

Synthesis of capped porphyrin 1Zn

To a solution of **$1H_2$** (25 mg, 0.019 mmol) in MeOH (1 mL) and $CHCl_3$ (2 mL), $Zn(OAc)_2$ (20 mg, 0.11 mmol) was added. After being refluxed for 4 hours, the reaction mixture was concentrated *in vacuo*. The crude product was purified by column chromatography on silica gel with CH_2Cl_2 to yield **1Zn** (21 mg, 0.016 mmol, 79%). M.p. >300 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.97 (d, *J* = 4.5 Hz, 4H), 8.80 (d, *J* = 4.5 Hz, 4H), 8.53 (d, *J* = 6.9 Hz, 2H), 8.25 (d, *J* = 7.9 Hz, 2H), 7.93 (d, *J* = 7.5 Hz, 2H), 7.88 (t, *J* = 7.7 Hz, 2H), 7.80 (d, *J* = 7.4 Hz, 2H), 7.77-7.71 (m, 4H), 7.69-7.63 (m, 4H), 7.11 (br s, 2H), 6.32 (s, 4H), 5.26 (br s, *J* = 7.6 Hz, 4H), 4.30 (br s, 2H), 3.77 (d, *J* = 12.0 Hz, 4H), 3.39 (t, *J* = 7.4 Hz, 4H), 3.30 (t, *J* = 7.4 Hz, 4H), 2.57 (d, *J* = 12.0 Hz, 4H), 1.70 (tq, *J* = 7.6, 7.6 Hz, 4H), 1.56 (tq, *J* = 7.6, 7.6 Hz, 4H), 0.78 (t, *J* = 7.6 Hz, 6H), 0.77 ppm (t, *J* = 7.6 Hz, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ = 167.3, 154.2, 151.5, 150.5, 150.0, 142.8, 140.4, 139.5, 136.6, 135.9, 135.3, 134.1, 133.3, 132.6, 131.4, 130.9, 128.4, 128.1, 126.7, 126.5, 126.2, 121.0, 120.4, 118.7, 117.7, 77.4, 76.5, 28.7, 22.9, 22.9, 10.2, 10.0 ppm; IR (KBr): 1/λ = 3533, 3399, 3060, 2959, 2927, 2870, 1680, 1597, 1467, 1228, 795, 751, 702 cm^{-1}; FAB-HRMS calcd for $C_{86}H_{74}N_6O_6Zn$: 1350.4961 [M^+]; found 1350.4948; elemental analysis calcd (%) for $C_{86}H_{74}N_6O_6Zn•2H_2O$: C 74.37, H 5.66, N 6.05; found: C 74.40, H 5.66, N 5.79.

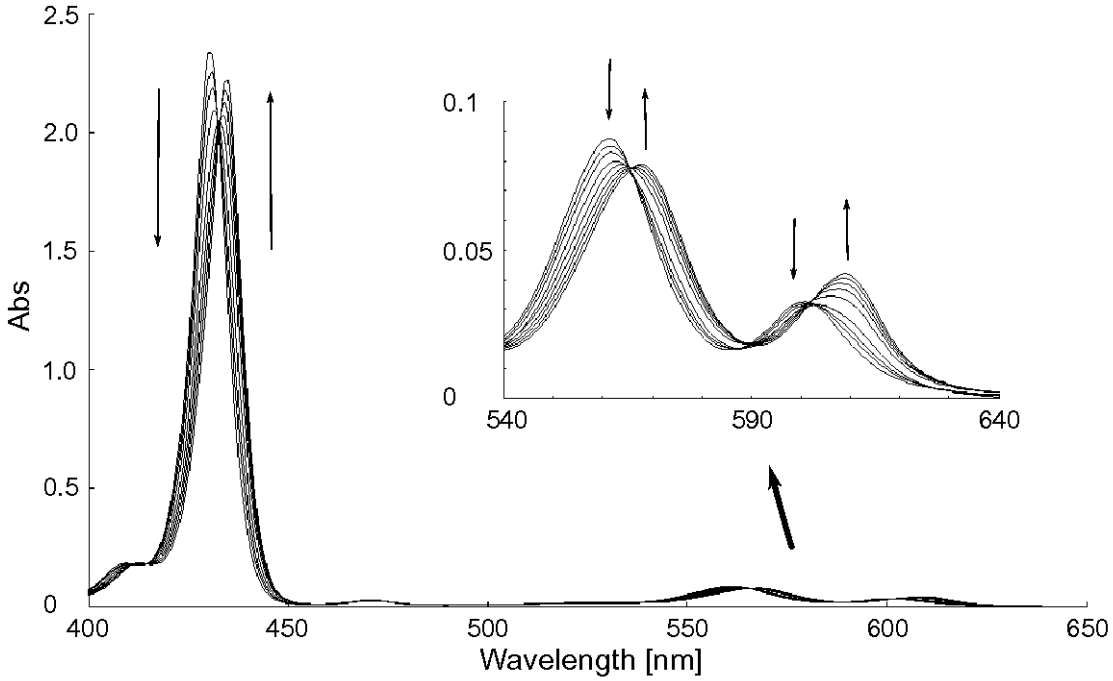


Figure S1 The absorption spectra of **1Zn** (5.0×10^{-6} mol l^{-1}) in chloroform upon the addition of pyridine (**7**) (a, 0.0; b, 2.5; c, 5.0; d, 10; e, 20; f, 31; g, 44; h, 60; i, 80×10^{-6} mol l^{-1}).

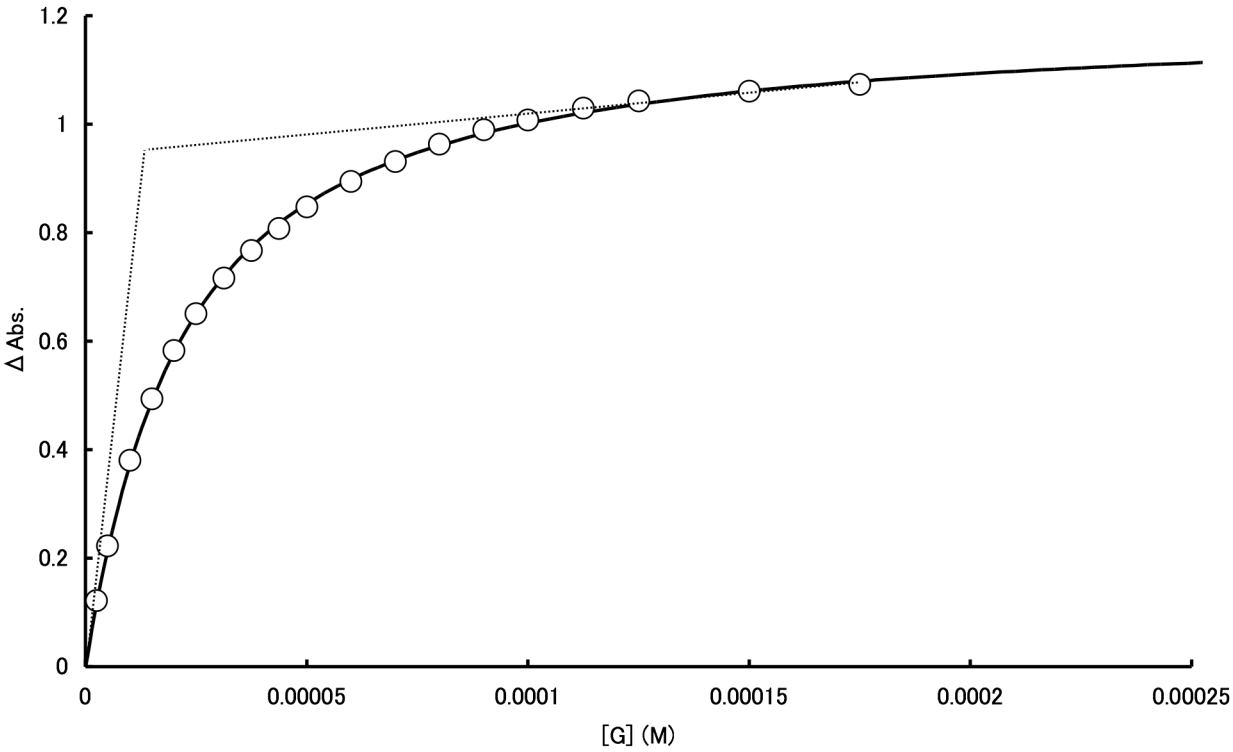


Figure S2. Absorption changes at 435 nm of **1Zn** (5.0×10^{-6} mol l^{-1}) in chloroform in the presence of various amounts of pyridine (**7**) and curve fitting analysis.

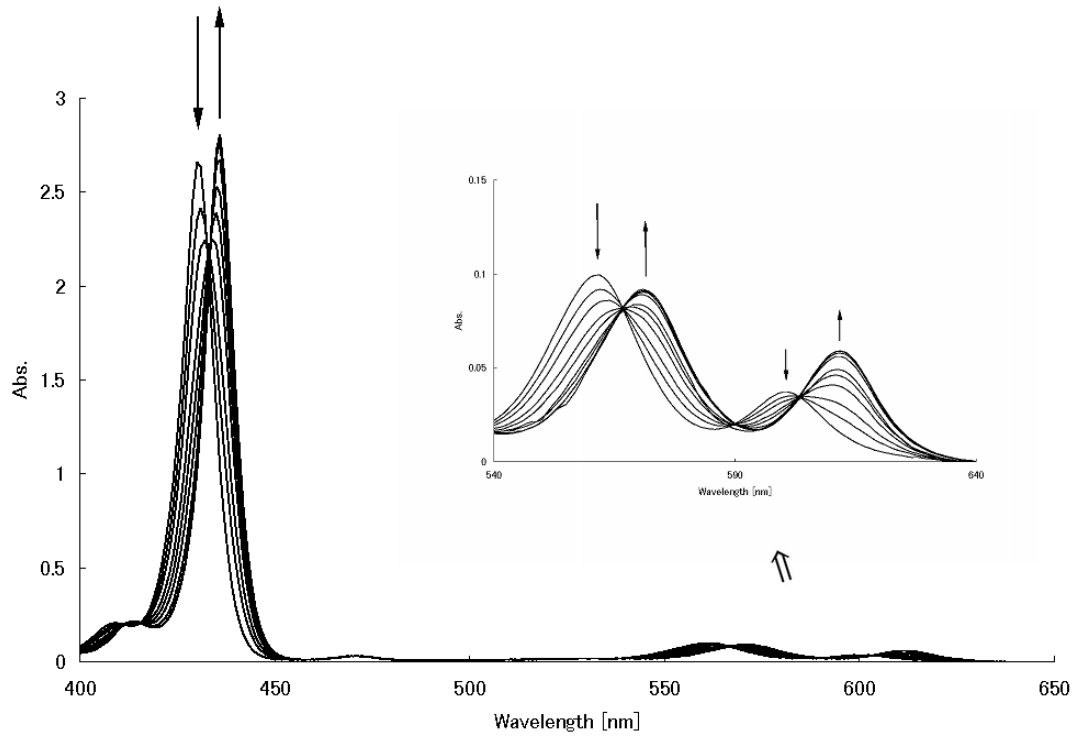


Figure S3. The absorption spectra of **1Zn** (2.5×10^{-6} mol l^{-1}) in chloroform upon the addition of imidazole (**9**) (a, 0.0; b, 0.5; c, 1.0; d, 1.75; e, 2.25; f, 2.75; g, 3.25; h, 4.0; i, 8.0; j, 10.0×10^{-6} mol l^{-1}).

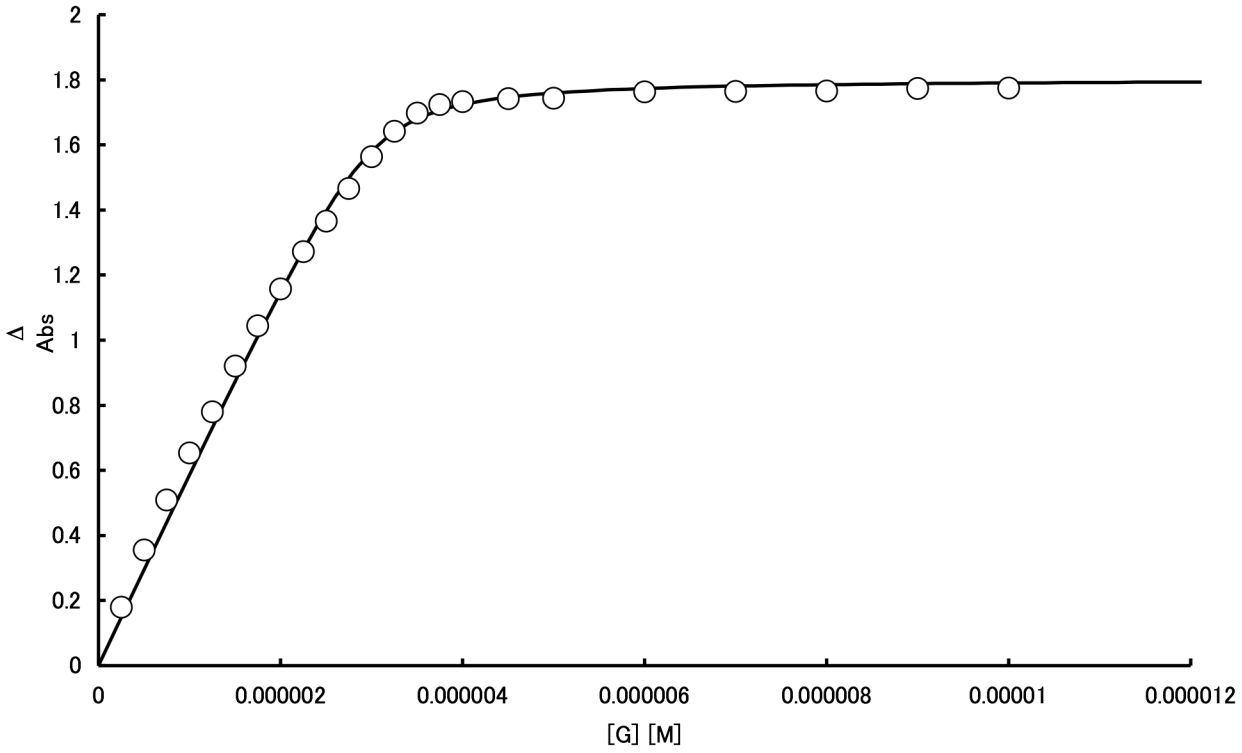


Figure S4. Absorption changes at 436 nm of **1Zn** (2.5×10^{-6} mol l^{-1}) in chloroform in the presence of various amounts of imidazole (**9**).

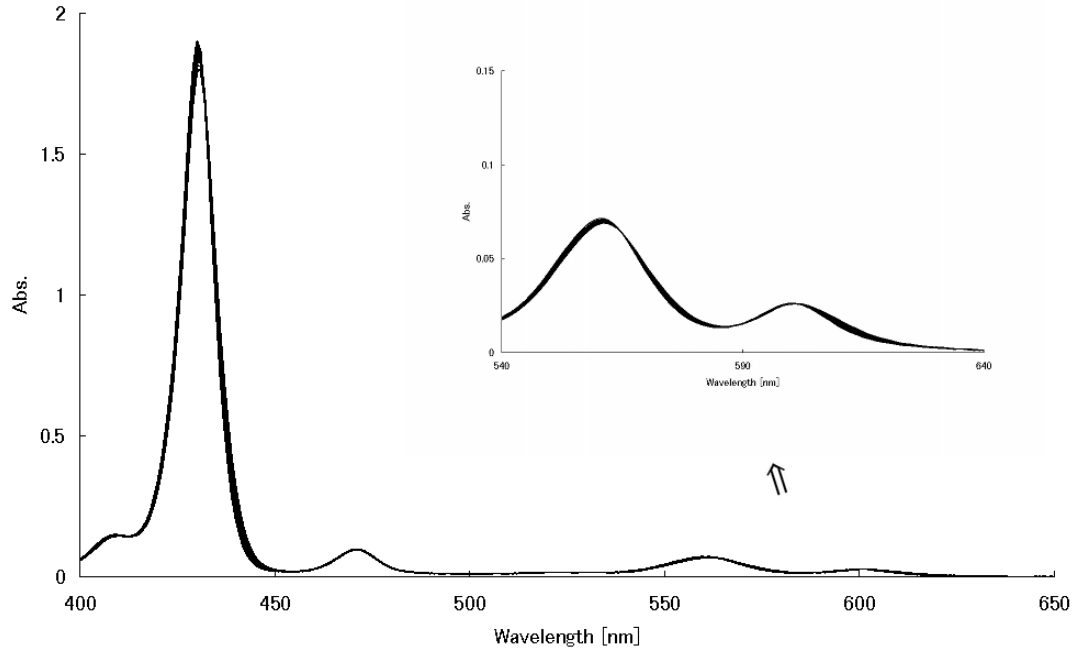


Figure S5. The absorption spectra of **1Zn** (5.0×10^{-6} mol l^{-1}) in chloroform upon the addition of 4-methylpyridine (**8**) (a, 0.0; b, 3.75; c, 10; d, 20; e, 30; f, 40; g, 60; h, 85×10^{-3} mol l^{-1}).

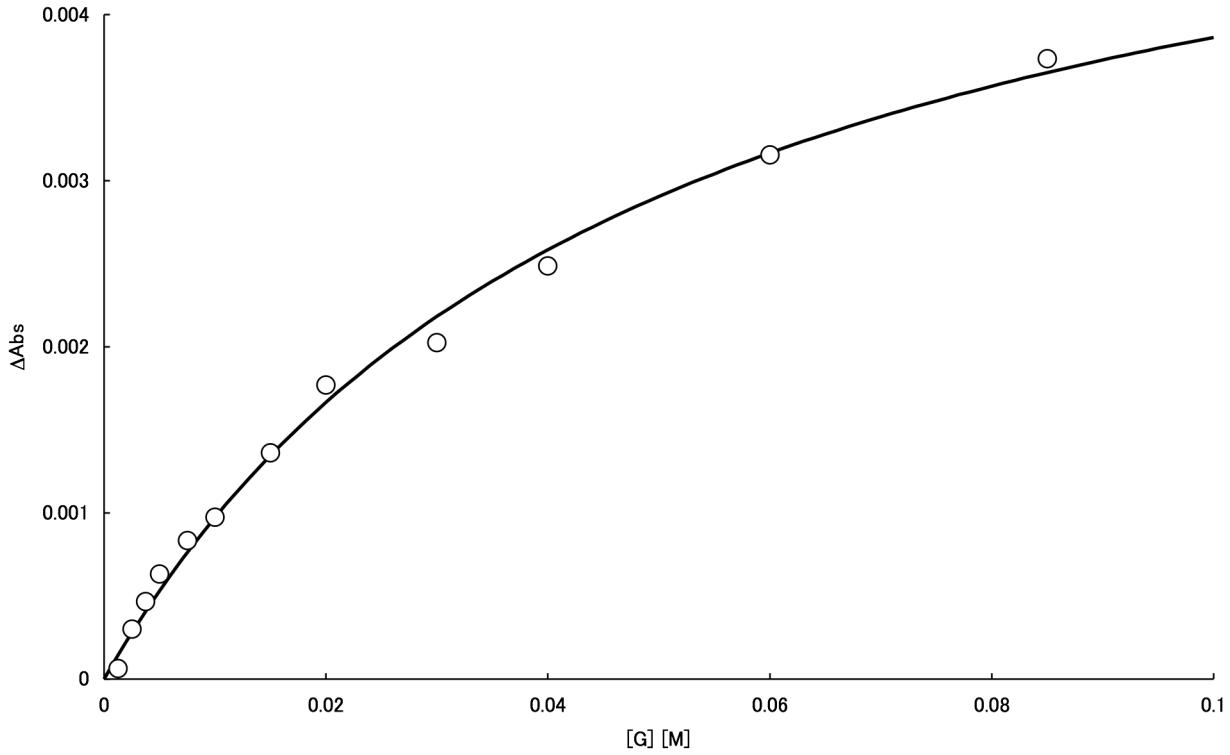


Figure S6. Absorption changes at 575 nm of **1Zn** (5.0×10^{-6} mol l^{-1}) in chloroform in the presence of various amounts of 4-methylpyridine (**8**).

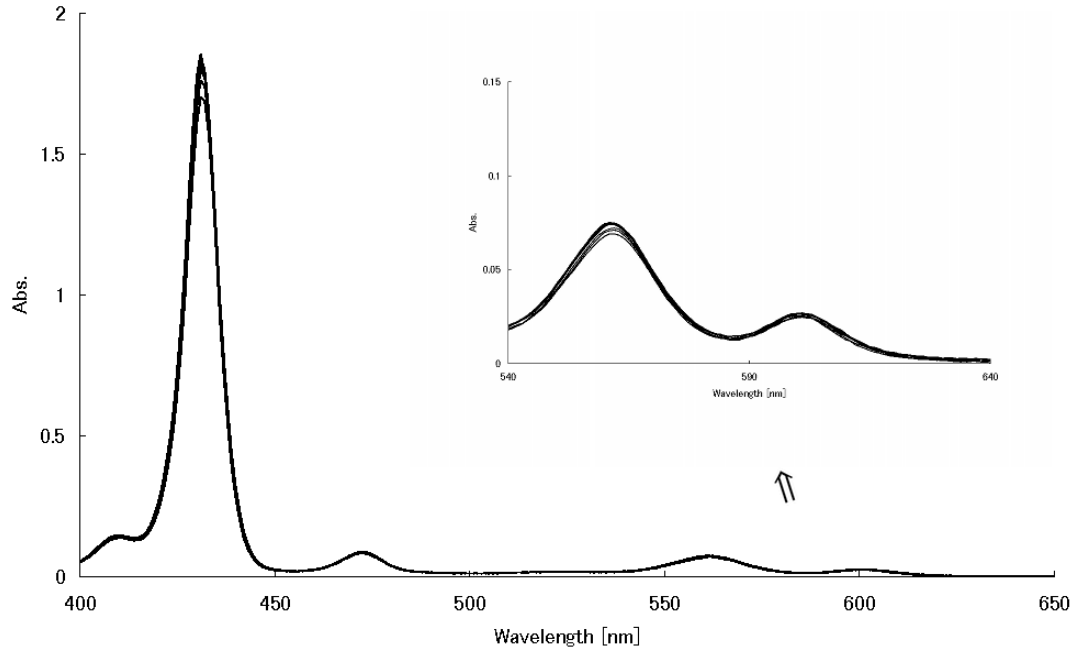


Figure S7. The absorption spectra of **1Zn** (5.0×10^{-6} mol l^{-1}) in chloroform upon the addition of *N*-methylimidazole (**10**) (a, 0.0; b, 1.0; c, 4.5; d, 7.5; e, 12.5; f, 17.5; g, 22.5; h, 27.5; i, 37.5; j, 42.5 $\times 10^{-3}$ mol l^{-1}).

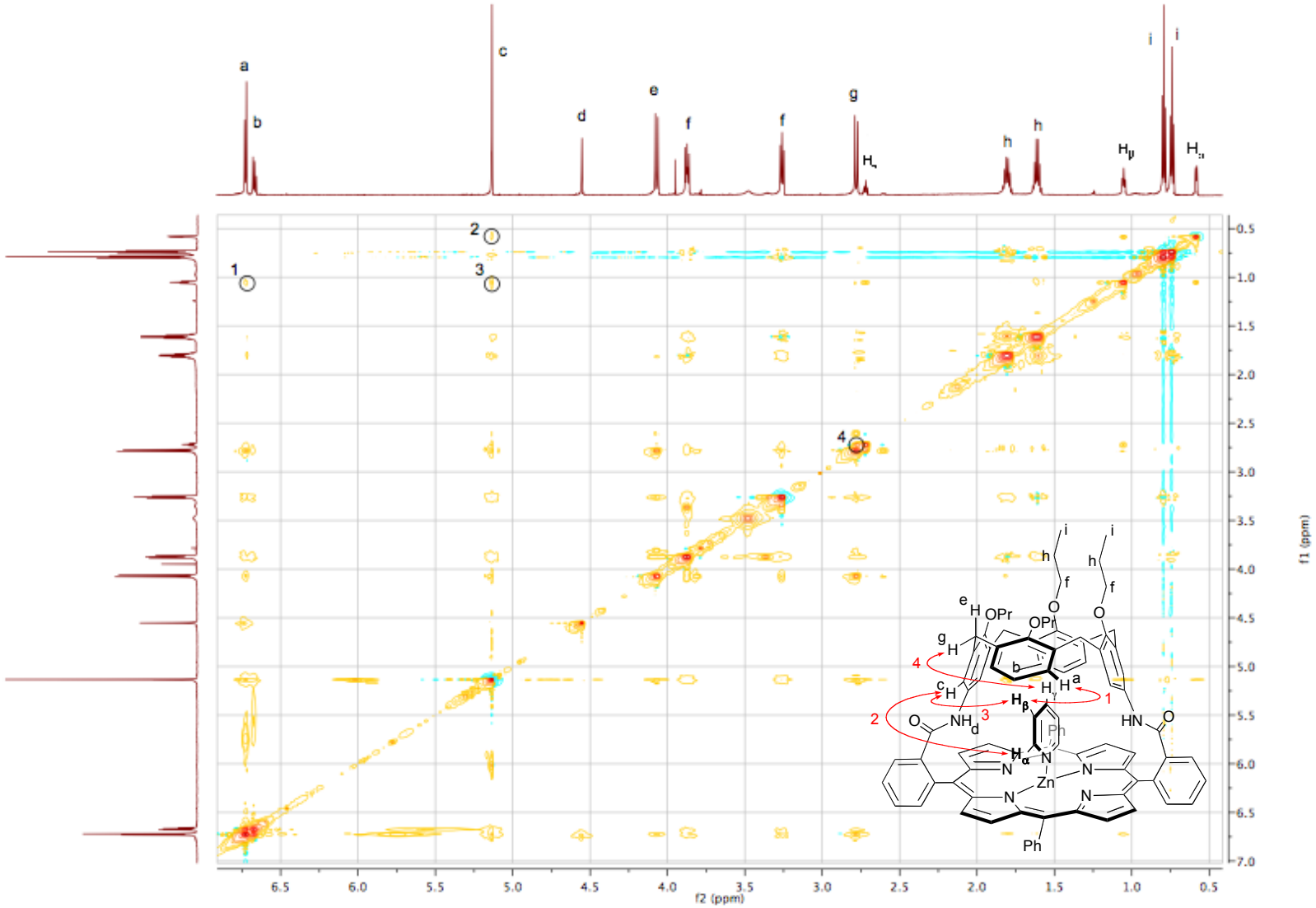


Figure S8. Partial NOESY NMR spectrum (700 MHz, $CDCl_3$, 297 K, mixing time = 800 ms) of **1Zn** (2.70 mM) and pyridine (**7**) (7.56 mM).

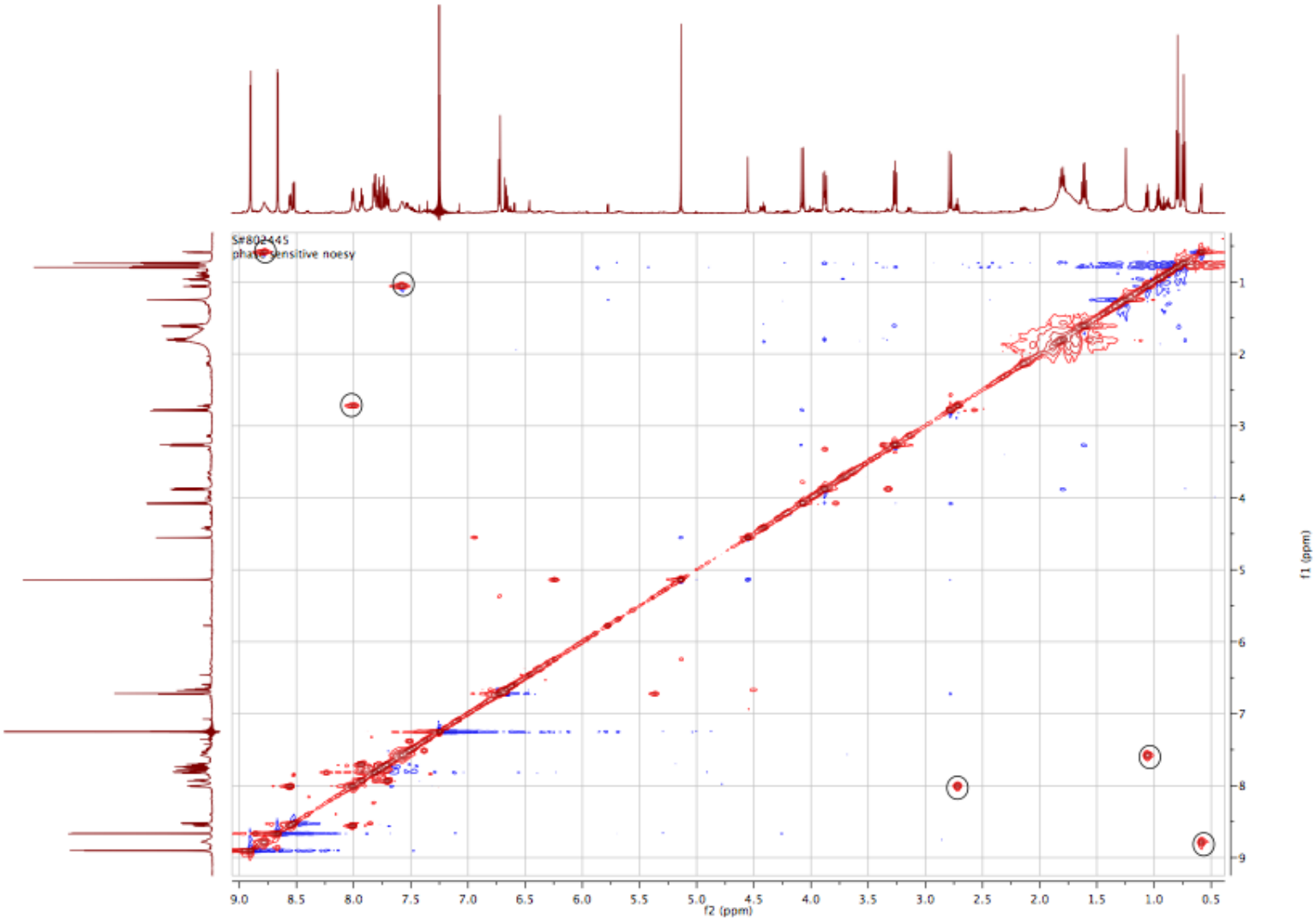


Figure S9. 2D EXSY spectrum (600 MHz, $CDCl_3$, 300 K, mixing time = 1000 ms) of a mixture of **1Zn** (2.66 mM) and pyridine (**7**) (5.32 mM). EXSY signals are marked with "o".

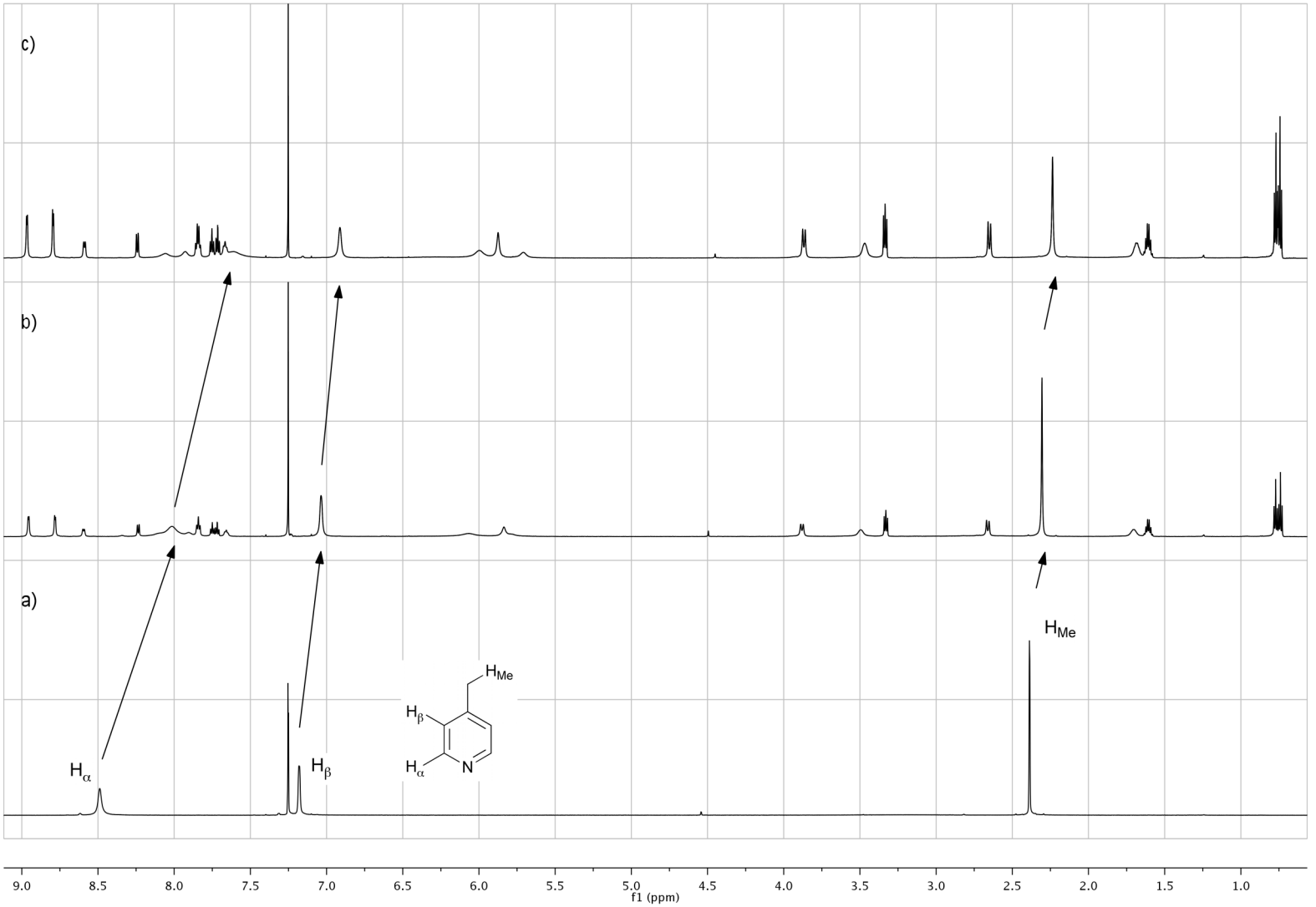


Figure S10. 1H-NMR spectra (700 MHz, $CDCl_3$, 297 K) of 4-methylpyridine (**8**) (5.58 mM) upon the addition of **1Zn** (a, 0.0; b, 1.59; c, 3.78 mM).

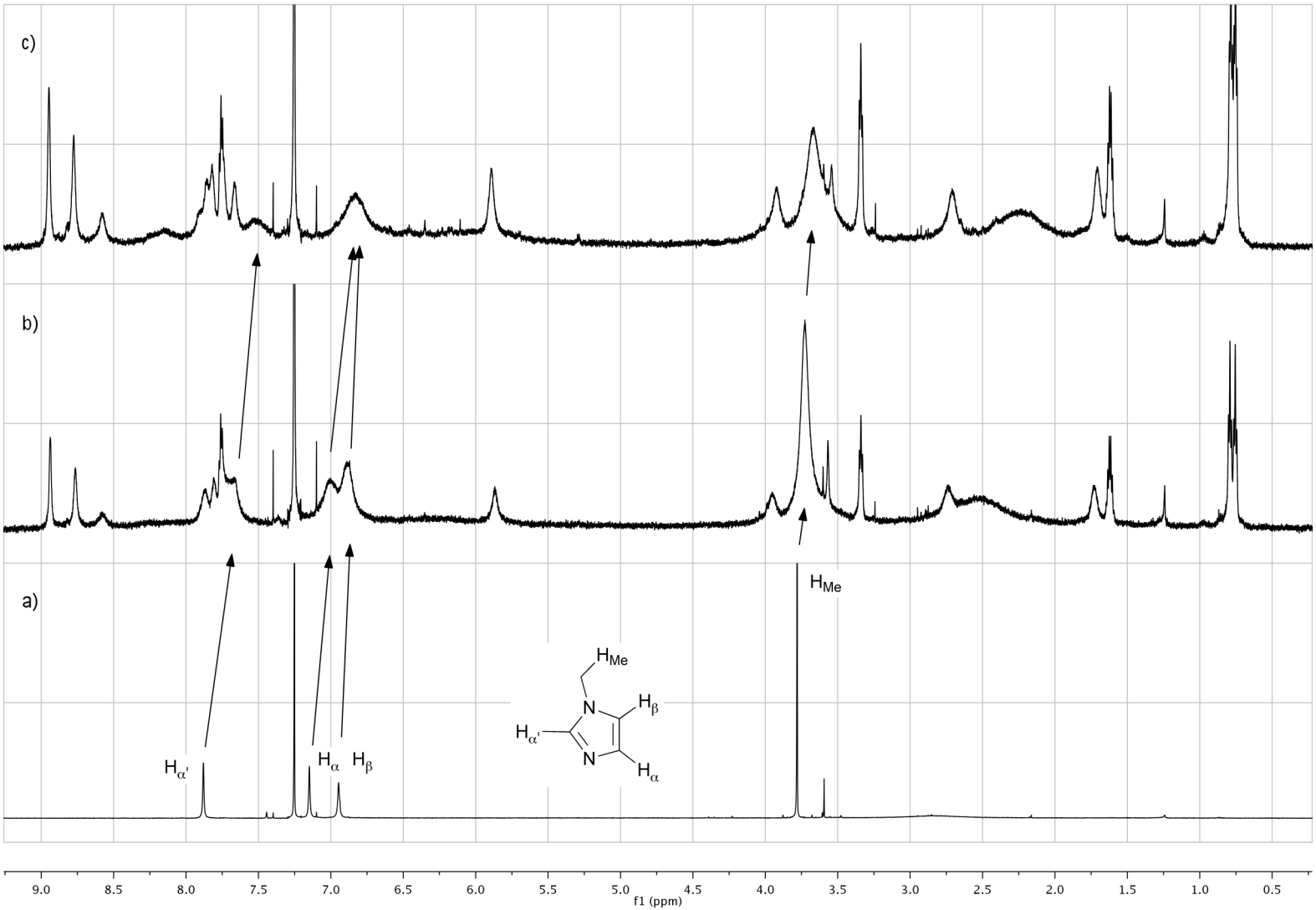


Figure S11. 1H-NMR spectra (700 MHz, $CDCl_3$, 297 K) of *N*-methylimidazole (**10**) (5.72 mM) upon the addition of **1Zn** (a, 0.0; b, 0.38; c, 0.91 mM).

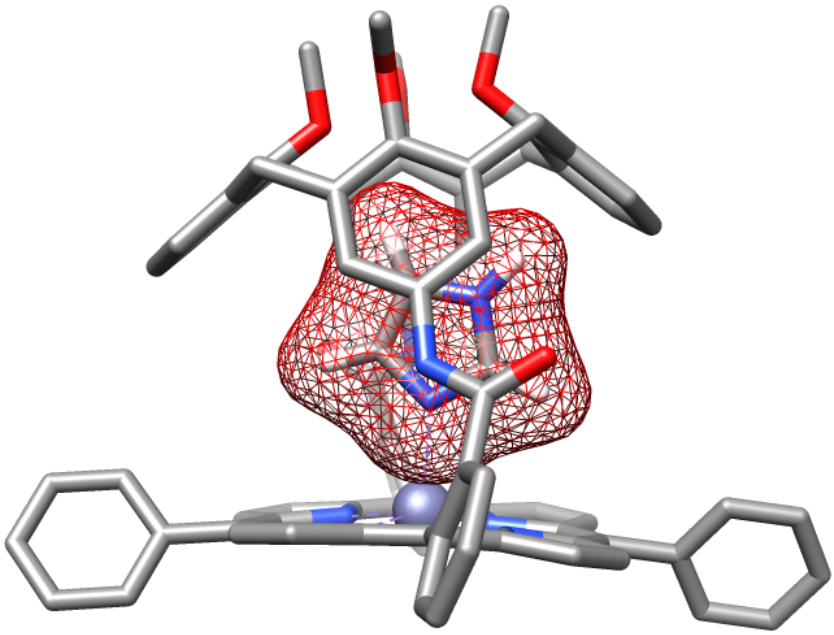
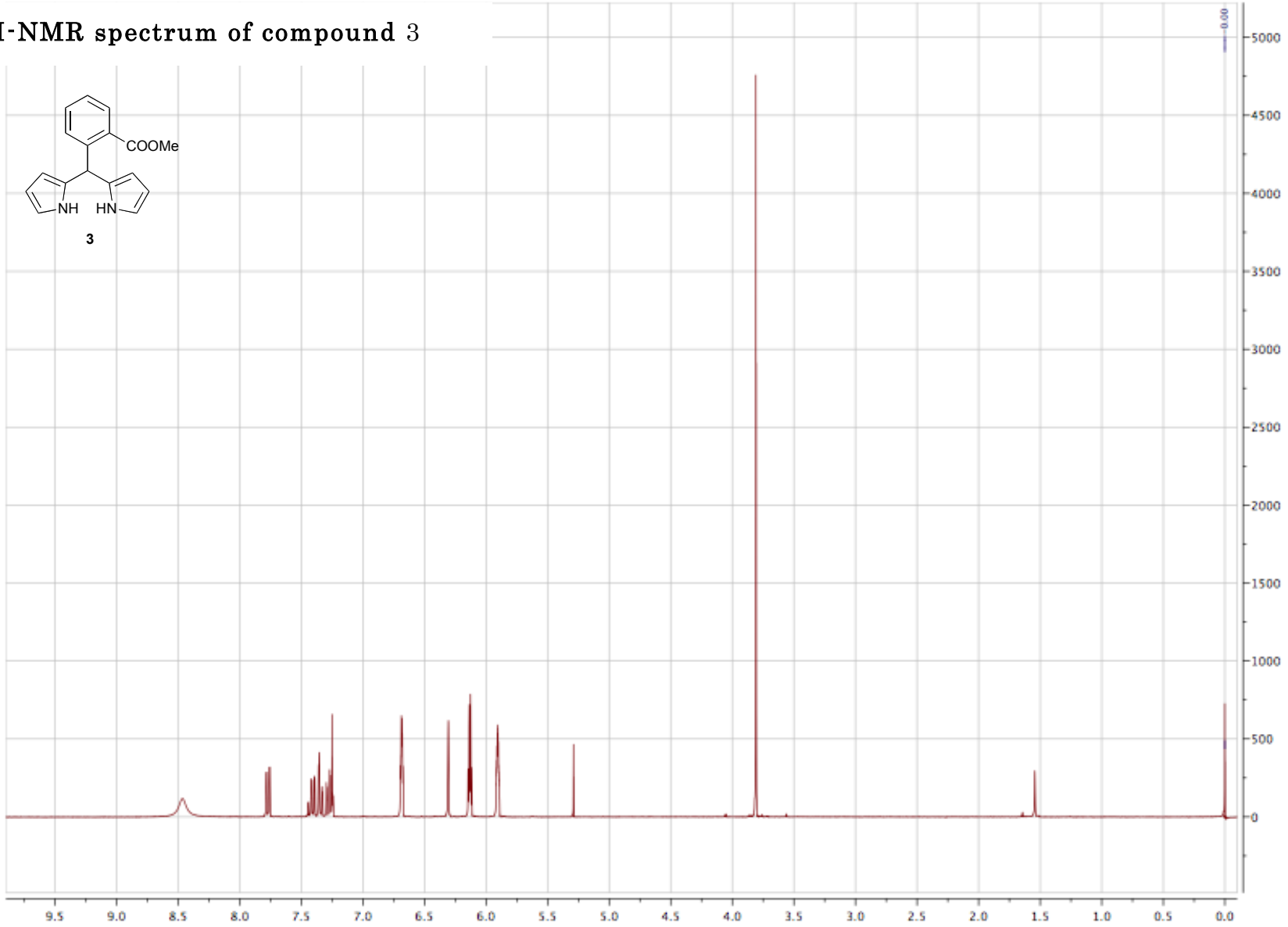


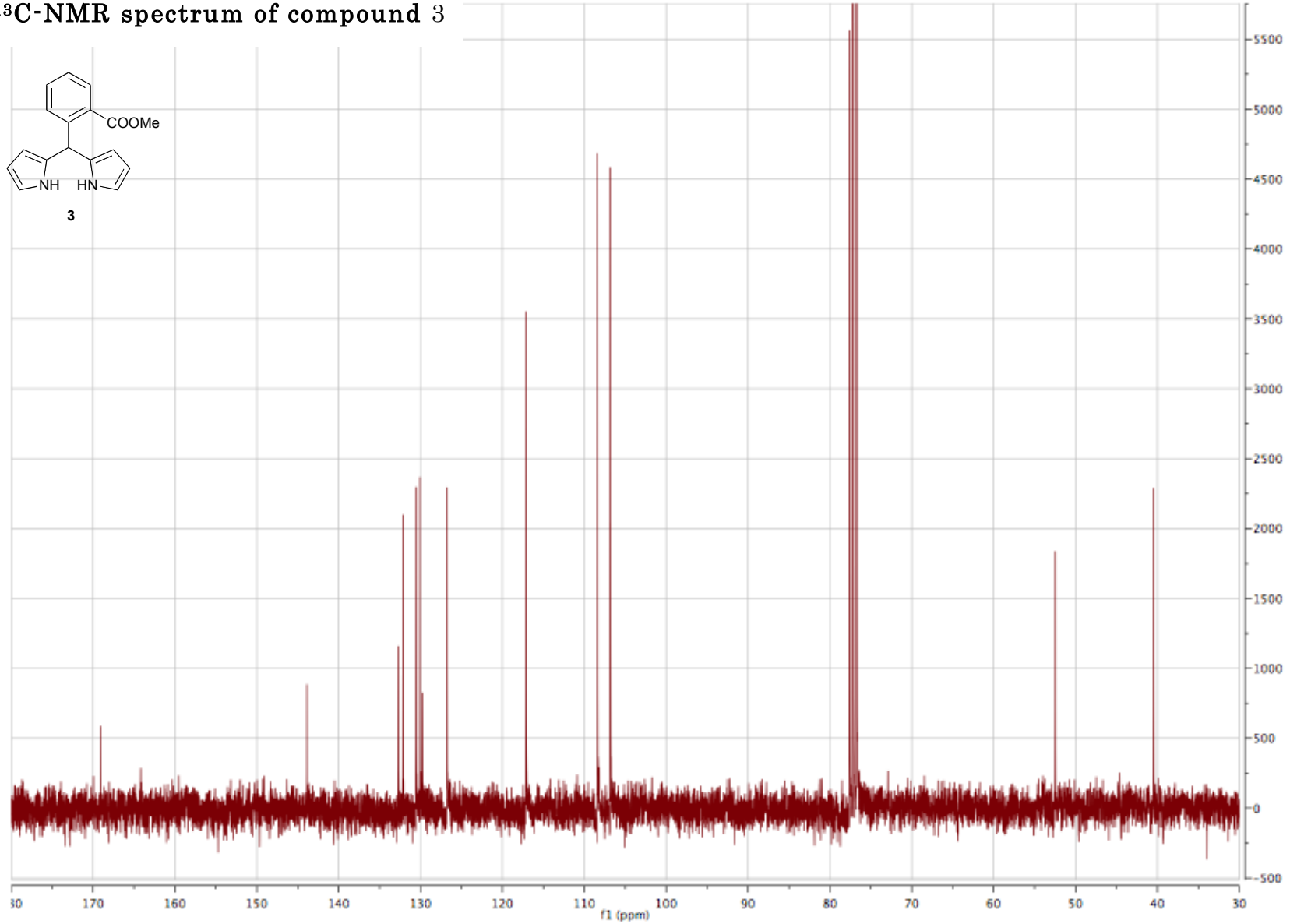
Figure S12. Optimized structure of encapsulation complex of **1Zn** with imidazole (**9**). For simplify and clarity of calculation, *n*-propyl groups were replaced to methyl groups.

^{1}H-NMR spectrum of compound 3

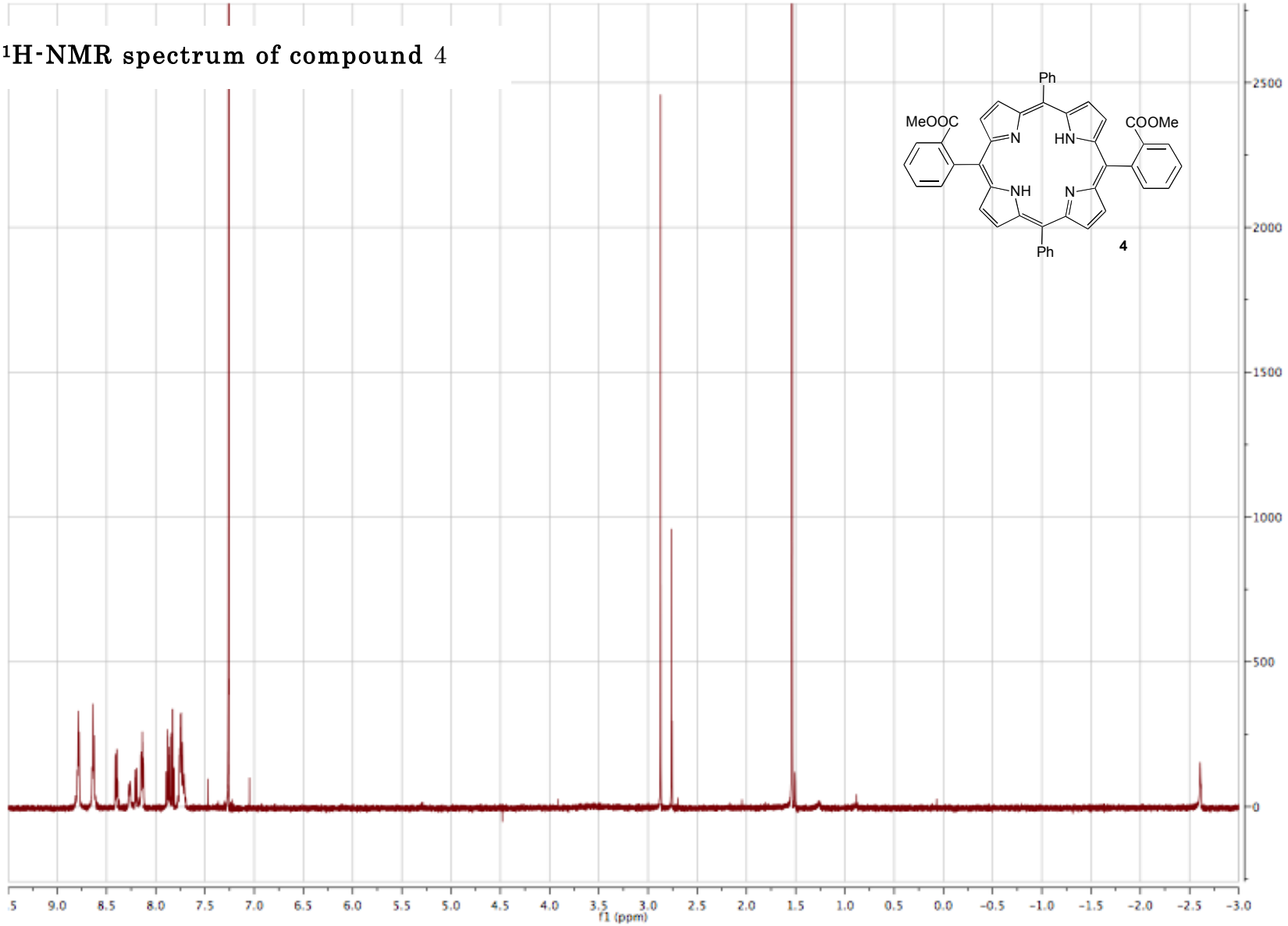
3



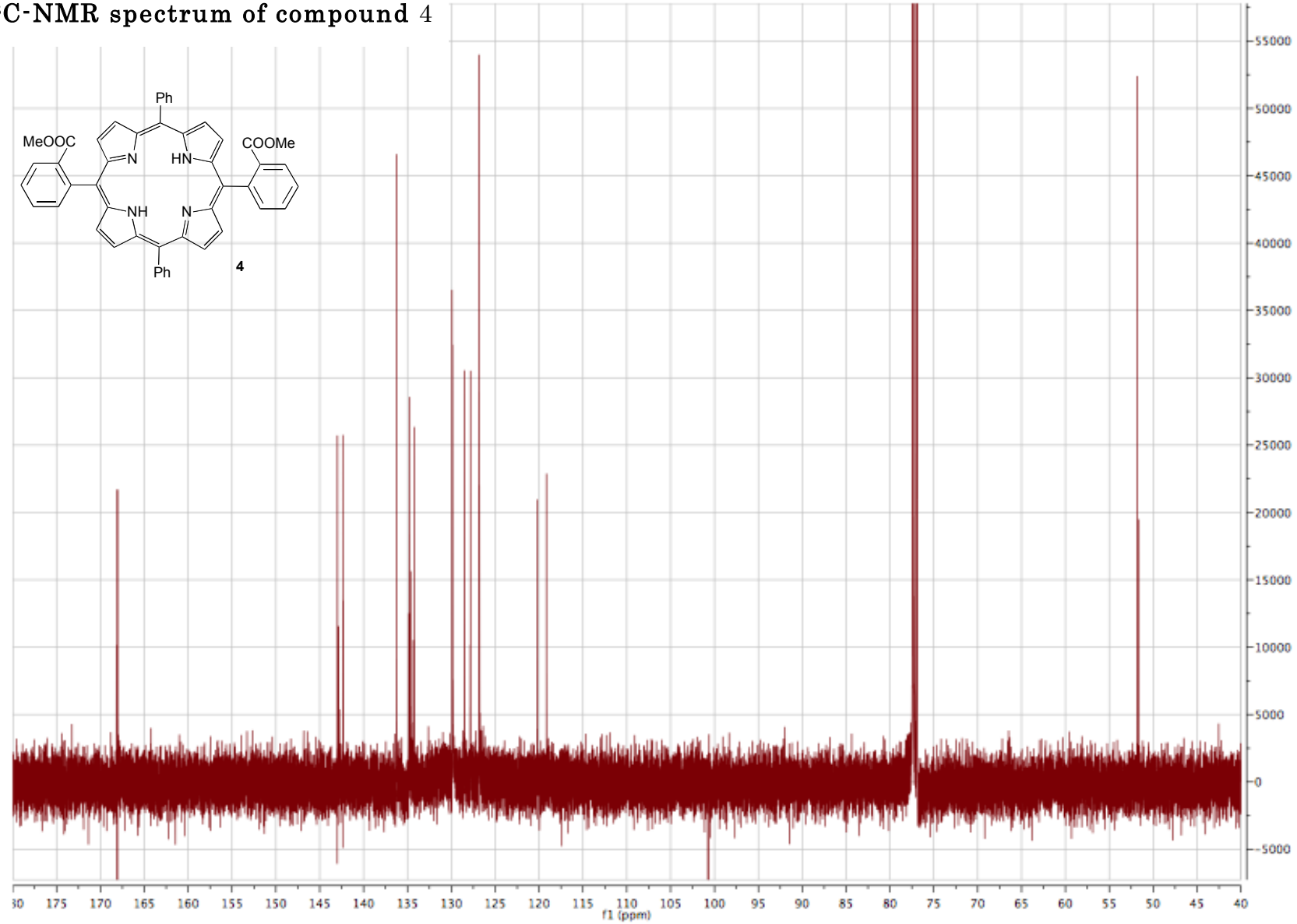
^{13}C-NMR spectrum of compound 3



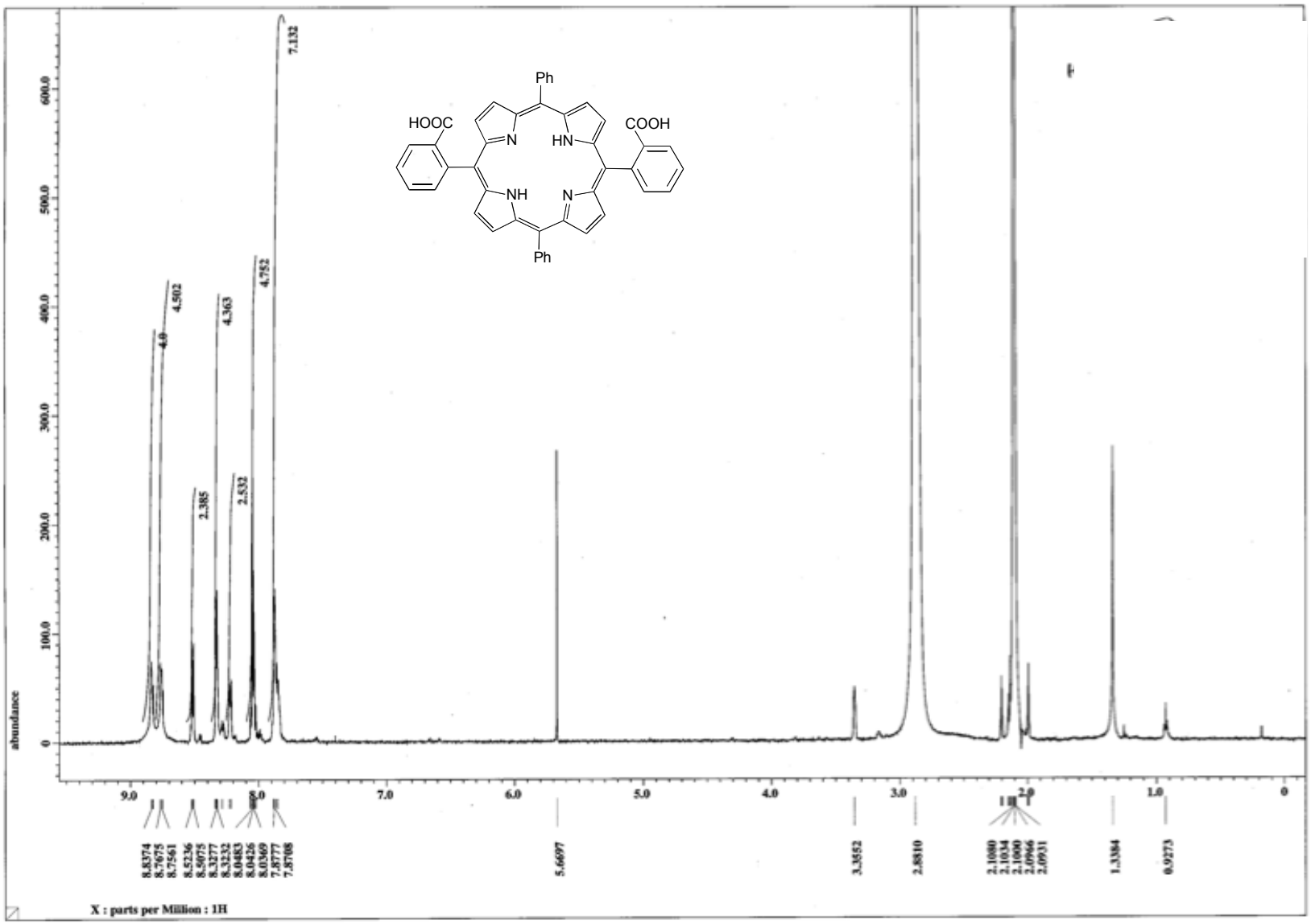
^{1}H-NMR spectrum of compound 4



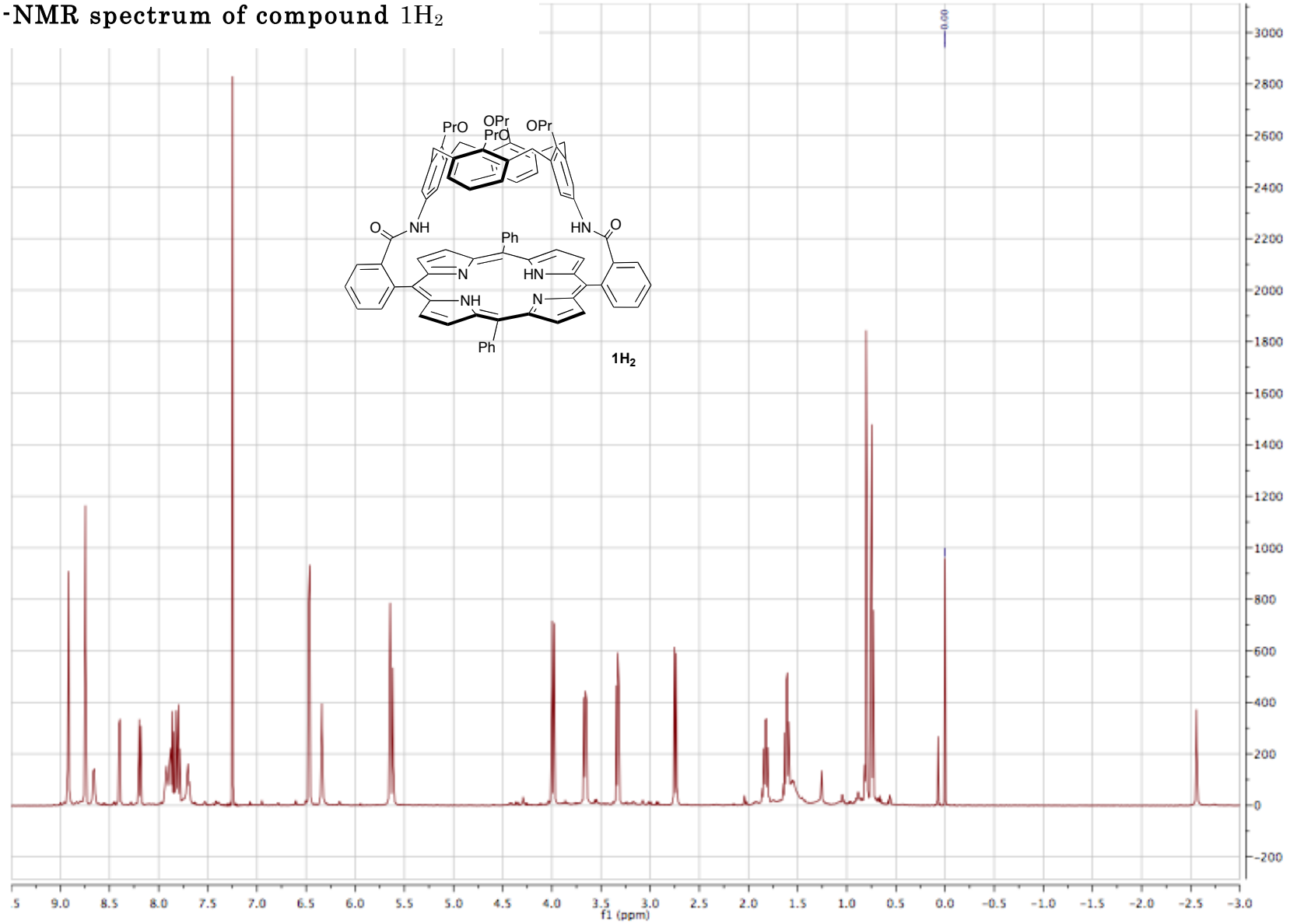
^{13}C-NMR spectrum of compound 4



^{1}H-NMR spectrum of 2,2'-(10,20-diphenyl-21H,23H-porphine-5,15-diyl)bisbenzoic acid stereoisomer



^{1}H-NMR spectrum of compound $1H_2$



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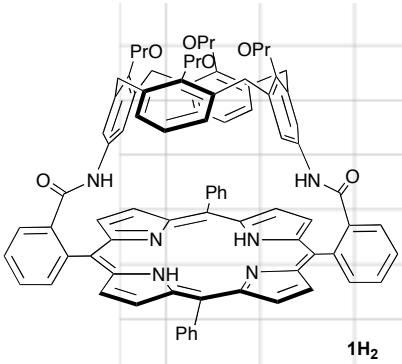
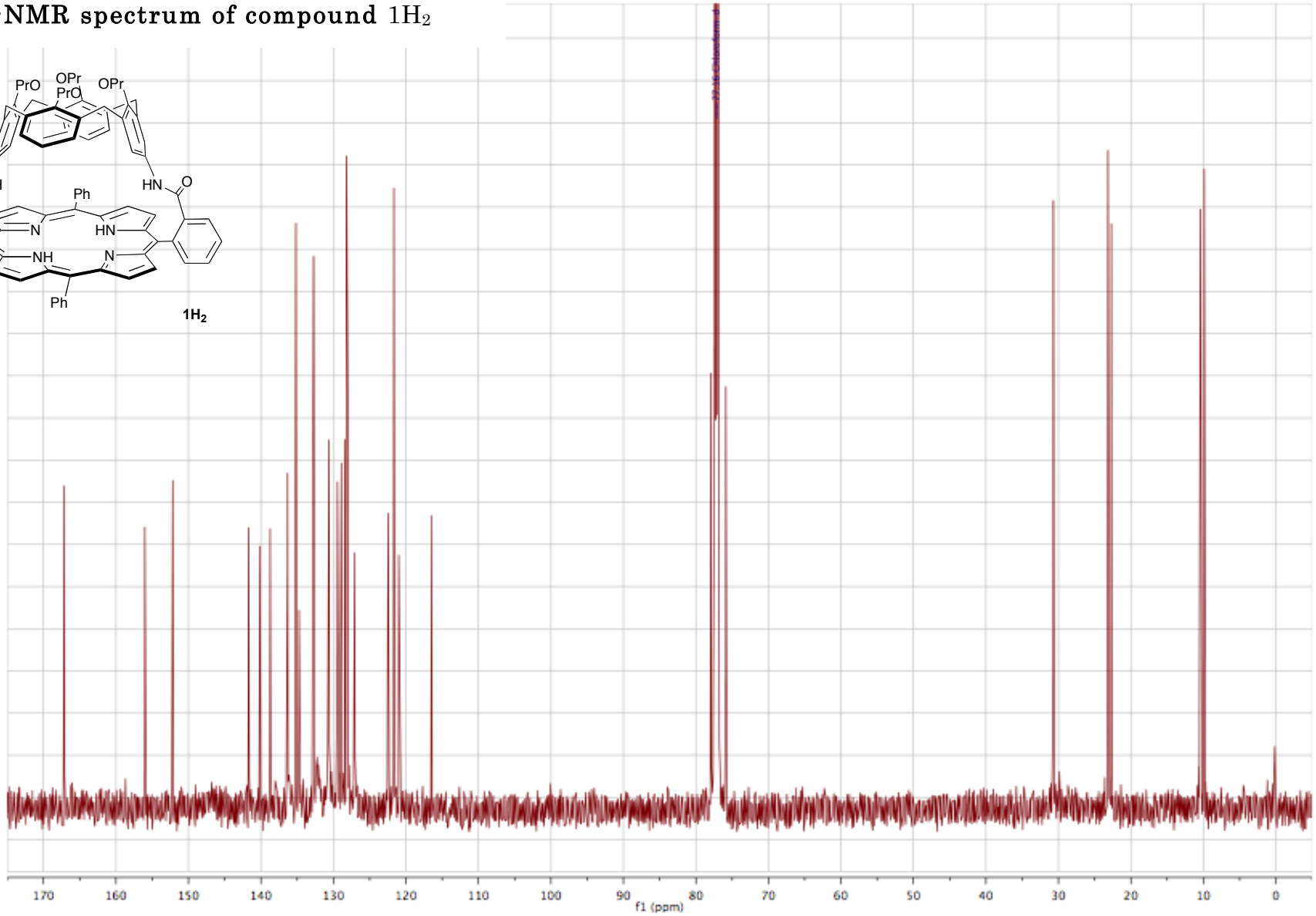
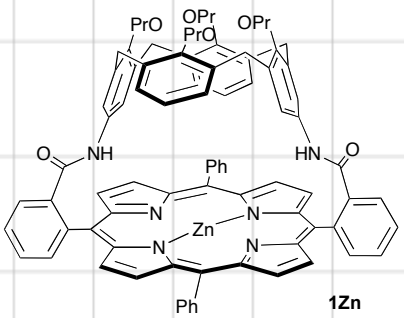


1H$_2$

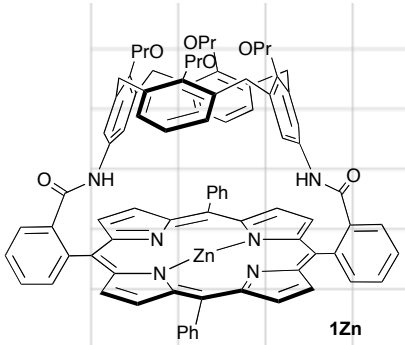


^{1}H-NMR spectrum of compound 1Zn

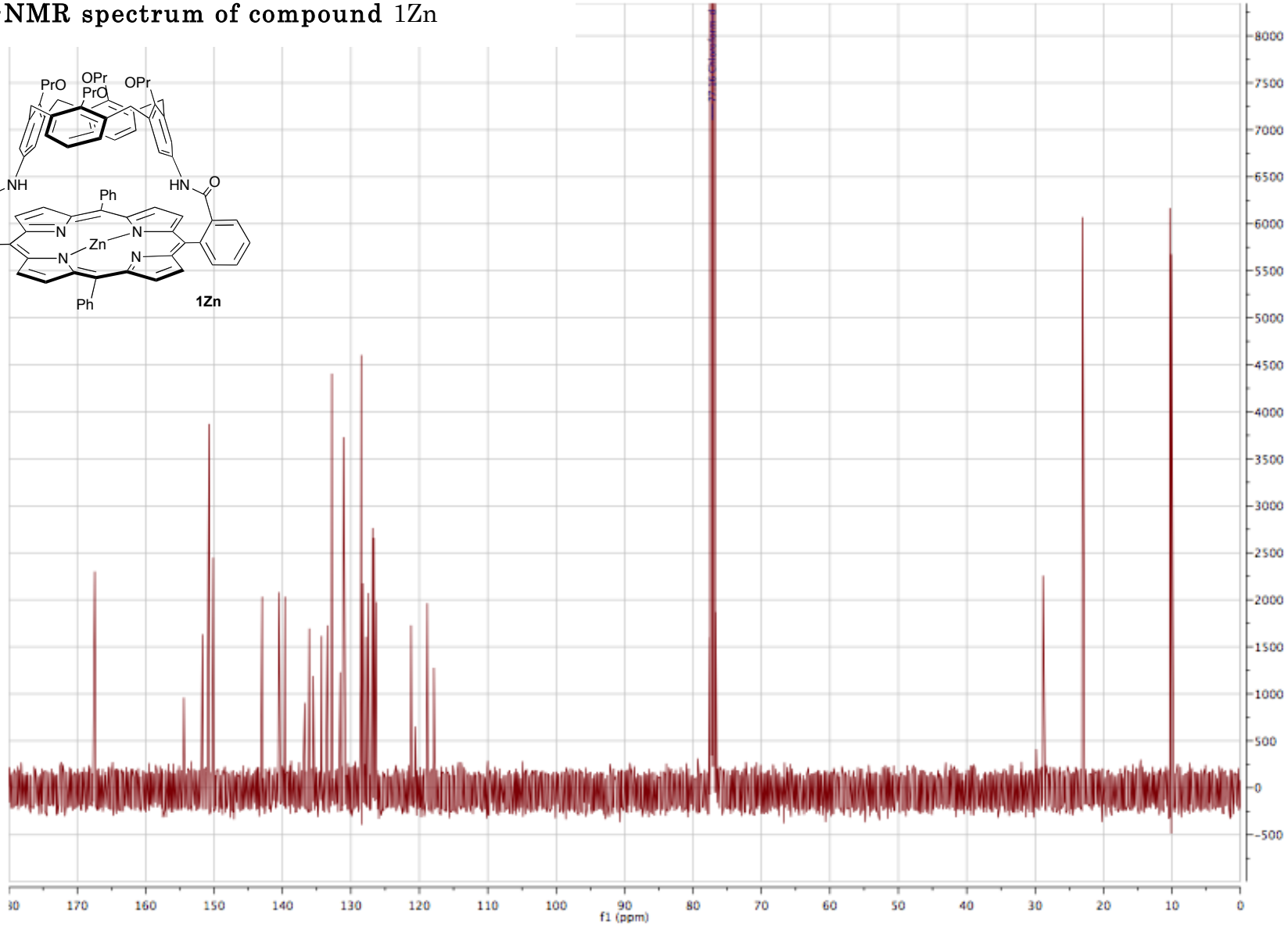


1Zn

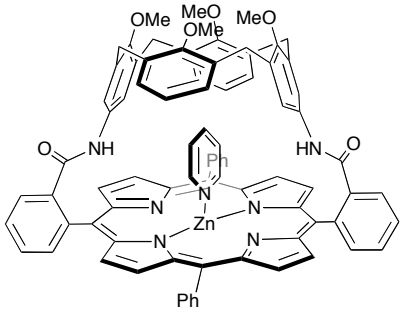
^{13}C-NMR spectrum of compound 1Zn



1Zn



Calculated Structures of 1Zn **with pyridine or imidazole, and electronic energies (au).**



1Zn encapsulating pyridine
Optimized: M06-2X/LANL2DZ
Energy: –4098.89241618
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.971139	1.971526	-2.358792
2	6	0	-2.864668	2.026367	-3.814862
3	6	0	-2.975866	0.738517	-4.273058
4	6	0	-3.139004	-0.121678	-3.103789
5	7	0	-3.134980	0.658959	-1.965508
6	6	0	-3.194783	-1.534766	-3.143804
7	6	0	-3.169879	-2.373967	-2.008964
8	6	0	-3.183078	-3.835647	-2.038819
9	6	0	-3.054053	-4.266898	-0.745889
10	6	0	-2.989390	-3.074682	0.097094
11	6	0	-2.971137	-1.971519	2.358803
12	6	0	-2.864660	-2.026359	3.814873
13	6	0	-2.975852	-0.738509	4.273070
14	6	0	-3.138990	0.121686	3.103801
15	6	0	-3.194763	1.534774	3.143816
16	6	0	-3.169861	2.373974	2.008975
17	6	0	-3.183055	3.835654	2.038831
18	6	0	-3.054036	4.266906	0.745901
19	6	0	-2.989380	3.074689	-0.097083
20	6	0	-2.884735	3.090593	-1.503898
21	7	0	-3.077660	1.951702	0.697099
22	7	0	-3.134974	-0.658950	1.965520
23	7	0	-3.077670	-1.951694	-0.697088
24	6	0	-2.884740	-3.090585	1.503909
25	6	0	-3.226760	2.181158	4.491577

26	6	0	-4.295595	1.936824	5.375099
27	6	0	-4.326179	2.535071	6.643049
28	6	0	-3.283567	3.383437	7.047778
29	6	0	-2.211563	3.629759	6.175205
30	6	0	-2.184543	3.033023	4.906631
31	6	0	-2.729746	-4.436450	2.140452
32	6	0	-3.819055	-4.984924	2.844529
33	6	0	-3.763416	-6.281288	3.369547
34	6	0	-2.612691	-7.062962	3.176727
35	6	0	-1.522765	-6.528976	2.481370
36	6	0	-1.563038	-5.212575	1.982910
37	6	0	-3.226789	-2.181149	-4.491565
38	6	0	-2.184579	-3.033022	-4.906623
39	6	0	-2.211607	-3.629758	-6.175197
40	6	0	-3.283613	-3.383428	-7.047766
41	6	0	-4.326217	-2.535055	-6.643034
42	6	0	-4.295626	-1.936809	-5.375084
43	6	0	-2.729742	4.436457	-2.140443
44	6	0	-1.563033	5.212580	-1.982907
45	6	0	-1.522759	6.528980	-2.481369
46	6	0	-2.612688	7.062968	-3.176721
47	6	0	-3.763416	6.281296	-3.369534
48	6	0	-3.819054	4.984932	-2.844514
49	6	0	-0.292859	-4.752401	1.307783
50	8	0	0.335414	-5.533328	0.556239
51	6	0	-0.292850	4.752405	-1.307785
52	8	0	0.335426	5.533332	-0.556245
53	7	0	0.190665	-3.511856	1.673816
54	7	0	0.190667	3.511857	-1.673815
55	6	0	1.529800	-3.068840	1.448070
56	6	0	2.248945	-3.426601	0.296777
57	6	0	3.600823	-3.075970	0.166482
58	6	0	4.231772	-2.386863	1.217033
59	6	0	3.502571	-1.922187	2.326839
60	6	0	2.149268	-2.277304	2.430766
61	6	0	1.529802	3.068838	-1.448074
62	6	0	2.248952	3.426595	-0.296784
63	6	0	3.600829	3.075961	-0.166493
64	6	0	4.231773	2.386853	-1.217048
65	6	0	3.502567	1.922179	-2.326851
66	6	0	2.149264	2.277301	-2.430773
67	6	0	4.352263	3.427203	1.112640

68	6	0	4.352250	-3.427214	-1.112655
69	6	0	3.868416	2.584890	2.284215
70	6	0	4.230455	1.227185	2.367367
71	6	0	3.754621	0.378740	3.383238
72	6	0	2.883615	0.921282	4.342505
73	6	0	2.506423	2.272666	4.283694
74	6	0	3.000722	3.099427	3.262002
75	6	0	3.868400	-2.584900	-2.284227
76	6	0	4.230441	-1.227196	-2.367380
77	6	0	3.754605	-0.378749	-3.383250
78	6	0	2.883595	-0.921290	-4.342515
79	6	0	2.506401	-2.272673	-4.283703
80	6	0	3.000702	-3.099435	-3.262012
81	6	0	4.172432	1.083824	-3.408642
82	6	0	4.172444	-1.083835	3.408627
83	8	0	5.012447	0.681427	1.351559
84	8	0	5.630691	-2.199101	1.180718
85	8	0	5.630692	2.199087	-1.180738
86	8	0	5.012439	-0.681440	-1.351576
87	6	0	6.357592	3.331922	-1.739502
88	6	0	6.458870	0.807423	1.482688
89	6	0	6.357591	-3.331938	1.739478
90	6	0	6.458861	-0.807438	-1.482712
91	30	0	-2.870967	0.000003	0.000006
92	6	0	1.327822	-0.656073	-1.008392
93	6	0	2.051582	-0.000002	-0.000005
94	6	0	1.327826	0.656069	1.008385
95	6	0	-0.067266	0.636232	0.977200
96	7	0	-0.748562	-0.000002	0.000001
97	6	0	-0.067270	-0.636236	-0.977202
98	1	0	-0.663045	-1.138196	-1.734221
99	1	0	-0.391773	-2.942158	2.281710
100	1	0	-0.391775	2.942159	-2.281705
101	1	0	-2.725735	2.925837	-4.397121
102	1	0	-2.926968	0.394216	-5.295238
103	1	0	-3.287591	-4.439472	-2.927301
104	1	0	-3.025252	-5.286604	-0.390649
105	1	0	-2.725727	-2.925830	4.397132
106	1	0	-2.926948	-0.394208	5.295249
107	1	0	-3.287561	4.439479	2.927314
108	1	0	-3.025233	5.286611	0.390660
109	1	0	-5.105882	1.287618	5.055835

110	1	0	-5.161345	2.343606	7.309027
111	1	0	-3.306461	3.846944	8.028709
112	1	0	-1.400173	4.282342	6.481559
113	1	0	-1.351611	3.216174	4.232931
114	1	0	-4.719876	-4.387519	2.948693
115	1	0	-4.616421	-6.685563	3.904492
116	1	0	-2.568018	-8.076403	3.561028
117	1	0	-1.351645	-3.216177	-4.232926
118	1	0	-1.400223	-4.282346	-6.481553
119	1	0	-3.306514	-3.846935	-8.028697
120	1	0	-5.161385	-2.343585	-7.309009
121	1	0	-5.105907	-1.287597	-5.055816
122	1	0	-2.568015	8.076408	-3.561023
123	1	0	-4.616422	6.685571	-3.904474
124	1	0	-4.719877	4.387529	-2.948672
125	1	0	1.759536	-3.993349	-0.485994
126	1	0	1.580333	-1.952912	3.300849
127	1	0	1.759547	3.993344	0.485990
128	1	0	1.580325	1.952911	-3.300854
129	1	0	5.422113	3.261520	0.953731
130	1	0	4.198980	4.485559	1.351567
131	1	0	5.422101	-3.261534	-0.953751
132	1	0	4.198964	-4.485570	-1.351582
133	1	0	2.501279	0.284833	5.136185
134	1	0	1.833037	2.678606	5.031527
135	1	0	2.703008	4.143401	3.212819
136	1	0	2.501259	-0.284840	-5.136194
137	1	0	1.833013	-2.678612	-5.031534
138	1	0	2.702986	-4.143409	-3.212829
139	1	0	5.256633	1.146547	-3.271682
140	1	0	3.929055	1.497543	-4.394345
141	1	0	5.256644	-1.146560	3.271662
142	1	0	3.929071	-1.497554	4.394332
143	1	0	7.419316	3.095286	-1.648624
144	1	0	6.094372	3.477205	-2.794738
145	1	0	6.129655	4.250965	-1.185444
146	1	0	6.717212	1.545069	2.253823
147	1	0	6.826740	1.134819	0.509117
148	1	0	6.866539	-0.174603	1.741707
149	1	0	6.094374	-3.477221	2.794715
150	1	0	6.129651	-4.250980	1.185420
151	1	0	7.419315	-3.095304	1.648598

152	1	0	6.866530	0.174588	-1.741735
153	1	0	6.826735	-1.134832	-0.509142
154	1	0	6.717198	-1.545086	-2.253847
155	1	0	-0.628452	-7.117654	2.306823
156	1	0	-0.628444	7.117657	-2.306827
157	1	0	1.820148	-1.186478	-1.809807
158	1	0	3.143617	-0.000003	-0.000007
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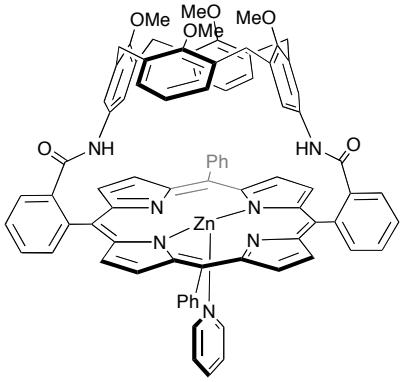
160	1	0	-0.663037	1.138192	1.734222



1Zn bound to pyridine outside

Optimized: M06-2X/LANL2DZ

Energy: –4098.86435803

Standard orientation:

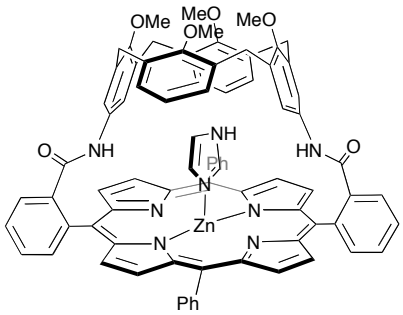
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.196141	-2.168307	2.431375
2	6	0	-2.395164	-3.604290	2.252497
3	6	0	-1.149987	-4.173758	2.181644
4	6	0	-0.175776	-3.096423	2.332745
5	7	0	-0.844535	-1.896536	2.472135
6	6	0	1.225697	-3.264207	2.301881
7	6	0	2.164355	-2.212804	2.364994
8	6	0	3.613570	-2.390623	2.377498
9	6	0	4.174775	-1.142826	2.431088
10	6	0	3.076267	-0.181925	2.451700
11	6	0	2.196141	2.168307	2.431375
12	6	0	2.395164	3.604290	2.252497
13	6	0	1.149987	4.173758	2.181644
14	6	0	0.175776	3.096423	2.332745
15	6	0	-1.225697	3.264207	2.301881
16	6	0	-2.164355	2.212804	2.364994
17	6	0	-3.613570	2.390623	2.377498
18	6	0	-4.174775	1.142826	2.431088
19	6	0	-3.076267	0.181925	2.451700
20	6	0	-3.236043	-1.217909	2.460517
21	7	0	-1.873392	0.861618	2.432698
22	7	0	0.844535	1.896536	2.472135
23	7	0	1.873392	-0.861618	2.432698
24	6	0	3.236043	1.217909	2.460517
25	6	0	-1.754309	4.654668	2.150532

26	6	0	-1.494858	5.638029	3.123804
27	6	0	-1.991057	6.941189	2.972709
28	6	0	-2.751298	7.278998	1.841993
29	6	0	-3.012563	6.304737	0.865343
30	6	0	-2.518462	5.001735	1.019295
31	6	0	4.641179	1.732951	2.426283
32	6	0	5.176751	2.354336	3.569227
33	6	0	6.514626	2.767917	3.604563
34	6	0	7.344937	2.544755	2.494019
35	6	0	6.821098	1.933548	1.348984
36	6	0	5.469397	1.549352	1.299659
37	6	0	1.754309	-4.654668	2.150532
38	6	0	2.518462	-5.001735	1.019295
39	6	0	3.012563	-6.304737	0.865343
40	6	0	2.751298	-7.278998	1.841993
41	6	0	1.991057	-6.941189	2.972709
42	6	0	1.494858	-5.638029	3.123804
43	6	0	-4.641179	-1.732951	2.426283
44	6	0	-5.469397	-1.549352	1.299659
45	6	0	-6.821098	-1.933548	1.348984
46	6	0	-7.344937	-2.544755	2.494019
47	6	0	-6.514626	-2.767917	3.604563
48	6	0	-5.176751	-2.354336	3.569227
49	6	0	5.001506	0.951778	-0.004919
50	8	0	5.742638	0.169561	-0.644601
51	6	0	-5.001506	-0.951778	-0.004919
52	8	0	-5.742638	-0.169561	-0.644601
53	7	0	3.787473	1.402876	-0.469183
54	7	0	-3.787473	-1.402876	-0.469183
55	6	0	3.273929	1.173224	-1.780202
56	6	0	3.483395	-0.033736	-2.459458
57	6	0	3.087118	-0.167883	-3.797445
58	6	0	2.498515	0.930752	-4.448424
59	6	0	2.170452	2.104021	-3.745807
60	6	0	2.566511	2.210954	-2.406357
61	6	0	-3.273929	-1.173224	-1.780202
62	6	0	-3.483395	0.033736	-2.459458
63	6	0	-3.087118	0.167883	-3.797445
64	6	0	-2.498515	-0.930752	-4.448424
65	6	0	-2.170452	-2.104021	-3.745807
66	6	0	-2.566511	-2.210954	-2.406357
67	6	0	-3.291961	1.500572	-4.502776

68	6	0	3.291961	-1.500572	-4.502776
69	6	0	-2.312580	2.550776	-3.998591
70	6	0	-0.962791	2.473243	-4.384865
71	6	0	0.000000	3.396470	-3.944231
72	6	0	-0.413090	4.425690	-3.083294
73	6	0	-1.754165	4.524689	-2.681332
74	6	0	-2.698381	3.591899	-3.138538
75	6	0	2.312580	-2.550776	-3.998591
76	6	0	0.962791	-2.473243	-4.384865
77	6	0	0.000000	-3.396470	-3.944231
78	6	0	0.413090	-4.425690	-3.083294
79	6	0	1.754165	-4.524689	-2.681332
80	6	0	2.698381	-3.591899	-3.138538
81	6	0	-1.438598	-3.257340	-4.416055
82	6	0	1.438598	3.257340	-4.416055
83	8	0	-0.562553	1.411705	-5.192526
84	8	0	2.288017	0.881572	-5.844055
85	8	0	-2.288017	-0.881572	-5.844055
86	8	0	0.562553	-1.411705	-5.192526
87	6	0	-3.456658	-1.317094	-6.595478
88	6	0	-0.652037	1.598720	-6.632709
89	6	0	3.456658	1.317094	-6.595478
90	6	0	0.652037	-1.598720	-6.632709
91	30	0	0.000000	0.000000	2.743181
92	6	0	-1.039990	0.618117	7.013264
93	6	0	0.000000	0.000000	7.723882
94	6	0	1.039990	-0.618117	7.013264
95	6	0	1.005100	-0.597208	5.613320
96	7	0	0.000000	0.000000	4.933140
97	6	0	-1.005100	0.597208	5.613320
98	1	0	-1.782486	1.057607	5.011718
99	1	0	3.278091	2.062757	0.110958
100	1	0	-3.278091	-2.062757	0.110958
101	1	0	-3.354485	-4.096409	2.178401
102	1	0	-0.906837	-5.213182	2.020868
103	1	0	4.123793	-3.341377	2.355999
104	1	0	5.225708	-0.894919	2.450918
105	1	0	3.354485	4.096409	2.178401
106	1	0	0.906837	5.213182	2.020868
107	1	0	-4.123793	3.341377	2.355999
108	1	0	-5.225708	0.894919	2.450918
109	1	0	-0.913226	5.372506	4.002234

110	1	0	-1.788592	7.687007	3.734663
111	1	0	-3.135280	8.287067	1.723882
112	1	0	-3.598778	6.558456	-0.012578
113	1	0	-2.708158	4.247876	0.259961
114	1	0	4.535740	2.488116	4.435588
115	1	0	6.910932	3.242700	4.496144
116	1	0	8.387273	2.844010	2.521581
117	1	0	2.708158	-4.247876	0.259961
118	1	0	3.598778	-6.558456	-0.012578
119	1	0	3.135280	-8.287067	1.723882
120	1	0	1.788592	-7.687007	3.734663
121	1	0	0.913226	-5.372506	4.002234
122	1	0	-8.387273	-2.844010	2.521581
123	1	0	-6.910932	-3.242700	4.496144
124	1	0	-4.535740	-2.488116	4.435588
125	1	0	3.983132	-0.853971	-1.957526
126	1	0	2.355918	3.129138	-1.860056
127	1	0	-3.983132	0.853971	-1.957526
128	1	0	-2.355918	-3.129138	-1.860056
129	1	0	-3.155826	1.358963	-5.579656
130	1	0	-4.313499	1.857070	-4.327866
131	1	0	3.155826	-1.358963	-5.579656
132	1	0	4.313499	-1.857070	-4.327866
133	1	0	0.314116	5.154611	-2.734163
134	1	0	-2.058924	5.331527	-2.021818
135	1	0	-3.738275	3.669808	-2.830315
136	1	0	-0.314116	-5.154611	-2.734163
137	1	0	2.058924	-5.331527	-2.021818
138	1	0	3.738275	-3.669808	-2.830315
139	1	0	-1.448368	-3.095063	-5.498349
140	1	0	-1.966614	-4.195665	-4.207794
141	1	0	1.448368	3.095063	-5.498349
142	1	0	1.966614	4.195665	-4.207794
143	1	0	-3.197993	-1.226092	-7.652299
144	1	0	-3.703819	-2.360007	-6.358712
145	1	0	-4.324211	-0.685264	-6.366756
146	1	0	-1.339062	2.419228	-6.882153
147	1	0	-1.030469	0.657019	-7.032668
148	1	0	0.348456	1.807631	-7.026546
149	1	0	3.703819	2.360007	-6.358712
150	1	0	4.324211	0.685264	-6.366756
151	1	0	3.197993	1.226092	-7.652299

152	1	0	-0.348456	-1.807631	-7.026546
153	1	0	1.030469	-0.657019	-7.032668
154	1	0	1.339062	-2.419228	-6.882153
155	1	0	7.442465	1.739834	0.480949
156	1	0	-7.442465	-1.739834	0.480949
157	1	0	-1.860594	1.105816	7.524949
158	1	0	0.000000	0.000000	8.808575
159	1	0	1.860594	-1.105816	7.524949
160	1	0	1.782486	-1.057607	5.011718



1Zn encapsulating imidazole

Optimized: M06-2X/LANL2DZ

Energy: –4076.85000085

Standard orientation:

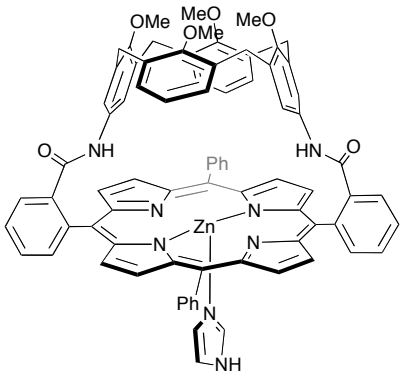
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.183595	2.123939	2.775462
2	6	0	1.712713	2.251690	4.151949
3	6	0	1.603177	0.980378	4.655880
4	6	0	2.008156	0.059483	3.595743
5	7	0	2.337719	0.787669	2.469754
6	6	0	2.021899	-1.351580	3.705134
7	6	0	2.325423	-2.239402	2.648416
8	6	0	2.421814	-3.694445	2.771433
9	6	0	2.718946	-4.186368	1.528957
10	6	0	2.829727	-3.038514	0.633538
11	6	0	3.398606	-2.035328	-1.598119
12	6	0	3.717341	-2.166823	-3.017787
13	6	0	3.860136	-0.896829	-3.512914
14	6	0	3.634143	0.024131	-2.402239
15	6	0	3.681794	1.432530	-2.499902
16	6	0	3.408673	2.314544	-1.434426
17	6	0	3.533925	3.768884	-1.503409
18	6	0	3.162917	4.262010	-0.283046
19	6	0	2.817870	3.113342	0.553636
20	6	0	2.402509	3.205821	1.897022
21	7	0	2.986308	1.951906	-0.169402
22	7	0	3.341050	-0.697972	-1.262176
23	7	0	2.591416	-1.881022	1.342119
24	6	0	3.160773	-3.120721	-0.733069
25	6	0	4.047648	2.029385	-3.820959
26	6	0	5.298297	1.762583	-4.410860

27	6	0	5.639837	2.325598	-5.648853
28	6	0	4.733078	3.162966	-6.317688
29	6	0	3.484100	3.435727	-5.737610
30	6	0	3.146160	2.873718	-4.498355
31	6	0	3.292057	-4.493238	-1.315718
32	6	0	4.575061	-4.998247	-1.598555
33	6	0	4.747544	-6.301155	-2.081285
34	6	0	3.628931	-7.129077	-2.272892
35	6	0	2.349288	-6.638120	-1.994374
36	6	0	2.171569	-5.319003	-1.536396
37	6	0	1.695980	-1.949280	5.035441
38	6	0	0.640577	-2.873338	5.166725
39	6	0	0.331596	-3.437912	6.411994
40	6	0	1.078684	-3.089970	7.548637
41	6	0	2.137355	-2.176054	7.427684
42	6	0	2.442246	-1.610427	6.181393
43	6	0	2.189187	4.595621	2.411913
44	6	0	1.159860	5.416905	1.901533
45	6	0	1.086977	6.770288	2.275016
46	6	0	2.001176	7.304534	3.190888
47	6	0	2.999613	6.481830	3.736777
48	6	0	3.095181	5.141748	3.338633
49	6	0	0.742881	-4.905575	-1.290552
50	8	0	-0.073866	-5.735730	-0.827584
51	6	0	0.059417	4.931388	0.989496
52	8	0	-0.404396	5.663172	0.084587
53	7	0	0.374442	-3.633528	-1.680085
54	7	0	-0.475585	3.704648	1.314546
55	6	0	-0.977835	-3.176043	-1.636380
56	6	0	-1.777270	-3.463350	-0.522701
57	6	0	-3.142747	-3.167781	-0.529940
58	6	0	-3.703777	-2.588770	-1.683173
59	6	0	-2.897177	-2.166801	-2.754997
60	6	0	-1.526256	-2.478301	-2.722598
61	6	0	-1.735563	3.205525	0.885493
62	6	0	-2.282593	3.469422	-0.379070
63	6	0	-3.580009	3.027678	-0.689046
64	6	0	-4.333135	2.366477	0.296880
65	6	0	-3.763301	2.012607	1.532918
66	6	0	-2.460326	2.434374	1.808040
67	6	0	-4.143578	3.241476	-2.089184
68	6	0	-3.968390	-3.459745	0.712513

69	6	0	-3.473349	2.322453	-3.100578
70	6	0	-3.784198	0.947432	-3.121618
71	6	0	-3.148437	0.041250	-3.995237
72	6	0	-2.166983	0.542544	-4.867539
73	6	0	-1.831823	1.906824	-4.861484
74	6	0	-2.484630	2.790083	-3.985201
75	6	0	-3.659567	-2.471903	1.828091
76	6	0	-4.138627	-1.155423	1.731522
77	6	0	-3.929275	-0.195930	2.736451
78	6	0	-3.179851	-0.570314	3.862495
79	6	0	-2.667200	-1.872314	3.974637
80	6	0	-2.911013	-2.818603	2.965727
81	6	0	-4.519837	1.194474	2.567174
82	6	0	-3.503258	-1.437911	-3.949960
83	8	0	-4.672075	0.441926	-2.178331
84	8	0	-5.107658	-2.483707	-1.790791
85	8	0	-5.696800	2.090874	0.056711
86	8	0	-4.817703	-0.764323	0.576979
87	6	0	-6.568487	3.175125	0.490706
88	6	0	-6.081045	0.368589	-2.548942
89	6	0	-5.713001	-3.699800	-2.319759
90	6	0	-6.270633	-0.899251	0.583141
91	30	0	2.464197	0.028822	0.521013
92	6	0	0.186212	0.714550	-1.262088
93	7	0	0.433294	0.098288	-0.101156
94	1	0	1.081420	-3.021812	-2.076554
95	1	0	-0.020876	3.181513	2.057408
96	1	0	1.499259	3.184120	4.654937
97	1	0	1.265178	0.688979	5.638787
98	1	0	2.305369	-4.252204	3.687888
99	1	0	2.874635	-5.217030	1.245060
100	1	0	3.817846	-3.101034	-3.551021
101	1	0	4.082873	-0.604671	-4.528002
102	1	0	3.881287	4.323518	-2.361748
103	1	0	3.145122	5.294781	0.031786
104	1	0	6.004157	1.125601	-3.885598
105	1	0	6.611097	2.116850	-6.085650
106	1	0	4.997475	3.599659	-7.275269
107	1	0	2.777798	4.083561	-6.246922
108	1	0	2.179050	3.083737	-4.048728
109	1	0	5.434133	-4.360092	-1.414701
110	1	0	5.745301	-6.673228	-2.289631

111	1	0	3.755218	-8.145381	-2.630607
112	1	0	0.063626	-3.138583	4.285078
113	1	0	-0.486743	-4.146657	6.494585
114	1	0	0.842929	-3.528316	8.512917
115	1	0	2.728219	-1.910206	8.298264
116	1	0	3.272312	-0.916532	6.085060
117	1	0	1.935973	8.348870	3.477071
118	1	0	3.712072	6.886293	4.448200
119	1	0	3.893805	4.510442	3.716558
120	1	0	-1.333311	-3.949167	0.339615
121	1	0	-0.895400	-2.214406	-3.569535
122	1	0	-1.706816	4.031467	-1.105680
123	1	0	-2.009707	2.180071	2.766534
124	1	0	-5.219818	3.045047	-2.073700
125	1	0	-3.985488	4.280591	-2.398412
126	1	0	-5.032778	-3.402772	0.463456
127	1	0	-3.753008	-4.474008	1.066462
128	1	0	-1.661981	-0.137745	-5.547705
129	1	0	-1.069836	2.279620	-5.537571
130	1	0	-2.223291	3.844529	-3.979448
131	1	0	-3.002560	0.153111	4.654102
132	1	0	-2.092495	-2.147100	4.853072
133	1	0	-2.529242	-3.832150	3.062639
134	1	0	-5.566060	1.112852	2.255890
135	1	0	-4.492609	1.708042	3.535427
136	1	0	-4.591328	-1.546076	-3.902147
137	1	0	-3.154766	-1.905286	-4.878337
138	1	0	-7.590047	2.861018	0.268960
139	1	0	-6.457180	3.354047	1.567363
140	1	0	-6.333445	4.099840	-0.050922
141	1	0	-6.620935	1.149183	-2.004535
142	1	0	-6.422048	-0.621970	-2.244330
143	1	0	-6.206197	0.498083	-3.631880
144	1	0	-5.343804	-3.906339	-3.332121
145	1	0	-5.485149	-4.558027	-1.675801
146	1	0	-6.790505	-3.525827	-2.343380
147	1	0	-6.663838	0.035290	0.180896
148	1	0	-6.542091	-1.742307	-0.058641
149	1	0	-6.640452	-1.059409	1.604619
150	1	0	1.470020	-7.261966	-2.114772
151	1	0	0.307757	7.383961	1.835286
152	1	0	0.926587	1.172263	-1.899076

153	6	0	-1.800973	0.040195	-0.483226
154	1	0	-2.877777	-0.095702	-0.470857
155	6	0	-0.800544	-0.329058	0.397830
156	1	0	-0.885602	-0.865777	1.329832
157	7	0	-1.147883	0.693262	-1.521376
158	1	0	-1.594384	1.115246	-2.324135



1Zn encapsulating imidazole

Optimized: M06-2X/LANL2DZ

Energy: –4076.813818

Standard orientation:

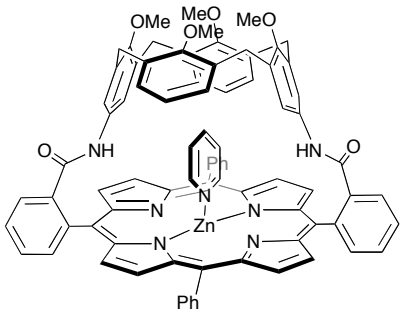
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.528936	-2.116118	2.201242
2	6	0	-2.347102	-2.308247	3.638444
3	6	0	-2.251700	-1.060489	4.198301
4	6	0	-2.391074	-0.091523	3.113908
5	7	0	-2.545176	-0.766068	1.920107
6	6	0	-2.341225	1.310686	3.272156
7	6	0	-2.399632	2.243427	2.215535
8	6	0	-2.380521	3.694571	2.384766
9	6	0	-2.425019	4.248646	1.134135
10	6	0	-2.471113	3.143545	0.180192
11	6	0	-2.445733	2.246139	-2.163250
12	6	0	-2.256399	2.432562	-3.599894
13	6	0	-2.205858	1.182424	-4.160652
14	6	0	-2.380543	0.218403	-3.077019
15	6	0	-2.383763	-1.184427	-3.236229
16	6	0	-2.473538	-2.116137	-2.179563
17	6	0	-2.527334	-3.565704	-2.349142
18	6	0	-2.593350	-4.118107	-1.097245
19	6	0	-2.580047	-3.013143	-0.143092
20	6	0	-2.586442	-3.162118	1.258939
21	7	0	-2.530198	-1.816298	-0.830505
22	7	0	-2.510043	0.898218	-1.882367
23	7	0	-2.479369	1.945830	0.867620
24	6	0	-2.466197	3.293553	-1.220293
25	6	0	-2.241502	-1.725798	-4.622850

26	6	0	-3.200851	-1.443490	-5.613788
27	6	0	-3.057975	-1.952273	-6.913035
28	6	0	-1.949247	-2.748888	-7.239844
29	6	0	-0.986309	-3.033188	-6.258406
30	6	0	-1.132117	-2.526083	-4.959465
31	6	0	-2.403884	4.694246	-1.745134
32	6	0	-3.536771	5.248545	-2.368514
33	6	0	-3.545910	6.583942	-2.791476
34	6	0	-2.418522	7.393263	-2.575855
35	6	0	-1.283397	6.850744	-1.962500
36	6	0	-1.260675	5.501002	-1.568891
37	6	0	-2.170452	1.845606	4.658136
38	6	0	-1.021625	2.588798	4.992917
39	6	0	-0.848928	3.088499	6.291461
40	6	0	-1.824244	2.853745	7.273801
41	6	0	-2.972419	2.114534	6.948337
42	6	0	-3.142262	1.612872	5.649517
43	6	0	-2.581015	-4.563989	1.783761
44	6	0	-1.478630	-5.422159	1.590160
45	6	0	-1.556759	-6.769805	1.983694
46	6	0	-2.705581	-7.260526	2.614957
47	6	0	-3.790620	-6.400212	2.849979
48	6	0	-3.727168	-5.066369	2.426820
49	6	0	0.034945	5.011655	-0.969141
50	8	0	0.691102	5.745973	-0.194167
51	6	0	-0.169545	-4.989930	0.975637
52	8	0	0.444467	-5.751491	0.192405
53	7	0	0.474252	3.784831	-1.410571
54	7	0	0.328180	-3.785059	1.414829
55	6	0	1.774818	3.248288	-1.173837
56	6	0	2.445992	3.438903	0.040527
57	6	0	3.775747	3.019154	0.184329
58	6	0	4.427179	2.426658	-0.911769
59	6	0	3.730298	2.117755	-2.093843
60	6	0	2.398779	2.537286	-2.210239
61	6	0	1.648816	-3.305306	1.167883
62	6	0	2.302571	-3.524331	-0.051152
63	6	0	3.647770	-3.160565	-0.204484
64	6	0	4.331433	-2.596162	0.886800
65	6	0	3.656742	-2.258545	2.073870
66	6	0	2.309660	-2.621432	2.199640
67	6	0	4.327501	-3.371548	-1.548695

68	6	0	4.472996	3.201199	1.523811
69	6	0	3.850380	-2.359809	-2.580180
70	6	0	4.284638	-1.026508	-2.491879
71	6	0	3.879313	-0.040518	-3.408466
72	6	0	3.004253	-0.412484	-4.441012
73	6	0	2.551043	-1.736509	-4.548183
74	6	0	2.973882	-2.703653	-3.622659
75	6	0	3.960263	2.209876	2.557943
76	6	0	4.341321	0.860555	2.468238
77	6	0	3.900786	-0.108719	3.386242
78	6	0	3.044032	0.297180	4.421395
79	6	0	2.643188	1.637962	4.529700
80	6	0	3.101079	2.587860	3.603053
81	6	0	4.360168	-1.549087	3.222186
82	6	0	4.396218	1.380552	-3.247092
83	8	0	5.105179	-0.644990	-1.433446
84	8	0	5.818924	2.194266	-0.847447
85	8	0	5.731003	-2.421599	0.811955
86	8	0	5.141695	0.446954	1.406270
87	6	0	6.459514	-3.603500	1.250430
88	6	0	6.543168	-0.705289	-1.647129
89	6	0	6.592315	3.346577	-1.287861
90	6	0	6.581746	0.449236	1.613446
91	30	0	-2.826813	0.073004	0.019885
92	6	0	-5.682085	-0.990476	-0.545186
93	7	0	-4.974392	0.014791	-0.036298
94	1	0	-0.116130	3.280579	-2.065273
95	1	0	-0.234343	-3.255399	2.074058
96	1	0	-2.287288	-3.265029	4.137473
97	1	0	-2.082448	-0.812480	5.235273
98	1	0	-2.344944	4.210000	3.332302
99	1	0	-2.421716	5.298087	0.879146
100	1	0	-2.163442	3.387147	-4.098125
101	1	0	-2.044730	0.929817	-5.197774
102	1	0	-2.520435	-4.082571	-3.296625
103	1	0	-2.639267	-5.166892	-0.843416
104	1	0	-4.061807	-0.832406	-5.357244
105	1	0	-3.808852	-1.730653	-7.664690
106	1	0	-1.837195	-3.142437	-8.244928
107	1	0	-0.124781	-3.646891	-6.503315
108	1	0	-0.382217	-2.732874	-4.200681
109	1	0	-4.415986	4.624008	-2.496011

110	1	0	-4.430188	6.994937	-3.267497
111	1	0	-2.425528	8.433888	-2.882238
112	1	0	-0.263766	2.758111	4.232718
113	1	0	0.042439	3.658424	6.535316
114	1	0	-1.691740	3.242097	8.278429
115	1	0	-3.733643	1.933015	7.700313
116	1	0	-4.034262	1.048135	5.393080
117	1	0	-2.755202	-8.299863	2.921762
118	1	0	-4.684068	-6.770047	3.342411
119	1	0	-4.573575	-4.401470	2.571891
120	1	0	1.944504	3.941974	0.859137
121	1	0	1.856981	2.341629	-3.134348
122	1	0	1.774604	-4.005863	-0.866083
123	1	0	1.783282	-2.402700	3.127439
124	1	0	5.410546	-3.277628	-1.421666
125	1	0	4.109870	-4.380792	-1.916494
126	1	0	5.550207	3.061210	1.389660
127	1	0	4.300624	4.218599	1.893047
128	1	0	2.681419	0.333043	-5.163491
129	1	0	1.877689	-2.010268	-5.354704
130	1	0	2.628254	-3.731177	-3.708887
131	1	0	2.693800	-0.435212	5.144578
132	1	0	1.982954	1.937835	5.337784
133	1	0	2.796014	3.628049	3.690123
134	1	0	5.438395	-1.568464	3.034816
135	1	0	4.166790	-2.086404	4.158459
136	1	0	5.475702	1.357023	-3.067368
137	1	0	4.217828	1.925372	-4.182012
138	1	0	7.521106	-3.369424	1.148953
139	1	0	6.226641	-3.837661	2.297156
140	1	0	6.205331	-4.470180	0.627049
141	1	0	6.938974	-1.596475	-1.148698
142	1	0	6.950326	0.199241	-1.192918
143	1	0	6.782111	-0.730941	-2.719434
144	1	0	6.360936	3.594033	-2.331858
145	1	0	6.379261	4.220758	-0.659556
146	1	0	7.644076	3.068320	-1.195850
147	1	0	6.950128	-0.472609	1.160786
148	1	0	7.011156	1.321813	1.109872
149	1	0	6.826620	0.469317	2.684507
150	1	0	-0.402885	7.455933	-1.773921
151	1	0	-0.707241	-7.413911	1.782206

152	1	0	-5.268162	-1.888385	-0.976319
153	6	0	-7.162265	0.531995	0.165375
154	1	0	-8.120237	0.979707	0.362210
155	6	0	-5.879274	0.974528	0.412005
156	1	0	-5.544791	1.891500	0.868291
157	7	0	-7.022016	-0.715859	-0.442064
158	1	0	-7.772916	-1.315065	-0.753525



1Zn encapsulating pyridine

Optimized: B3LYP/LANL2DZ

Energy: –4078.36658393

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.002654	2.131394	2.236173
2	6	0	2.952754	2.269985	3.690949
3	6	0	3.151737	1.016563	4.225093
4	6	0	3.297472	0.086311	3.106931
5	7	0	3.204052	0.794642	1.916208
6	6	0	3.419825	-1.325764	3.232953
7	6	0	3.344297	-2.244024	2.152617
8	6	0	3.392144	-3.701712	2.270312
9	6	0	3.180493	-4.219890	1.014922
10	6	0	3.042832	-3.088826	0.098874
11	6	0	3.002659	-2.131395	-2.236172
12	6	0	2.952761	-2.269986	-3.690948
13	6	0	3.151747	-1.016565	-4.225092
14	6	0	3.297479	-0.086312	-3.106930
15	6	0	3.419831	1.325764	-3.232951
16	6	0	3.344300	2.244024	-2.152615
17	6	0	3.392145	3.701712	-2.270310
18	6	0	3.180493	4.219889	-1.014919
19	6	0	3.042829	3.088825	-0.098873
20	6	0	2.880528	3.197389	1.307205
21	7	0	3.157133	1.906848	-0.816888
22	7	0	3.204056	-0.794643	-1.916205
23	7	0	3.157132	-1.906849	0.816890
24	6	0	2.880533	-3.197390	-1.307204
25	6	0	3.598015	1.878660	-4.618393
26	6	0	4.750286	1.555574	-5.373270

27	6	0	4.929671	2.066271	-6.671901
28	6	0	3.953602	2.904395	-7.245195
29	6	0	2.799153	3.228279	-6.506131
30	6	0	2.625422	2.722097	-5.204899
31	6	0	2.680503	-4.584358	-1.857692
32	6	0	3.764868	-5.211210	-2.517337
33	6	0	3.681807	-6.534730	-2.977103
34	6	0	2.501021	-7.273276	-2.766723
35	6	0	1.416772	-6.669201	-2.113027
36	6	0	1.482810	-5.324400	-1.676433
37	6	0	3.598006	-1.878660	4.618395
38	6	0	2.625411	-2.722094	5.204901
39	6	0	2.799138	-3.228275	6.506134
40	6	0	3.953587	-2.904393	7.245199
41	6	0	4.929659	-2.066273	6.671905
42	6	0	4.750277	-1.555576	5.373273
43	6	0	2.680501	4.584357	1.857692
44	6	0	1.482811	5.324403	1.676431
45	6	0	1.416774	6.669203	2.113026
46	6	0	2.501023	7.273275	2.766726
47	6	0	3.681807	6.534724	2.977108
48	6	0	3.764865	5.211205	2.517341
49	6	0	0.216755	-4.822597	-1.006579
50	8	0	-0.303376	-5.477741	-0.064073
51	6	0	0.216756	4.822603	1.006574
52	8	0	-0.303365	5.477741	0.064058
53	7	0	-0.389367	-3.713629	-1.581357
54	7	0	-0.389369	3.713635	1.581350
55	6	0	-1.727451	-3.256695	-1.355029
56	6	0	-2.438492	-3.539687	-0.170423
57	6	0	-3.789304	-3.164149	-0.037208
58	6	0	-4.436273	-2.547594	-1.133701
59	6	0	-3.705954	-2.117637	-2.268469
60	6	0	-2.352667	-2.495251	-2.366993
61	6	0	-1.727452	3.256699	1.355022
62	6	0	-2.438497	3.539690	0.170418
63	6	0	-3.789309	3.164149	0.037208
64	6	0	-4.436274	2.547593	1.133702
65	6	0	-3.705950	2.117637	2.268468
66	6	0	-2.352663	2.495253	2.366988
67	6	0	-4.515399	3.407941	-1.293107
68	6	0	-4.515388	-3.407942	1.293109

69	6	0	-4.046735	2.472986	-2.416478
70	6	0	-4.441394	1.111999	-2.444133
71	6	0	-3.957003	0.194180	-3.407655
72	6	0	-3.091926	0.688585	-4.406479
73	6	0	-2.714402	2.045058	-4.427812
74	6	0	-3.183364	2.927325	-3.435551
75	6	0	-4.046720	-2.472986	2.416478
76	6	0	-4.441380	-1.111999	2.444132
77	6	0	-3.956989	-0.194180	3.407655
78	6	0	-3.091911	-0.688585	4.406478
79	6	0	-2.714387	-2.045057	4.427811
80	6	0	-3.183349	-2.927324	3.435551
81	6	0	-4.369879	1.282901	3.372198
82	6	0	-4.369890	-1.282902	-3.372197
83	8	0	-5.267304	0.635819	-1.420765
84	8	0	-5.848253	-2.371429	-1.105837
85	8	0	-5.848253	2.371428	1.105845
86	8	0	-5.267289	-0.635819	1.420764
87	6	0	-6.573757	3.543222	1.613606
88	6	0	-6.717192	0.780370	-1.596082
89	6	0	-6.573758	-3.543223	-1.613596
90	6	0	-6.717177	-0.780374	1.596077
91	30	0	2.902891	0.000000	0.000001
92	6	0	-1.329332	-0.612257	1.039780
93	6	0	-2.049189	-0.000002	-0.000006
94	6	0	-1.329329	0.612256	-1.039789
95	6	0	0.068574	0.594762	-1.005533
96	7	0	0.756761	0.000002	0.000000
97	6	0	0.068571	-0.594759	1.005530
98	1	0	0.661068	-1.065479	1.782456
99	1	0	0.117337	-3.263472	-2.337343
100	1	0	0.117333	3.263481	2.337339
101	1	0	2.804407	3.195267	4.229321
102	1	0	3.173476	0.744148	5.270116
103	1	0	3.566487	-4.250639	3.183528
104	1	0	3.143590	-5.262397	0.733993
105	1	0	2.804413	-3.195268	-4.229321
106	1	0	3.173490	-0.744149	-5.270115
107	1	0	3.566488	4.250640	-3.183526
108	1	0	3.143588	5.262397	-0.733991
109	1	0	5.510975	0.916613	-4.931586
110	1	0	5.827819	1.813580	-7.230827

111	1	0	4.090448	3.298669	-8.249471
112	1	0	2.036850	3.871316	-6.940295
113	1	0	1.728084	2.969956	-4.643335
114	1	0	4.688090	-4.651164	-2.639786
115	1	0	4.533965	-6.990328	-3.475521
116	1	0	2.429281	-8.305204	-3.100972
117	1	0	1.728073	-2.969951	4.643336
118	1	0	2.036833	-3.871310	6.940297
119	1	0	4.090432	-3.298667	8.249475
120	1	0	5.827807	-1.813583	7.230832
121	1	0	5.510967	-0.916617	4.931589
122	1	0	2.429286	8.305202	3.100975
123	1	0	4.533965	6.990321	3.475528
124	1	0	4.688086	4.651157	2.639792
125	1	0	-1.941472	-4.067118	0.633003
126	1	0	-1.786034	-2.205395	-3.251161
127	1	0	-1.941480	4.067121	-0.633010
128	1	0	-1.786027	2.205397	3.251153
129	1	0	-5.589476	3.280648	-1.133088
130	1	0	-4.342860	4.442332	-1.617250
131	1	0	-5.589466	-3.280649	1.133094
132	1	0	-4.342847	-4.442332	1.617252
133	1	0	-2.715553	0.011574	-5.171109
134	1	0	-2.053450	2.410974	-5.209508
135	1	0	-2.870185	3.969336	-3.445744
136	1	0	-2.715539	-0.011573	5.171108
137	1	0	-2.053434	-2.410972	5.209507
138	1	0	-2.870170	-3.969335	3.445744
139	1	0	-5.453543	1.344971	3.236061
140	1	0	-4.129971	1.722268	4.349797
141	1	0	-5.453552	-1.344974	-3.236057
142	1	0	-4.129983	-1.722269	-4.349797
143	1	0	-7.637701	3.302469	1.532022
144	1	0	-6.315289	3.740953	2.663637
145	1	0	-6.346683	4.437367	1.016415
146	1	0	-6.951613	1.510951	-2.383017
147	1	0	-7.105724	1.124895	-0.636240
148	1	0	-7.137254	-0.198617	-1.852861
149	1	0	-6.315295	-3.740953	-2.663627
150	1	0	-6.346681	-4.437369	-1.016406
151	1	0	-7.637702	-3.302471	-1.532006
152	1	0	-7.137243	0.198615	1.852842

153	1	0	-7.105704	-1.124912	0.636236
154	1	0	-6.951598	-1.510946	2.383019
155	1	0	0.506443	-7.231170	-1.925296
156	1	0	0.506448	7.231175	1.925293
157	1	0	-1.830815	-1.102553	1.860754
158	1	0	-3.135162	-0.000003	-0.000009
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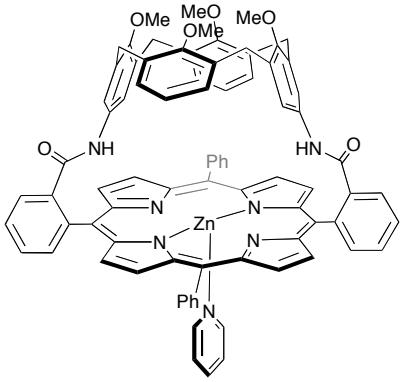


1Zn encapsulating pyridine

Optimized: B3LYP/LANL2DZ

Energy: –4078.35891789

Standard orientation:

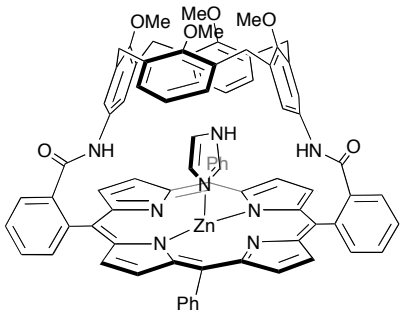
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.443130	-1.908506	2.436675
2	6	0	-2.794054	-3.319746	2.287880
3	6	0	-1.617577	-4.032702	2.304889
4	6	0	-0.530438	-3.070161	2.464438
5	7	0	-1.063230	-1.788544	2.539689
6	6	0	0.848585	-3.403301	2.484538
7	6	0	1.908236	-2.461920	2.504492
8	6	0	3.329151	-2.801377	2.500094
9	6	0	4.031893	-1.620778	2.474659
10	6	0	3.053478	-0.536740	2.473100
11	6	0	2.443130	1.908506	2.436675
12	6	0	2.794054	3.319746	2.287880
13	6	0	1.617577	4.032702	2.304889
14	6	0	0.530438	3.070161	2.464438
15	6	0	-0.848585	3.403301	2.484538
16	6	0	-1.908236	2.461920	2.504492
17	6	0	-3.329151	2.801377	2.500094
18	6	0	-4.031893	1.620778	2.474659
19	6	0	-3.053478	0.536740	2.473100
20	6	0	-3.374803	-0.841725	2.424978
21	7	0	-1.771520	1.075427	2.515593
22	7	0	1.063230	1.788544	2.539689
23	7	0	1.771520	-1.075427	2.515593
24	6	0	3.374803	0.841725	2.424978
25	6	0	-1.209165	4.861643	2.433661

26	6	0	-0.880543	5.725090	3.504083
27	6	0	-1.217923	7.090644	3.459012
28	6	0	-1.884154	7.618697	2.336131
29	6	0	-2.210613	6.768828	1.261191
30	6	0	-1.877815	5.402682	1.310830
31	6	0	4.835081	1.200060	2.356415
32	6	0	5.458678	1.724138	3.512310
33	6	0	6.834649	2.004284	3.539168
34	6	0	7.622241	1.745539	2.400107
35	6	0	7.017838	1.228070	1.244504
36	6	0	5.627633	0.973589	1.201636
37	6	0	1.209165	-4.861643	2.433661
38	6	0	1.877815	-5.402682	1.310830
39	6	0	2.210613	-6.768828	1.261191
40	6	0	1.884154	-7.618697	2.336131
41	6	0	1.217923	-7.090644	3.459012
42	6	0	0.880543	-5.725090	3.504083
43	6	0	-4.835081	-1.200060	2.356415
44	6	0	-5.627633	-0.973589	1.201636
45	6	0	-7.017838	-1.228070	1.244504
46	6	0	-7.622241	-1.745539	2.400107
47	6	0	-6.834649	-2.004284	3.539168
48	6	0	-5.458678	-1.724138	3.512310
49	6	0	5.108562	0.444849	-0.119115
50	8	0	5.766822	-0.422382	-0.755660
51	6	0	-5.108562	-0.444849	-0.119115
52	8	0	-5.766822	0.422382	-0.755660
53	7	0	3.957267	1.037460	-0.608786
54	7	0	-3.957267	-1.037460	-0.608786
55	6	0	3.426863	0.867850	-1.927521
56	6	0	3.525529	-0.352411	-2.619303
57	6	0	3.129001	-0.444539	-3.965482
58	6	0	2.668532	0.721156	-4.621122
59	6	0	2.412413	1.911658	-3.900120
60	6	0	2.806542	1.969579	-2.550099
61	6	0	-3.426863	-0.867850	-1.927521
62	6	0	-3.525529	0.352411	-2.619303
63	6	0	-3.129001	0.444539	-3.965482
64	6	0	-2.668532	-0.721156	-4.621122
65	6	0	-2.412413	-1.911658	-3.900120
66	6	0	-2.806542	-1.969579	-2.550099
67	6	0	-3.182620	1.804808	-4.665409

68	6	0	3.182620	-1.804808	-4.665409
69	6	0	-2.085216	2.750086	-4.166696
70	6	0	-0.747050	2.581366	-4.595097
71	6	0	0.313367	3.374309	-4.099508
72	6	0	0.000000	4.394079	-3.177288
73	6	0	-1.327178	4.603046	-2.758001
74	6	0	-2.360818	3.781935	-3.246222
75	6	0	2.085216	-2.750086	-4.166696
76	6	0	0.747050	-2.581366	-4.595097
77	6	0	-0.313367	-3.374309	-4.099508
78	6	0	0.000000	-4.394079	-3.177288
79	6	0	1.327178	-4.603046	-2.758001
80	6	0	2.360818	-3.781935	-3.246222
81	6	0	-1.751830	-3.125562	-4.559302
82	6	0	1.751830	3.125562	-4.559302
83	8	0	-0.456890	1.532232	-5.475911
84	8	0	2.483943	0.706827	-6.031986
85	8	0	-2.483943	-0.706827	-6.031986
86	8	0	0.456890	-1.532232	-5.475911
87	6	0	-3.711680	-1.036527	-6.764972
88	6	0	-0.571178	1.799303	-6.908977
89	6	0	3.711680	1.036527	-6.764972
90	6	0	0.571178	-1.799303	-6.908977
91	30	0	0.000000	0.000000	2.844784
92	6	0	-1.027682	0.642725	7.183678
93	6	0	0.000000	0.000000	7.899547
94	6	0	1.027682	-0.642725	7.183678
95	6	0	0.991962	-0.620113	5.779287
96	7	0	0.000000	0.000000	5.088427
97	6	0	-0.991962	0.620113	5.779287
98	1	0	-1.760873	1.100713	5.183625
99	1	0	3.525584	1.755958	-0.036559
100	1	0	-3.525584	-1.755958	-0.036559
101	1	0	-3.797207	-3.708703	2.184719
102	1	0	-1.493911	-5.100209	2.197758
103	1	0	3.731986	-3.802953	2.512044
104	1	0	5.104782	-1.498649	2.454500
105	1	0	3.797207	3.708703	2.184719
106	1	0	1.493911	5.100209	2.197758
107	1	0	-3.731986	3.802953	2.512044
108	1	0	-5.104782	1.498649	2.454500
109	1	0	-0.371466	5.320764	4.375791

110	1	0	-0.963768	7.737086	4.295981
111	1	0	-2.144139	8.674023	2.299011
112	1	0	-2.721363	7.167851	0.387713
113	1	0	-2.122109	4.751716	0.475185
114	1	0	4.852746	1.890468	4.399303
115	1	0	7.289517	2.404255	4.442216
116	1	0	8.691182	1.942949	2.414106
117	1	0	2.122109	-4.751716	0.475185
118	1	0	2.721363	-7.167851	0.387713
119	1	0	2.144139	-8.674023	2.299011
120	1	0	0.963768	-7.737086	4.295981
121	1	0	0.371466	-5.320764	4.375791
122	1	0	-8.691182	-1.942949	2.414106
123	1	0	-7.289517	-2.404255	4.442216
124	1	0	-4.852746	-1.890468	4.399303
125	1	0	3.938188	-1.218820	-2.117945
126	1	0	2.661581	2.893908	-1.992599
127	1	0	-3.938188	1.218820	-2.117945
128	1	0	-2.661581	-2.893908	-1.992599
129	1	0	-3.081976	1.652208	-5.743042
130	1	0	-4.156581	2.275547	-4.477994
131	1	0	3.081976	-1.652208	-5.743042
132	1	0	4.156581	-2.275547	-4.477994
133	1	0	0.795486	5.029283	-2.791199
134	1	0	-1.551966	5.402682	-2.055862
135	1	0	-3.384114	3.937515	-2.909191
136	1	0	-0.795486	-5.029283	-2.791199
137	1	0	1.551966	-5.402682	-2.055862
138	1	0	3.384114	-3.937515	-2.909191
139	1	0	-1.766036	-2.976409	-5.642324
140	1	0	-2.341751	-4.025069	-4.336000
141	1	0	1.766036	2.976409	-5.642324
142	1	0	2.341751	4.025069	-4.336000
143	1	0	-3.456920	-0.979288	-7.827375
144	1	0	-4.058534	-2.050768	-6.518930
145	1	0	-4.514726	-0.321749	-6.535274
146	1	0	-1.334952	2.563371	-7.116157
147	1	0	-0.864147	0.850483	-7.360754
148	1	0	0.398016	2.127521	-7.306769
149	1	0	4.058534	2.050768	-6.518930
150	1	0	4.514726	0.321749	-6.535274
151	1	0	3.456920	0.979288	-7.827375

152	1	0	-0.398016	-2.127521	-7.306769
153	1	0	0.864147	-0.850483	-7.360754
154	1	0	1.334952	-2.563371	-7.116157
155	1	0	7.608022	1.006579	0.360363
156	1	0	-7.608022	-1.006579	0.360363
157	1	0	-1.839585	1.150888	7.694393
158	1	0	0.000000	0.000000	8.986421
159	1	0	1.839585	-1.150888	7.694393
160	1	0	1.760873	-1.100713	5.183625



1Zn encapsulating imidazole

Optimized: B3LYP/LANL2DZ

Energy: –4100.41656698

Standard orientation:

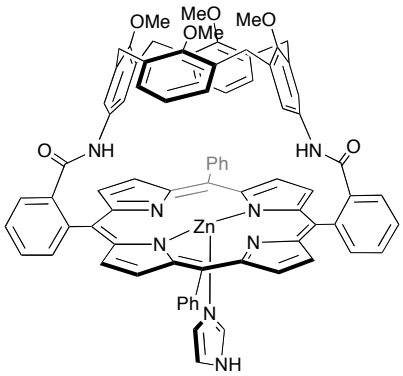
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.569980	-2.137523	2.496334
2	6	0	-2.201529	-2.448647	3.876652
3	6	0	-2.020568	-1.248188	4.526578
4	6	0	-2.259227	-0.186178	3.550596
5	7	0	-2.586388	-0.759296	2.328879
6	6	0	-2.116967	1.204745	3.808631
7	6	0	-2.216168	2.226440	2.828621
8	6	0	-2.090229	3.660842	3.089384
9	6	0	-2.214425	4.307665	1.883351
10	6	0	-2.445319	3.282310	0.867165
11	6	0	-3.121591	2.592249	-1.464122
12	6	0	-3.432440	2.894196	-2.861378
13	6	0	-3.849755	1.720551	-3.445336
14	6	0	-3.784679	0.679710	-2.420930
15	6	0	-4.086434	-0.691725	-2.638550
16	6	0	-3.889383	-1.722968	-1.684119
17	6	0	-4.193714	-3.138283	-1.895849
18	6	0	-3.812041	-3.811181	-0.760324
19	6	0	-3.298535	-2.814729	0.178344
20	6	0	-2.863042	-3.099084	1.496932
21	7	0	-3.361243	-1.558120	-0.408309
22	7	0	-3.330358	1.238603	-1.232926
23	7	0	-2.444054	2.033000	1.470793
24	6	0	-2.688147	3.543552	-0.505767
25	6	0	-4.646208	-1.073117	-3.979906
26	6	0	-5.898823	-0.569654	-4.403649

27	6	0	-6.433427	-0.922931	-5.656150
28	6	0	-5.720695	-1.782467	-6.514700
29	6	0	-4.471048	-2.287611	-6.106176
30	6	0	-3.942193	-1.938166	-4.850009
31	6	0	-2.583044	4.975454	-0.958051
32	6	0	-3.779474	5.682955	-1.225341
33	6	0	-3.767847	7.040199	-1.582598
34	6	0	-2.542089	7.729756	-1.664801
35	6	0	-1.347345	7.045947	-1.398438
36	6	0	-1.350108	5.670281	-1.065243
37	6	0	-1.827697	1.619317	5.223473
38	6	0	-0.614816	2.264129	5.561250
39	6	0	-0.348246	2.650516	6.887623
40	6	0	-1.293275	2.403227	7.902409
41	6	0	-2.505358	1.763354	7.578015
42	6	0	-2.767167	1.372483	6.251949
43	6	0	-2.795424	-4.555493	1.875171
44	6	0	-1.774775	-5.420757	1.400667
45	6	0	-1.849776	-6.807841	1.666285
46	6	0	-2.895001	-7.339209	2.437216
47	6	0	-3.889915	-6.480415	2.944040
48	6	0	-3.839079	-5.107184	2.653297
49	6	0	0.021495	5.083049	-0.810311
50	8	0	0.873502	5.745803	-0.158488
51	6	0	-0.560637	-4.986270	0.605641
52	8	0	-0.195973	-5.625574	-0.418528
53	7	0	0.317457	3.864205	-1.406663
54	7	0	0.175975	-3.945011	1.148800
55	6	0	1.616092	3.261379	-1.424352
56	6	0	2.481850	3.374598	-0.319977
57	6	0	3.800200	2.896992	-0.386000
58	6	0	4.255396	2.337847	-1.603618
59	6	0	3.358910	2.052681	-2.660789
60	6	0	2.038564	2.541578	-2.561402
61	6	0	1.497554	-3.544601	0.786905
62	6	0	2.057336	-3.790376	-0.483849
63	6	0	3.401641	-3.458715	-0.747419
64	6	0	4.197736	-2.953872	0.306914
65	6	0	3.619759	-2.563184	1.539164
66	6	0	2.266108	-2.870188	1.760310
67	6	0	3.964697	-3.597069	-2.170170
68	6	0	4.685294	2.965030	0.862074

69	6	0	3.389625	-2.539483	-3.123924
70	6	0	3.918965	-1.221978	-3.178680
71	6	0	3.310994	-0.188241	-3.940162
72	6	0	2.197235	-0.529143	-4.737531
73	6	0	1.690370	-1.842526	-4.752336
74	6	0	2.272732	-2.833404	-3.938860
75	6	0	4.256828	1.979816	1.957224
76	6	0	4.495792	0.591717	1.817415
77	6	0	4.111096	-0.353867	2.797631
78	6	0	3.466948	0.125575	3.956476
79	6	0	3.218805	1.501416	4.123754
80	6	0	3.613815	2.420237	3.133088
81	6	0	4.435079	-1.842070	2.616998
82	6	0	3.823172	1.257751	-3.890381
83	8	0	5.035885	-0.911565	-2.387839
84	8	0	5.642499	2.077109	-1.779260
85	8	0	5.604233	-2.853809	0.129205
86	8	0	5.059982	0.113122	0.629884
87	6	0	6.310642	-4.095243	0.469442
88	6	0	6.336802	-1.091770	-3.031795
89	6	0	6.382766	3.252038	-2.258150
90	6	0	6.529589	0.099367	0.509903
91	30	0	-2.596430	0.206079	0.458218
92	6	0	-0.220187	-0.767907	-1.219725
93	7	0	-0.568242	-0.073588	-0.126410
94	1	0	-0.417696	3.414498	-1.942884
95	1	0	-0.211795	-3.497909	1.974139
96	1	0	-2.117256	-3.441607	4.296014
97	1	0	-1.739419	-1.096202	5.558317
98	1	0	-1.943766	4.109228	4.060670
99	1	0	-2.179510	5.372466	1.703892
100	1	0	-3.355604	3.866563	-3.326280
101	1	0	-4.154427	1.569506	-4.470462
102	1	0	-4.647378	-3.554620	-2.782842
103	1	0	-3.893090	-4.871050	-0.567611
104	1	0	-6.457930	0.085759	-3.740549
105	1	0	-7.402530	-0.532007	-5.957705
106	1	0	-6.132368	-2.055060	-7.483685
107	1	0	-3.910587	-2.950398	-6.761732
108	1	0	-2.974658	-2.328214	-4.543481
109	1	0	-4.724595	5.156170	-1.124672
110	1	0	-4.704178	7.557598	-1.777189

111	1	0	-2.519826	8.784816	-1.925762
112	1	0	0.120836	2.450008	4.782740
113	1	0	0.591547	3.142961	7.127867
114	1	0	-1.089681	2.705477	8.927084
115	1	0	-3.245626	1.573246	8.351837
116	1	0	-3.709324	0.889615	6.004715
117	1	0	-2.935104	-8.406800	2.638317
118	1	0	-4.706715	-6.878351	3.541289
119	1	0	-4.627856	-4.447005	3.004287
120	1	0	2.130355	3.856364	0.583636
121	1	0	1.347240	2.385781	-3.388293
122	1	0	1.448188	-4.253822	-1.249505
123	1	0	1.811057	-2.601326	2.712662
124	1	0	5.051691	-3.501108	-2.123012
125	1	0	3.721590	-4.589952	-2.569981
126	1	0	5.721396	2.764204	0.574714
127	1	0	4.645802	3.978539	1.281584
128	1	0	1.724728	0.238022	-5.347351
129	1	0	0.840671	-2.089719	-5.383220
130	1	0	1.859145	-3.839328	-3.931600
131	1	0	3.165563	-0.575705	4.732393
132	1	0	2.728714	1.854651	5.027821
133	1	0	3.422534	3.482722	3.271287
134	1	0	5.495507	-1.943256	2.364904
135	1	0	4.275158	-2.339415	3.583069
136	1	0	4.915985	1.256746	-3.893566
137	1	0	3.482598	1.766932	-4.801653
138	1	0	7.372030	-3.899951	0.291524
139	1	0	6.151391	-4.362059	1.523886
140	1	0	5.972467	-4.927279	-0.163957
141	1	0	6.491597	-2.140796	-3.322920
142	1	0	7.075720	-0.798384	-2.285801
143	1	0	6.430790	-0.452621	-3.921081
144	1	0	6.014141	3.572374	-3.242949
145	1	0	6.291666	4.090410	-1.553782
146	1	0	7.428929	2.942184	-2.335177
147	1	0	6.805741	-0.931083	0.277310
148	1	0	6.791469	0.771517	-0.310470
149	1	0	7.000885	0.425106	1.447865
150	1	0	-0.393656	7.563822	-1.432701
151	1	0	-1.080297	-7.455314	1.256254
152	1	0	-0.901966	-1.252708	-1.897673

153	6	0	1.695869	-0.091043	-0.276689
154	1	0	2.761420	0.022890	-0.163848
155	6	0	0.621059	0.355563	0.472715
156	1	0	0.620435	0.947601	1.372653
157	7	0	1.139931	-0.791606	-1.341288
158	1	0	1.660284	-1.278322	-2.058274



1Zn encapsulating imidazole

Optimized: B3LYP/LANL2DZ

Energy: –4100.42088822

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.526820	2.381908	-1.961168
2	6	0	-2.459165	2.646364	-3.397768
3	6	0	-2.575875	1.434217	-4.037626
4	6	0	-2.718373	0.410840	-3.004112
5	7	0	-2.677169	1.016895	-1.754477
6	6	0	-2.835371	-0.981730	-3.253886
7	6	0	-2.837759	-1.985879	-2.252398
8	6	0	-2.928450	-3.422904	-2.506099
9	6	0	-2.837733	-4.058748	-1.291652
10	6	0	-2.704509	-3.021627	-0.271575
11	6	0	-2.448094	-2.280168	2.123514
12	6	0	-2.211958	-2.560549	3.538889
13	6	0	-2.123699	-1.346921	4.181437
14	6	0	-2.305798	-0.308130	3.170189
15	6	0	-2.249174	1.086836	3.423098
16	6	0	-2.303656	2.093858	2.426491
17	6	0	-2.230966	3.530410	2.684074
18	6	0	-2.272262	4.166886	1.466526
19	6	0	-2.377235	3.130650	0.442033
20	6	0	-2.414465	3.372209	-0.953966
21	7	0	-2.419730	1.882949	1.054605
22	7	0	-2.497244	-0.906414	1.930807
23	7	0	-2.731665	-1.772200	-0.881017
24	6	0	-2.559792	-3.268096	1.115051
25	6	0	-2.073667	1.525153	4.850390

26	6	0	-3.090787	1.299820	5.806495
27	6	0	-2.929052	1.710736	7.142807
28	6	0	-1.740436	2.348368	7.548157
29	6	0	-0.717472	2.570550	6.605596
30	6	0	-0.883364	2.164442	5.268638
31	6	0	-2.521109	-4.709421	1.548685
32	6	0	-3.671262	-5.268058	2.151738
33	6	0	-3.727624	-6.627420	2.501145
34	6	0	-2.625994	-7.463645	2.233000
35	6	0	-1.475919	-6.923334	1.637721
36	6	0	-1.401925	-5.549039	1.313989
37	6	0	-2.920978	-1.422304	-4.688171
38	6	0	-1.899835	-2.210800	-5.268471
39	6	0	-1.977641	-2.616557	-6.613231
40	6	0	-3.083044	-2.245254	-7.403375
41	6	0	-4.107185	-1.462118	-6.836410
42	6	0	-4.023613	-1.052050	-5.492872
43	6	0	-2.342168	4.807311	-1.402695
44	6	0	-1.169647	5.597342	-1.282454
45	6	0	-1.210536	6.969866	-1.620197
46	6	0	-2.383404	7.557631	-2.117097
47	6	0	-3.541911	6.770953	-2.271329
48	6	0	-3.515419	5.414653	-1.908400
49	6	0	-0.090265	-5.095406	0.707926
50	8	0	0.481662	-5.799989	-0.168279
51	6	0	0.171100	5.095712	-0.789063
52	8	0	0.862207	5.803994	-0.007268
53	7	0	0.465229	-3.948141	1.246652
54	7	0	0.613020	3.896437	-1.319950
55	6	0	1.789776	-3.460492	1.014299
56	6	0	2.457971	-3.657816	-0.207659
57	6	0	3.806073	-3.281814	-0.352615
58	6	0	4.488401	-2.760767	0.769869
59	6	0	3.794481	-2.407882	1.951537
60	6	0	2.439838	-2.770457	2.058775
61	6	0	1.927887	3.352213	-1.160711
62	6	0	2.645645	3.489380	0.041182
63	6	0	3.984365	3.069544	0.122131
64	6	0	4.603219	2.543319	-1.035183
65	6	0	3.853893	2.244388	-2.196269
66	6	0	2.513312	2.672282	-2.247127
67	6	0	4.728629	3.170918	1.452853

68	6	0	4.482931	-3.383973	-1.724391
69	6	0	4.267676	2.139178	2.488156
70	6	0	4.556912	0.761454	2.329113
71	6	0	4.140492	-0.209035	3.273296
72	6	0	3.418302	0.230574	4.402017
73	6	0	3.120119	1.593575	4.582721
74	6	0	3.545695	2.538918	3.631836
75	6	0	3.938625	-2.311773	-2.674141
76	6	0	4.522813	-1.024055	-2.737084
77	6	0	3.927069	0.039536	-3.456858
78	6	0	2.775900	-0.243732	-4.220922
79	6	0	2.221495	-1.535406	-4.239257
80	6	0	2.788327	-2.554338	-3.454333
81	6	0	4.473285	1.466621	-3.363379
82	6	0	4.499202	-1.689232	3.103025
83	8	0	5.195515	0.331260	1.158783
84	8	0	5.897230	-2.592001	0.716630
85	8	0	6.004620	2.312930	-1.030917
86	8	0	5.715676	-0.778783	-2.019710
87	6	0	6.776872	3.474866	-1.481539
88	6	0	6.658988	0.287880	1.151723
89	6	0	6.634586	-3.814946	1.048121
90	6	0	6.939924	-1.029398	-2.778361
91	30	0	-2.912261	0.068480	0.110502
92	6	0	-5.771071	1.197112	0.875243
93	7	0	-5.096161	0.203310	0.287636
94	1	0	-0.064310	-3.476115	1.972641
95	1	0	-0.000930	3.421798	-1.973972
96	1	0	-2.337455	3.619832	-3.851434
97	1	0	-2.546192	1.247062	-5.100840
98	1	0	-3.043226	-3.880515	-3.477134
99	1	0	-2.855578	-5.122714	-1.106536
100	1	0	-2.130061	-3.545011	3.978070
101	1	0	-1.934430	-1.169774	5.229909
102	1	0	-2.153706	3.987107	3.659431
103	1	0	-2.228129	5.230432	1.283609
104	1	0	-4.011801	0.811258	5.497055
105	1	0	-3.726016	1.535055	7.861927
106	1	0	-1.612826	2.665198	8.580681
107	1	0	0.206382	3.057362	6.910001
108	1	0	-0.085386	2.325414	4.548232
109	1	0	-4.530900	-4.625583	2.324526

110	1	0	-4.625462	-7.032779	2.961587
111	1	0	-2.664419	-8.520909	2.483181
112	1	0	-1.042969	-2.495767	-4.663258
113	1	0	-1.179018	-3.217926	-7.041518
114	1	0	-3.145184	-2.560970	-8.442183
115	1	0	-4.967734	-1.173478	-7.435746
116	1	0	-4.820444	-0.453440	-5.058106
117	1	0	-2.395535	8.612536	-2.379501
118	1	0	-4.458565	7.212396	-2.655251
119	1	0	-4.415331	4.811220	-1.995773
120	1	0	1.932004	-4.124007	-1.030277
121	1	0	1.899726	-2.546272	2.977780
122	1	0	2.170284	3.947815	0.899644
123	1	0	1.929831	2.499686	-3.149878
124	1	0	5.799491	3.050052	1.266070
125	1	0	4.576153	4.170451	1.880693
126	1	0	5.559745	-3.256743	-1.597166
127	1	0	4.292895	-4.374206	-2.158929
128	1	0	3.093733	-0.497049	5.144006
129	1	0	2.568840	1.915304	5.463521
130	1	0	3.317697	3.593834	3.774349
131	1	0	2.314263	0.550166	-4.805160
132	1	0	1.344225	-1.739062	-4.848332
133	1	0	2.335009	-3.543354	-3.441540
134	1	0	5.555409	1.441244	-3.220243
135	1	0	4.258713	1.986632	-4.307024
136	1	0	5.578538	-1.780079	2.947310
137	1	0	4.259329	-2.199398	4.045845
138	1	0	7.828954	3.181835	-1.420519
139	1	0	6.523405	3.741100	-2.518106
140	1	0	6.593660	4.346733	-0.836834
141	1	0	7.081643	1.287233	1.319877
142	1	0	6.910673	-0.066390	0.154988
143	1	0	7.031420	-0.413074	1.910285
144	1	0	6.411877	-4.144870	2.073673
145	1	0	6.387132	-4.629391	0.352400
146	1	0	7.695298	-3.562211	0.961282
147	1	0	7.765603	-0.790207	-2.103547
148	1	0	7.006702	-2.082289	-3.090384
149	1	0	6.993424	-0.389915	-3.671943
150	1	0	-0.621113	-7.552662	1.408661
151	1	0	-0.309854	7.559688	-1.479024

152	1	0	-5.330252	2.064690	1.339305
153	6	0	-7.314892	-0.257217	0.136147
154	1	0	-8.290681	-0.674222	-0.050653
155	6	0	-6.045473	-0.711954	-0.178521
156	1	0	-5.752289	-1.611296	-0.695497
157	7	0	-7.124850	0.956611	0.805455
158	1	0	-7.851457	1.554581	1.175185