Design of oxophilic metalloporphyrins: An experimental and DFT study of methanol binding
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1: Porphyrin metallation

All free bases where obtained commercially and metallated as follows:

Al(III)TPPCl:
Al(III)TPPCl was prepared according to the literature (1). TPP (308 mg, 0.49 mmol) was weighed into a dry round bottom flask and dissolved in 20 mL dry DCM. A solution of Et_2AlCl (1M in propane, 1.2 mL, 1.2 mmol) was added dropwise. The solution was left stirring at room temperature for 2 h, and the reaction was followed by TLC. Then solvent and any volatile by-products were removed by evaporation, and the crude product was purified by column chromatography with DCM (0 % -> 10 % MeOH) as eluent over basic alumina. The solvent was reduced by evaporation. Excess pentane was added and the precipitate collected by filtration. The received greenish solid was dried under high vacuum. Yield 188 mg, 57%. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.05 (s, 8H, pyrrole), 8.20 (m, 8H, aromatic), 7.77 (m, 12H, aromatic). UV–Vis in CH_2Cl_2, λ_{max} (nm): 418, 548. MS (MALDI-TOF, negative mode) calculated for $C_{44}H_{30}AlClN_4$: m/z = 676, found: m/z = 674.

Co(III)TPPCl:
Co(III)TPPCl was prepared according to the literature (2),(3). TPP (530 mg, 0.86 mmol) and cobalt(II) acetate tetrahydrate (1.12 g, 4.5 mmol) were dissolved in 100 mL DMF and heated to 130 °C for 4.5 h. The reaction was followed by UV-vis and TLC. The reaction mixture was concentrated and water was added (50 mL). The product was extracted with chloroform (4x100 mL). The organic phase was washed with water (2x75 mL) and brine (75 mL) and dried over $MgSO_4$. The solvent was removed by

evaporation. The resulting purple solid was suspended in pentane, filtered, washed with more pentane and dried under vacuum. The Co(II)TPP (405 mg, 0.60 mmol) was dissolved in 300 mL 1:1 MeOH/chloroform. HCl (3 mL) was added and the reaction was stirred at room temperature overnight. The solution was concentrated under vacuum and washed with water. The organic phase was dried over $MgSO_4$ and purified by column chromatography with $CHCl_3$ (0 %-> 10 % MeOH) as eluent over silica. The solvent was removed by evaporation and the product dried under high vacuum. Yield 214 mg, 39%. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.10 (pyrrole), 9.05 (pyrrole), 8.20 (aromatic), 7.76 (aromatic). UV–Vis in CH_2Cl_2, λ_{max} (nm): 426, 545. MS (MALDI-TOF, positive mode) calculated for $C_{44}H_{30}ClCoN_4$: m/z = 708, found: m/z: 706.

Co(III)TPFPPCl:
The synthesis of Co(III)TPFPPCl followed the same procedure as the synthesis of Co(III)TPPCl. Yield 378 mg, 73%. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.08 (s, 8H, pyrrole). UV–Vis in CH_2Cl_2, λ_{max} (nm): 424, 543. MS (MALDI-TOF, positive mode) calculated for $C_{44}H_{10}ClCoF_{20}N_4$: m/z = 1068, found: m/z: 1066.

Fe(II)TPP:
Fe(II)TPP was prepared according to the literature (4). TPP (503 mg, 0.82 mmol) was dissolved in DMF (250 mL) and heated to reflux. Iron chloride (1.635 g, 8.0 mmol) was added and the reaction was refluxed for 4 h. The solvent was removed by evaporation and the received black solid was purified by column chromatography with DCM/pentane (1:1 -> 1:0) as eluent over silica. The solvent was removed by evaporation and the black product dried under high vacuum. Yield 466 mg, 85 %. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 13.48 (s, 8H, pyrrole), 7.79 (m, 8H, aromatic), 7.66 (m, 12H, aromatic). UV–Vis in CH_2Cl_2, λ_{max} (nm): 313, 402.5, 564.5, 605. MS (MALDI-TOF, positive mode) calculated for $C_{44}H_{30}FeN_4$: m/z = 670, found: m/z: 668.

Mg(II)TPP:
Mg(II)TPP was prepared according to the literature (5). TPP (106 mg, 0.17 mmol) was dissolved in DCM (10 mL) and triethylamine (1 mL) was added. To the solution $MgBr_2$ (1,2 g, 7.0 mmol) was added and the solution was stirred at room temperature for 15 min. Additional DCM was added (~20 mL) and the solution was washed with dilute $NaHCO_3$ (2x 25 mL) and dried over $NaSO_4$. The solvent was removed by evaporation and the crude product was purified by column chromatography with 1:1 acetone/chloroform as eluent over basic alumina. The product solution was concentrated and pentane was added to initiate precipitation. The resulting solid was collected by filtration and dried under high vacuum overnight. Yield 109 mg, 64%. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.88 (s, 8H, pyrrole), 8.23 (m, 8H, aromatic), 7.74 (m, 12H, aromatic). UV–Vis in CH_2Cl_2, λ_{max} (nm): 425, 564, 603. MS (MALDI-TOF, positive mode) calculated for $C_{44}H_{30}MgN_4$: m/z = 638, found: m/z: 637.

Mg(II)TPFPP:
Mg(II)TPFPP was prepared according to the literature (6). TPFPP (100 mg, 0.1 mmol) was dissolved in DCM (8 mL) and diisopropylethylamine (0.7 mL) was added. To the solution MgI_2 (0.57 g, 2.0 mmol) was added and the solution was stirred at room temperature for 2 h. Additional DCM added (~25 mL) and the solution was washed with dilute $NaHCO_3$ (2x 25 mL) and dried over $NaSO_4$. The solution was concentrated to 3 mL and the crude product was purified by column chromatography with DCM as eluent over basic alumina. The product solution was collected and the solvent removed by

evaporation. To remove grease the product was further purified by column chromatography over a short silica plug with diethyl ether as eluent. The solvent was removed by evaporation and the product dried under high vacuum overnight. Yield 64 mg, 63%. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.92 (s, 8H, pyrrole). UV–Vis in CH_2Cl_2, λ_{max} (nm): 392.5, 414, 550. MS (MALDI-TOF, positive mode) calculated for $C_{44}H_{10}F_{20}MgN_4$: m/z = 998, found: m/z: 996.

Mg(II)TPPBr$_8$:
The synthesis of Mg(II)TPPBr$_8$ followed the same procedure as the synthesis of Mg(II)TPP. Yield 49 mg, 40%. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.16 (m, 8H, aromatic), 7.76 (m, 12H, aromatic). UV–Vis in CH_2Cl_2, λ_{max} (nm): 370, 463.5, 639,5**.** MS (MALDI-TOF, positive mode) calculated for $C_{44}H_{22}Br_8MgN_4$: m/z = 1268 (at maximum of isotope cluster), found: m/z: 1268.

Sn(IV)TPP(OH)$_2$:
Sn(IV)TPP(OH)$_2$ was prepared according to the literature (7). Sn(TPP)Cl_2 (52.3 mg, 0.065 mmol) and K_2CO_3 (184 mg, 1 mmol) were dissolved in a mixture of water (8 mL) and THF (60 mL) and heated to 70^{o}C. The solution was left stirring overnight. The organic solvent was evaporated, causing the porphyrin to crystallize. The crystals were collected, washed with water, then pentane and dried under high vacuum. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.14 (s, 8H, pyrrole), 8.35 (m, 8H, aromatic), 7.83 (m, 12H, aromatic). UV–Vis in CH_2Cl_2, λ_{max} (nm): 426, 560, 599, 625. MS (MALDI-TOF, positive mode) calculated for $C_{44}H_{31}N_4OSn$: m/z = 751 found: m/z: 749 ($[M - OH]^+$).

O=Ti(IV)TPP:
O=Ti(IV)TPP was prepared according to the literature (8). TPP (119 mg, 0.19 mmol) was placed in a flame dried 100 mL Schlenk flask under argon. Dry toluene (50 mL) was added. BuLi (0.15 mL, 2.5 M in hexane, 0.39 mmol) was added dropwise. The solution was stirred at room temperature. The colour changed from dark red to dark green. TCl_4 (0.1 mL, 0.95 mmol) was added dropwise and the solution was heated to 50 ^{o}C for 2.5 h. The colour changed to forest green. The solution was cooled to room temperature, opened to the atmosphere and stirred overnight. The colour gradually changed to brown. The solution was concentrated and the product separated by column chromatography with toluene/chloroform (1:0 -> 0:1) as eluent over basic alumina. The solvent was evaporated and the purple product dried under high vacuum. Yield, 52mg, 47%. ^{1}H NMR (500 MHz, $CDCl_3$) δ = δ = 9.14 (s, 8H, pyrrole), 8.48 (m, 4H, aromatic), 8.13 (m, 4H, aromatic), 7.84 (m, 8H, aromatic), 7.77 (m, 4H, aromatic). UV–Vis in CH_2Cl_2, λ_{max} (nm): 423, 551. MS (MALDI-TOF, positive mode) calculated for $C_{44}H_{30}N_4OTi$: m/z = 678, found: m/z: 677.

Zn(II)TPP:
Zn(II)TPP was prepared according to the literature (9). TPP (1.539 g, 2 mmol) was dissolved in 300 mL 2:1 chloroform/methanol. Zinc acetate (1.31 g, 7 mmol) was added and the mixture was refluxed for 3.5 h. The mixture was cooled to room temperature and the solvent removed by evaporation. The crude product was dissolved in chloroform and filtered through a short silica plug with chloroform as eluent. The solvent was evaporated and the resulting purple solid suspended in pentane, filtered and dried under vacuum. Yield 1.58 g, 93%. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.95 (s, 8H, pyrrole), 8.23 (m, 8H, aromatic), 7.76 (m, 12H, aromatic). UV–Vis in CH_2Cl_2, λ_{max} (nm): 424, 554, 593. MS (MALDI-TOF, positive mode) calculated for $C_{44}H_{30}N_4Zn$: m/z = 678, found: m/z: 677.

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Zn(II)TPPBr$_8$:
The synthesis of Zn(II)TPPBr$_8$ followed the same procedure as the synthesis of Zn(II)TPP. Yield 31 mg, 30%. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.12 (m, 8H, aromatic), 7.86 (m, 12H, aromatic). UV–Vis in CH_2Cl_2, λ_{max} (nm): 355, 460.5 598, 649. MS (MALDI-TOF, positive mode) calculated for $C_{44}H_{22}Br_8N_4Zn$: m/z = 1309 (maximum of isotope cluster), found: m/z: 1308.

2: Raw titration data

For NMR titrations, aliquots of freshly prepared ligand solutions (solvent $CDCl_3$, AlOx-filtered, dried over 3Å molecular sieves) were added to a solution of the porphyrin in an NMR tube. All NMR spectra were recorded on a 500 MHz spectrometer with d1 = 5 and nt = 32. The precise host/ligand ratios were calculated from the integrals at the estimated 1:1 ratio. *Since some of the metalloporphyrins were available only in minute amounts, a small quantity was weighed in, and in order to maintain the same methanol:metalloporphyrin ratio for all titrations, this was followed by preparation of a corresponding stock solution of methanol in deuterochloroform, with the methanol concentration varying slightly in order to keep the methanol:metalloporphyrin ratio the same for all titrations. The actual methanol:metalloporphyrin ratios were determined by NMR spectroscopy. Therefore, the actual concentrations of methanol stock solutions varied between 2.22×10^{-2} to 4.71×10^{-2} mol×L^{-1} for the entire series of metalloporphyrin titrations.*

Table 1: AlTPPCl-MeOH titration.

[AlTPPCl] (M)	[MeOH] (M)	δ CH_3 (ppm)	addition (mL)	tot. Vol (mL)	G/H
1.17E-02	0.00E+00	-	0.00	0.50	0.00
1.14E-02	4.36E-04	3.18	0.01	0.51	0.04
1.12E-02	8.55E-04	3.16	0.02	0.52	0.08
1.10E-02	1.26E-03	3.14	0.03	0.53	0.11
1.08E-02	1.65E-03	3.13	0.04	0.54	0.15
1.06E-02	2.02E-03	3.11	0.05	0.55	0.19
1.04E-02	2.38E-03	3.10	0.06	0.56	0.23
1.02E-02	2.73E-03	3.09	0.07	0.57	0.27
1.01E-02	3.06E-03	3.08	0.08	0.58	0.30
9.88E-03	3.39E-03	3.07	0.09	0.59	0.34
9.72E-03	3.70E-03	3.06	0.10	0.60	0.38
9.41E-03	4.30E-03	3.04	0.12	0.62	0.46
9.11E-03	4.86E-03	3.04	0.14	0.64	0.53
8.84E-03	5.39E-03	3.02	0.16	0.66	0.61
8.58E-03	5.88E-03	3.04	0.18	0.68	0.69
8.33E-03	6.35E-03	3.04	0.20	0.70	0.76
7.78E-03	7.41E-03	3.01	0.25	0.75	0.95
7.29E-03	8.33E-03	3.03	0.30	0.80	1.14
6.48E-03	9.87E-03	3.07	0.40	0.90	1.52
5.83E-03	1.11E-02	3.10	0.50	1.00	1.90

Table 2: AlTPPCl-AcOH titration.

[AlTPPCl] (M)	[AcOH] (M)	δ CH_3 (ppm)	addition (mL)	tot. Vol (mL)	G/H
3.33E-03	0.00E+00	-	0.00	0.50	0.00
3.27E-03	4.36E-04	2.082	0.01	0.51	0.13
3.20E-03	8.55E-04	2.084	0.02	0.52	0.27
3.14E-03	1.26E-03	2.085	0.03	0.53	0.40
3.09E-03	1.65E-03	2.085	0.04	0.54	0.53
3.03E-03	2.02E-03	2.086	0.05	0.55	0.67
2.98E-03	2.38E-03	2.087	0.06	0.56	0.80
2.92E-03	2.73E-03	2.087	0.07	0.57	0.93
2.87E-03	3.06E-03	2.088	0.08	0.58	1.07
2.82E-03	3.39E-03	2.089	0.09	0.59	1.20
2.78E-03	3.70E-03	2.089	0.10	0.60	1.33
2.69E-03	4.30E-03	2.090	0.12	0.62	1.60
2.60E-03	4.86E-03	2.091	0.14	0.64	1.87
2.52E-03	5.39E-03	2.092	0.16	0.66	2.13
2.45E-03	5.88E-03	2.093	0.18	0.68	2.40
2.38E-03	6.35E-03	2.093	0.20	0.70	2.67
2.22E-03	7.41E-03	2.095	0.25	0.75	3.33
2.08E-03	8.33E-03	2.096	0.30	0.80	4.00
1.85E-03	9.87E-03	2.099	0.40	0.90	5.33
1.67E-03	1.11E-02	2.100	0.50	1.00	6.67

Table 3: CoTPPCl-MeOH titration.

[CoTPPCl] (M)	[MeOH] (M)	δ CH_3 (ppm)	addition (mL)	tot. Vol (mL)	G/H
2.63E-03	0.00E+00	-	0.00	0.50	0.00
2.58E-03	8.60E-04	3.4728	0.01	0.51	0.33
2.53E-03	1.69E-03	3.4728	0.02	0.52	0.67
2.48E-03	2.48E-03	3.4730	0.03	0.53	1.00
2.44E-03	3.25E-03	3.4729	0.04	0.54	1.33
2.39E-03	3.99E-03	3.4729	0.05	0.55	1.67
2.35E-03	4.70E-03	3.4731	0.06	0.56	2.00
2.31E-03	5.38E-03	3.4730	0.07	0.57	2.33
2.27E-03	6.05E-03	3.4730	0.08	0.58	2.67
2.23E-03	6.69E-03	3.4731	0.09	0.59	3.00
2.19E-03	7.31E-03	3.4734	0.10	0.60	3.33
2.12E-03	8.49E-03	3.4734	0.12	0.62	4.00
2.06E-03	9.59E-03	3.4734	0.14	0.64	4.67
1.99E-03	1.06E-02	3.4736	0.16	0.66	5.33
1.93E-03	1.16E-02	3.4736	0.18	0.68	6.00
1.88E-03	1.25E-02	3.4737	0.20	0.70	6.67
1.64E-03	1.64E-02	3.4743	0.30	0.80	10.00

Table 4: CoTPPCl-AcOH titration.

[CoTPPCl] (M)	[AcOH] (M)	δ CH_3 (ppm)	addition (mL)	tot. Vol (mL)	G/H
4.24E-03	0.00E+00	-	0.00	0.50	0.00
4.16E-03	8.32E-04	2.027	0.01	0.51	0.20
4.08E-03	1.63E-03	2.041	0.02	0.52	0.40
4.00E-03	2.40E-03	2.051	0.03	0.53	0.60
3.93E-03	3.14E-03	2.061	0.04	0.54	0.80
3.86E-03	3.86E-03	2.069	0.05	0.55	1.00
3.79E-03	4.55E-03	2.076	0.06	0.56	1.20
3.72E-03	5.21E-03	2.083	0.07	0.57	1.40
3.66E-03	5.85E-03	2.088	0.08	0.58	1.60
3.60E-03	6.47E-03	2.092	0.09	0.59	1.80
3.54E-03	7.07E-03	2.096	0.10	0.60	2.00
3.42E-03	8.21E-03	2.105	0.12	0.62	2.40
3.31E-03	9.28E-03	2.109	0.14	0.64	2.80
3.21E-03	1.03E-02	2.114	0.16	0.66	3.20
3.12E-03	1.12E-02	2.117	0.18	0.68	3.60
3.03E-03	1.21E-02	2.118	0.20	0.70	4.00
2.65E-03	1.59E-02	2.118	0.30	0.80	6.00

Table 5: CoTPFPPCl-MeOH titration.

[CoTPFPPCl] (M)	[MeOH] (M)	δ CH_3 (ppm)	addition (mL)	tot. Vol (mL)	G/H
5.62E-03	0.00E+00	-	-	0.000	0.00
5.60E-03	1.41E-03	1.068	1.068	0.002	0.25
5.58E-03	2.80E-03	1.100	1.100	0.004	0.50
5.56E-03	4.18E-03	1.122	1.122	0.006	0.75
5.54E-03	5.56E-03	1.147	1.147	0.008	1.00
5.51E-03	6.92E-03	1.166	1.166	0.010	1.26
5.49E-03	8.27E-03	1.188	1.188	0.012	1.51
5.47E-03	9.61E-03	1.205	1.205	0.014	1.76
5.45E-03	1.09E-02	1.220	1.220	0.016	2.01
5.43E-03	1.23E-02	1.235	1.235	0.018	2.26
5.41E-03	1.36E-02	1.251	1.251	0.020	2.51
5.37E-03	1.62E-02	1.258	1.258	0.024	3.01
5.33E-03	1.87E-02	1.276	1.276	0.028	3.51
5.29E-03	2.12E-02	1.293	1.293	0.032	4.02
5.25E-03	2.37E-02	1.304	1.304	0.036	4.52
5.21E-03	2.61E-02	1.312	1.312	0.040	5.02
5.11E-03	3.21E-02	1.334	1.334	0.050	6.28
5.02E-03	3.78E-02	1.352	1.352	0.060	7.53
4.93E-03	4.33E-02	1.364	1.364	0.070	8.79
4.85E-03	4.87E-02	1.377	1.377	0.080	10.04
4.77E-03	5.38E-02	1.386	1.386	0.090	11.30

4.69E-03	5.88E-02	1.394	1.394	0.100	12.55
4.33E-03	8.14E-02	1.428	1.428	0.150	18.83
4.02E-03	1.01E-01	1.448	1.448	0.200	25.10

Table 6: CoTPFPPCl-AcOH titration.

[CoTPFPPCl] (M)	[AcOH] (M)	δ CH_3 (ppm)	addition (mL)	tot. Vol (mL)	G/H
2.11E-05	0.00E+00	-	0.000	0.500	0.00
2.10E-05	4.27E-06	2.083	0.002	0.502	0.20
2.09E-05	8.51E-06	2.085	0.004	0.504	0.41
2.08E-05	1.27E-05	2.086	0.006	0.506	0.61
2.08E-05	1.69E-05	2.087	0.008	0.508	0.81
2.06E-05	2.51E-05	2.089	0.012	0.512	1.22
2.05E-05	2.92E-05	2.089	0.014	0.514	1.42
2.04E-05	3.32E-05	2.090	0.016	0.516	1.63
2.04E-05	3.73E-05	2.091	0.018	0.518	1.83
2.03E-05	4.12E-05	2.092	0.020	0.520	2.03
2.01E-05	5.11E-05	2.093	0.025	0.525	2.54
1.99E-05	6.07E-05	2.093	0.030	0.530	3.05
1.97E-05	7.01E-05	2.094	0.035	0.535	3.56
1.95E-05	7.94E-05	2.095	0.040	0.540	4.07
1.92E-05	9.75E-05	2.096	0.050	0.550	5.08
1.88E-05	1.15E-04	2.097	0.060	0.560	6.10
1.85E-05	1.32E-04	2.098	0.070	0.570	7.11
1.82E-05	1.48E-04	2.099	0.080	0.580	8.13

Table 7: MgTPP-MeOH titration.

[MgTPP] (M)	[MeOH] (M)	δ CH_3 (ppm)	addition (mL)	tot. Vol (mL)	G/H
6.40E-03	0.00E+00	-	0.00	0.50	0.00
6.28E-03	9.23E-04	1.754	0.01	0.51	0.15
6.16E-03	1.81E-03	1.866	0.02	0.52	0.29
6.04E-03	2.67E-03	1.964	0.03	0.53	0.44
5.93E-03	3.49E-03	2.051	0.04	0.54	0.59
5.82E-03	4.28E-03	2.124	0.05	0.55	0.74
5.72E-03	5.05E-03	2.190	0.06	0.56	0.88
5.62E-03	5.78E-03	2.250	0.07	0.57	1.03
5.52E-03	6.50E-03	2.306	0.08	0.58	1.18
5.43E-03	7.18E-03	2.355	0.09	0.59	1.32
5.34E-03	7.85E-03	2.397	0.10	0.60	1.47
5.17E-03	9.11E-03	2.479	0.12	0.62	1.76
5.00E-03	1.03E-02	2.554	0.14	0.64	2.06
4.85E-03	1.14E-02	2.620	0.16	0.66	2.35
4.71E-03	1.25E-02	2.680	0.18	0.68	2.65

4.57E-03	1.35E-02	2.734	0.20	0.70	2.94
4.27E-03	1.57E-02	2.829	0.25	0.75	3.68
4.00E-03	1.77E-02	2.904	0.30	0.80	4.41
3.56E-03	2.09E-02	3.007	0.40	0.90	5.88
3.20E-03	2.35E-02	3.079	0.50	1.00	7.35
2.29E-03	3.03E-02	3.224	0.90	1.40	13.24

Table 8: MgTPP-Acetone titration.

[MgTPP] (M)	[CH_3OCH_3] (M)	δ CH_3 (ppm)	addition (mL)	tot. Vol (mL)	G/H
6.69E-03	0.00E+00	-	0.00	0.50	0.00
6.56E-03	9.23E-04	1.995	0.01	0.51	0.14
6.43E-03	1.81E-03	2.000	0.02	0.52	0.28
6.31E-03	2.67E-03	2.004	0.03	0.53	0.42
6.19E-03	3.49E-03	2.008	0.04	0.54	0.56
6.08E-03	4.28E-03	2.011	0.05	0.55	0.70
5.97E-03	5.05E-03	2.015	0.06	0.56	0.85
5.87E-03	5.78E-03	2.018	0.07	0.57	0.99
5.76E-03	6.50E-03	2.021	0.08	0.58	1.13
5.67E-03	7.18E-03	2.024	0.09	0.59	1.27
5.57E-03	7.85E-03	2.027	0.10	0.60	1.41
5.39E-03	9.11E-03	2.031	0.12	0.62	1.69
5.22E-03	1.03E-02	2.035	0.14	0.64	1.97
5.07E-03	1.14E-02	2.039	0.16	0.66	2.25
4.92E-03	1.25E-02	2.043	0.18	0.68	2.54
4.78E-03	1.35E-02	2.047	0.20	0.70	2.82
4.46E-03	1.57E-02	2.055	0.25	0.75	3.52
4.18E-03	1.77E-02	2.061	0.30	0.80	4.23
3.72E-03	2.09E-02	2.072	0.40	0.90	5.63
3.34E-03	2.35E-02	2.079	0.50	1.00	7.04
2.57E-03	2.90E-02	2.096	0.80	1.30	11.27

Table 9: MgTPP-Pyridine titration.

[MgTPP] (M)	[Pyr] (M)	CH21	CH22	CH1	addition (mL)	tot. Vol (mL)	G/H
7.53E-03	0.00E+00	-			0.00	0.50	0.00
7.39E-03	9.23E-04	5.658	3.04	6.47	0.01	0.51	0.13
7.25E-03	1.81E-03	5.692	3.15	6.49	0.02	0.52	0.25
7.11E-03	2.67E-03	5.724	3.27	6.52	0.03	0.53	0.38
6.98E-03	3.49E-03	5.776	3.45	6.56	0.04	0.54	0.50
6.85E-03	4.28E-03	5.830	3.63	6.60	0.05	0.55	0.63
6.73E-03	5.05E-03	5.893	3.84	6.64	0.06	0.56	0.75
6.61E-03	5.78E-03	5.960	4.08	6.69	0.07	0.57	0.88
6.50E-03	6.50E-03	6.031	4.32	6.75	0.08	0.58	1.00

6.39E-03	7.18E-03	6.104	4.56	6.80	0.09	0.59	1.13
6.28E-03	7.85E-03	6.170	4.80	6.85	0.10	0.60	1.25
6.08E-03	9.11E-03	6.294	5.22	6.94	0.12	0.62	1.50
5.89E-03	1.03E-02	6.408	5.61	7.03	0.14	0.64	1.75
5.71E-03	1.14E-02	6.514	5.97	7.10	0.16	0.66	2.00
5.54E-03	1.25E-02	6.583	6.20	7.16	0.18	0.68	2.25
5.38E-03	1.35E-02	6.650	6.43	7.21	0.20	0.70	2.50
5.02E-03	1.57E-02	6.769	6.84	7.29	0.25	0.75	3.13
4.71E-03	1.77E-02	6.853	7.13	7.36	0.30	0.80	3.75
4.19E-03	2.09E-02	6.955	7.48	7.43	0.40	0.90	5.00
3.77E-03	2.35E-02	7.017	7.68	7.48	0.50	1.00	6.25
3.14E-03	2.75E-02	7.086	7.93	7.53	0.70	1.20	8.75

Table 10: MgTPFPP-MeOH titration.

[MgTPFPP] (M)	[MeOH] (M)	δ CH_3 (ppm)	addition (mL)	tot. Vol (mL)	G/H
5.56E-03	0.00E+00	-	0.00	0.50	0.00
5.46E-03	5.90E-04	-0.122	0.01	0.51	0.11
5.35E-03	1.16E-03	0.073	0.02	0.52	0.22
5.25E-03	1.70E-03	0.257	0.03	0.53	0.32
5.15E-03	2.23E-03	0.457	0.04	0.54	0.43
5.06E-03	2.74E-03	0.706	0.05	0.55	0.54
4.97E-03	3.22E-03	0.868	0.06	0.56	0.65
4.88E-03	3.70E-03	1.025	0.07	0.57	0.76
4.80E-03	4.15E-03	1.147	0.08	0.58	0.87
4.72E-03	4.59E-03	1.268	0.09	0.59	0.97
4.64E-03	5.02E-03	1.376	0.10	0.60	1.08
4.49E-03	5.83E-03	1.534	0.12	0.62	1.30
4.35E-03	6.58E-03	1.671	0.14	0.64	1.51
4.22E-03	7.30E-03	1.791	0.16	0.66	1.73
4.09E-03	7.97E-03	1.896	0.18	0.68	1.95
3.97E-03	8.60E-03	1.990	0.20	0.70	2.16
3.71E-03	1.00E-02	2.172	0.25	0.75	2.70
3.48E-03	1.13E-02	2.326	0.30	0.80	3.25
3.09E-03	1.34E-02	2.523	0.40	0.90	4.33
2.78E-03	1.50E-02	2.666	0.50	1.00	5.41
2.32E-03	1.76E-02	2.817	0.70	1.20	7.57
1.99E-03	1.93E-02	2.940	0.90	1.40	9.74

Table 11: MgTPFPP-Acetone titration.

[MgTPFPP] (M)	[CH_3OCH_3] (M)	δ CH_3 (ppm)	addition (mL)	tot. Vol (mL)	G/H
6.35E-03	0.00E+00	-	0.00	0.50	0.00
6.23E-03	5.90E-04	0.605	0.01	0.51	0.09

6.11E-03	1.16E-03	0.739	0.02	0.52	0.19
5.99E-03	1.70E-03	0.851	0.03	0.53	0.28
5.88E-03	2.23E-03	0.948	0.04	0.54	0.38
5.77E-03	2.74E-03	1.038	0.05	0.55	0.47
5.67E-03	3.22E-03	1.113	0.06	0.56	0.57
5.57E-03	3.70E-03	1.187	0.07	0.57	0.66
5.48E-03	4.15E-03	1.245	0.08	0.58	0.76
5.38E-03	4.59E-03	1.298	0.09	0.59	0.85
5.29E-03	5.02E-03	1.347	0.10	0.60	0.95
5.12E-03	5.83E-03	1.421	0.12	0.62	1.14
4.96E-03	6.58E-03	1.481	0.14	0.64	1.33
4.81E-03	7.30E-03	1.534	0.16	0.66	1.52
4.67E-03	7.97E-03	1.578	0.18	0.68	1.71
4.54E-03	8.60E-03	1.617	0.20	0.70	1.90
4.23E-03	1.00E-02	1.694	0.25	0.75	2.37
3.97E-03	1.13E-02	1.754	0.30	0.80	2.84
3.53E-03	1.34E-02	1.828	0.40	0.90	3.79
3.18E-03	1.50E-02	1.881	0.50	1.00	4.74
2.65E-03	1.76E-02	1.931	0.70	1.20	6.63
2.27E-03	1.93E-02	1.971	0.90	1.40	8.53

Table 12: MgTPFPP-AcOH titration.

[MgTPFPP] (M)	**[AcOH] (M)**	**δ CH_3 (ppm)**	**addition (mL)**	**tot. Vol (mL)**	**G/H**
9.26E-03	0.00E+00	-	0.00	0.50	0.00
9.08E-03	5.90E-04	0.620	0.01	0.51	0.07
8.90E-03	1.16E-03	0.802	0.02	0.52	0.13
8.74E-03	1.70E-03	0.947	0.03	0.53	0.20
8.57E-03	2.23E-03	1.060	0.04	0.54	0.26
8.42E-03	2.74E-03	1.164	0.05	0.55	0.33
8.27E-03	3.22E-03	1.249	0.06	0.56	0.39
8.12E-03	3.70E-03	1.319	0.07	0.57	0.46
7.98E-03	4.15E-03	1.379	0.08	0.58	0.52
7.85E-03	4.59E-03	1.433	0.09	0.59	0.59
7.72E-03	5.02E-03	1.474	0.10	0.60	0.65
7.47E-03	5.83E-03	1.543	0.12	0.62	0.78
7.23E-03	6.58E-03	1.596	0.14	0.64	0.91
7.02E-03	7.30E-03	1.678	0.16	0.66	1.04
6.81E-03	7.97E-03	1.709	0.18	0.68	1.17
6.61E-03	8.60E-03	1.767	0.20	0.70	1.30
6.17E-03	1.00E-02	1.811	0.25	0.75	1.63
5.79E-03	1.13E-02	1.863	0.30	0.80	1.95
5.14E-03	1.34E-02	1.862	0.40	0.90	2.60
4.63E-03	1.50E-02	1.897	0.50	1.00	3.25

3.86E-03	1.76E-02	1.933	0.70	1.20	4.55
3.31E-03	1.93E-02	1.963	0.90	1.40	5.85

Table 13: MgTPFPP-Pyridine titration.

[MgTPFPP] (M)	[Pyr] (M)	CH21	CH22	CH1	addition (mL)	tot. Vol (mL)	G/H
5.12E-03	0.00E+00	-	-	-	0.00	0.50	0.00
7.06E-03	5.90E-04	5.533	2.540	6.391	0.01	0.51	0.08
6.92E-03	1.16E-03	5.537	2.553	3.394	0.02	0.52	0.17
6.79E-03	1.70E-03	5.545	2.571	3.399	0.03	0.53	0.25
6.67E-03	2.23E-03	5.550	2.595	6.404	0.04	0.54	0.33
6.55E-03	2.74E-03	5.558	2.622	6.410	0.05	0.55	0.42
6.43E-03	3.22E-03	5.571	2.658	6.419	0.06	0.56	0.50
6.32E-03	3.70E-03	5.585	2.704	6.428	0.07	0.57	0.59
6.21E-03	4.15E-03	5.562	2.763	6.442	0.08	0.58	0.67
6.10E-03	4.59E-03	5.626	2.848	6.462	0.09	0.59	0.75
6.00E-03	5.02E-03	5.663	2.960	6.487	0.10	0.60	0.84
5.81E-03	5.83E-03	5.770	3.266	6.568	0.12	0.62	1.00
5.63E-03	6.58E-03	5.932	3.716	6.675	0.14	0.64	1.17
5.46E-03	7.30E-03	6.102	4.206	6.783	0.16	0.66	1.34
5.30E-03	7.97E-03	6.256	4.707	6.879	0.18	0.68	1.50
5.14E-03	8.60E-03	6.368	5.091	6.959	0.20	0.70	1.67
4.80E-03	1.00E-02	6.658	5.903	7.128	0.25	0.75	2.09
4.50E-03	1.13E-02	6.862	6.700	7.289	0.30	0.80	2.51
4.00E-03	1.34E-02	7.084	7.641	7.390	0.40	0.90	3.34
3.60E-03	1.50E-02	7.199	8.138	7.466	0.50	1.00	4.18
3.00E-03	1.76E-02	7.348	8.503	7.544	0.70	1.20	5.85
2.57E-03	1.93E-02	7.414	8.600	7.594	0.90	1.40	7.52

Table 14: $MgTPPBr_8$-MeOH titration.

[$MgTPPBr_8$] (M)	[MeOH] (M)	δ CH_3 (ppm)	addition (mL)	tot. Vol (mL)	G/H
2.96E-03	0.00E+00	-	0.00	0.50	0.00
2.90E-03	4.64E-04	1.049	0.01	0.51	0.16
2.84E-03	9.10E-04	1.254	0.02	0.52	0.32
2.79E-03	1.34E-03	1.402	0.03	0.53	0.48
2.74E-03	1.75E-03	1.534	0.04	0.54	0.64
2.69E-03	2.15E-03	1.654	0.05	0.55	0.80
2.64E-03	2.53E-03	1.764	0.06	0.56	0.96
2.59E-03	2.91E-03	1.860	0.07	0.57	1.12
2.55E-03	3.26E-03	1.945	0.08	0.58	1.28
2.51E-03	3.61E-03	2.024	0.09	0.59	1.44
2.46E-03	3.94E-03	2.099	0.10	0.60	1.60
2.38E-03	4.58E-03	2.218	0.12	0.62	1.92

2.31E-03	5.17E-03	2.319	0.14	0.64	2.24
2.24E-03	5.73E-03	2.399	0.16	0.66	2.56
2.17E-03	6.26E-03	2.471	0.18	0.68	2.88
2.11E-03	6.76E-03	2.535	0.20	0.70	3.20
1.97E-03	7.89E-03	2.689	0.25	0.75	4.00
1.85E-03	8.87E-03	2.781	0.30	0.80	4.80
1.64E-03	1.05E-02	2.911	0.40	0.90	6.40
1.48E-03	1.18E-02	3.003	0.50	1.00	8.00
1.23E-03	1.38E-02	3.095	0.70	1.20	11.20
1.06E-03	1.52E-02	3.179	0.90	1.40	14.40

Table 15: MgTPPBr8-AcOH titration.

[MgTPPBr$_8$] (M)	**[AcOH] (M)**	**δ CH$_3$ (ppm)**	**addition (mL)**	**tot. Vol (mL)**	**G/H**	**Comment**
4.73E-03	0.00E+00	-	0.00	0.50	0.00	
4.64E-03	4.64E-04	-	0.01	0.51	0.10	signal overlap
4.55E-03	9.10E-04	-	0.02	0.52	0.20	signal overlap
4.46E-03	1.34E-03	-	0.03	0.53	0.30	signal overlap
4.38E-03	1.75E-03	-	0.04	0.54	0.40	signal overlap
4.30E-03	2.15E-03	-	0.05	0.55	0.50	signal overlap
4.22E-03	2.53E-03	-	0.06	0.56	0.60	signal overlap
4.15E-03	2.91E-03	1.438	0.07	0.57	0.70	
4.08E-03	3.26E-03	1.493	0.08	0.58	0.80	
4.01E-03	3.61E-03	1.599	0.09	0.59	0.90	
3.94E-03	3.94E-03	1.641	0.10	0.60	1.00	
3.82E-03	4.58E-03	1.733	0.12	0.62	1.20	
3.70E-03	5.17E-03	1.805	0.14	0.64	1.40	
3.58E-03	5.73E-03	1.880	0.16	0.66	1.60	
3.48E-03	6.26E-03	1.946	0.18	0.68	1.80	
3.38E-03	6.76E-03	1.985	0.20	0.70	2.00	
3.15E-03	7.89E-03	2.025	0.25	0.75	2.50	
2.96E-03	8.87E-03	2.050	0.30	0.80	3.00	
2.63E-03	1.05E-02	2.071	0.40	0.90	4.00	
2.37E-03	1.18E-02	2.084	0.50	1.00	5.00	
1.97E-03	1.38E-02	2.092	0.70	1.20	7.00	
1.69E-03	1.52E-02	2.099	0.90	1.40	9.00	

Table 16: MgTPPBr$_8$-Acetone titration.

[MgTPPBr$_8$] (M)	**[CH$_3$OCH$_3$] (M)**	**δ CH$_3$ (ppm)**	**addition (mL)**	**tot. Vol (mL)**	**G/H**
4.73E-03	0.00E+00	-	0.00	0.50	0.00
4.64E-03	4.64E-04	1.005	0.01	0.51	0.10
4.55E-03	9.10E-04	1.106	0.02	0.52	0.20
4.46E-03	1.34E-03	1.191	0.03	0.53	0.30

4.38E-03	1.75E-03	1.266	0.04	0.54	0.40
4.30E-03	2.15E-03	1.330	0.05	0.55	0.50
4.22E-03	2.53E-03	1.387	0.06	0.56	0.60
4.15E-03	2.91E-03	1.438	0.07	0.57	0.70
4.08E-03	3.26E-03	1.483	0.08	0.58	0.80
4.01E-03	3.61E-03	1.526	0.09	0.59	0.90
3.94E-03	3.94E-03	1.564	0.10	0.60	1.00
3.82E-03	4.58E-03	1.620	0.12	0.62	1.20
3.70E-03	5.17E-03	1.665	0.14	0.64	1.40
3.58E-03	5.73E-03	1.703	0.16	0.66	1.60
3.48E-03	6.26E-03	1.735	0.18	0.68	1.80
3.38E-03	6.76E-03	1.765	0.20	0.70	2.00
3.15E-03	7.89E-03	1.817	0.25	0.75	2.50
2.96E-03	8.87E-03	1.859	0.30	0.80	3.00
2.63E-03	1.05E-02	1.914	0.40	0.90	4.00
2.37E-03	1.18E-02	1.956	0.50	1.00	5.00
1.97E-03	1.38E-02	2.000	0.70	1.20	7.00
1.69E-03	1.52E-02	2.025	0.90	1.40	9.00

Table 17: $MgTPPBr_8$-Pyridine titration.

[$MgTPPBr_8$] (M)	[Pyr] (M)	CH21	CH22	CH1	addition (mL)	tot. Vol (mL)	G/H
4.07E-03	0.00E+00	-	-	-	0.00	0.50	0.00
3.99E-03	4.64E-04	3.156	5.832	6.636	0.01	0.51	0.12
3.91E-03	9.10E-04	3.188	5.840	6.641	0.02	0.52	0.23
3.84E-03	1.34E-03	3.225	5.853	6.650	0.03	0.53	0.35
3.77E-03	1.75E-03	3.275	5.865	6.658	0.04	0.54	0.47
3.70E-03	2.15E-03	3.344	5.884	6.675	0.05	0.55	0.58
3.63E-03	2.53E-03	3.460	5.915	6.696	0.06	0.56	0.70
3.57E-03	2.91E-03	3.616	5.957	6.726	0.07	0.57	0.81
3.51E-03	3.26E-03	3.856	6.020	6.773	0.08	0.58	0.93
3.45E-03	3.61E-03	4.146	6.100	6.828	0.09	0.59	1.05
3.39E-03	3.94E-03	4.464	6.184	6.890	0.10	0.60	1.16
3.28E-03	4.58E-03	5.018	6.352	6.994	0.12	0.62	1.40
3.18E-03	5.17E-03	5.465	6.451	7.078	0.14	0.64	1.63
3.08E-03	5.73E-03	5.831	6.547	7.147	0.16	0.66	1.86
2.99E-03	6.26E-03	6.116	6.623	7.204	0.18	0.68	2.09
2.91E-03	6.76E-03	6.356	6.686	7.248	0.20	0.70	2.33
2.71E-03	7.89E-03	6.798	6.792	7.328	0.25	0.75	2.91
2.54E-03	8.87E-03	7.070	6.881	7.386	0.30	0.80	3.49
2.26E-03	1.05E-02	7.461	6.995	7.464	0.40	0.90	4.65
2.03E-03	1.18E-02	7.734	7.067	7.511	0.50	1.00	5.81
1.70E-03	1.38E-02	8.035	7.146	7.561	0.70	1.20	8.14

Table 18: $SnTPP(OH)_2$-Pyridine titration.

[$SnTPP(OH)_2$] (M)	[Pyr] (M)	CH1	addition (mL)	tot. Vol (mL)	G/H
7.84E-03	0.00E+00	-	0.00	0.50	0.00
7.68E-03	7.68E-04	8.577	0.01	0.51	0.10
7.54E-03	1.51E-03	8.593	0.02	0.52	0.20
7.39E-03	2.22E-03	8.606	0.03	0.53	0.30
7.26E-03	2.90E-03	8.610	0.04	0.54	0.40
7.13E-03	3.56E-03	8.613	0.05	0.55	0.50
7.00E-03	4.20E-03	8.615	0.06	0.56	0.60
6.88E-03	4.81E-03	8.617	0.07	0.57	0.70
6.76E-03	5.41E-03	8.618	0.08	0.58	0.80
6.64E-03	5.98E-03	8.619	0.09	0.59	0.90
6.53E-03	6.53E-03	8.620	0.10	0.60	1.00
6.32E-03	7.59E-03	8.622	0.12	0.62	1.20
6.12E-03	8.57E-03	8.622	0.14	0.64	1.40
5.94E-03	9.50E-03	8.623	0.16	0.66	1.60
5.76E-03	1.04E-02	8.624	0.18	0.68	1.80
5.60E-03	1.12E-02	8.624	0.20	0.70	2.00
5.23E-03	1.31E-02	8.625	0.25	0.75	2.50
4.90E-03	1.47E-02	8.625	0.30	0.80	3.00
4.35E-03	1.74E-02	8.626	0.40	0.90	4.00
3.92E-03	1.96E-02	8.626	0.50	1.00	5.00

Table 19: O=TiTPP-AcOH titration.

[O=TiTPP] (M)	[AcOH] (M)	δ CH_3 (ppm)	addition (mL)	tot. Vol (mL)	G/H
8.87E-03	0.00E+00	-	0.00	0.50	0.00
8.69E-03	8.69E-04	2.078	0.01	0.51	0.10
8.53E-03	1.71E-03	2.082	0.02	0.52	0.20
8.37E-03	2.51E-03	2.085	0.03	0.53	0.30
8.21E-03	3.28E-03	2.087	0.04	0.54	0.40
8.06E-03	4.03E-03	2.089	0.05	0.55	0.50
7.92E-03	4.75E-03	2.090	0.06	0.56	0.60
7.78E-03	5.45E-03	2.091	0.07	0.57	0.70
7.64E-03	6.12E-03	2.092	0.08	0.58	0.80
7.52E-03	6.76E-03	2.093	0.09	0.59	0.90
7.39E-03	7.39E-03	2.094	0.10	0.60	1.00
7.15E-03	8.58E-03	2.095	0.12	0.62	1.20
6.93E-03	9.70E-03	2.097	0.14	0.64	1.40
6.72E-03	1.07E-02	2.098	0.16	0.66	1.60
6.52E-03	1.17E-02	2.098	0.18	0.68	1.80
6.33E-03	1.27E-02	2.099	0.20	0.70	2.00
5.91E-03	1.48E-02	2.100	0.25	0.75	2.50
5.54E-03	1.66E-02	2.101	0.30	0.80	3.00

4.93E-03	1.97E-02	2.102	0.40	0.90	4.00
4.43E-03	2.22E-02	2.103	0.50	1.00	5.00

Table 20: ZnTPP-MeOH titration.

[ZnTPP] (M)	[MeOH] (M)	δ CH_3 (ppm)	addition (mL)	tot. Vol (mL)	G/H
8.85E-03	0.00E+00	-	0.00	0.50	0.00
8.67E-03	8.67E-04	3.309	0.01	0.51	0.10
8.51E-03	1.70E-03	3.313	0.02	0.52	0.20
8.35E-03	2.50E-03	3.316	0.03	0.53	0.30
8.19E-03	3.28E-03	3.319	0.04	0.54	0.40
8.04E-03	4.02E-03	3.321	0.05	0.55	0.50
7.90E-03	4.74E-03	3.323	0.06	0.56	0.60
7.76E-03	5.43E-03	3.327	0.07	0.57	0.70
7.63E-03	6.10E-03	3.329	0.08	0.58	0.80
7.50E-03	6.75E-03	3.331	0.09	0.59	0.90
7.37E-03	7.37E-03	3.334	0.10	0.60	1.00
7.14E-03	8.56E-03	3.339	0.12	0.62	1.20
6.91E-03	9.68E-03	3.345	0.14	0.64	1.40
6.70E-03	1.07E-02	3.350	0.16	0.66	1.60
6.51E-03	1.17E-02	3.355	0.18	0.68	1.80
6.32E-03	1.26E-02	3.361	0.20	0.70	2.00
5.90E-03	1.47E-02	3.370	0.25	0.75	2.50
5.53E-03	1.66E-02	3.378	0.30	0.80	3.00
4.92E-03	1.97E-02	3.391	0.40	0.90	4.00
4.42E-03	2.21E-02	3.401	0.50	1.00	5.00
4.02E-03	2.41E-02	3.410	0.60	1.10	6.00

Table 21: ZnTPP-AcOH titration.

[ZnTPP] (M)	[AcOH] (M)	δ CH_3 (ppm)	addition (mL)	tot. Vol (mL)	G/H
7.96E-03	0.00E+00	-	0.00	0.50	0.00
7.81E-03	8.67E-04	2.073	0.01	0.51	0.11
7.66E-03	1.70E-03	2.078	0.02	0.52	0.22
7.51E-03	2.50E-03	2.081	0.03	0.53	0.33
7.37E-03	3.28E-03	2.083	0.04	0.54	0.44
7.24E-03	4.02E-03	2.084	0.05	0.55	0.56
7.11E-03	4.74E-03	2.085	0.06	0.56	0.67
6.99E-03	5.43E-03	2.086	0.07	0.57	0.78
6.86E-03	6.10E-03	2.087	0.08	0.58	0.89
6.75E-03	6.75E-03	2.088	0.09	0.59	1.00
6.64E-03	7.37E-03	2.089	0.10	0.60	1.11
6.42E-03	8.56E-03	2.090	0.12	0.62	1.33
6.22E-03	9.68E-03	2.091	0.14	0.64	1.56

6.03E-03	1.07E-02	2.092	0.16	0.66	1.78
5.86E-03	1.17E-02	2.093	0.18	0.68	2.00
5.69E-03	1.26E-02	2.093	0.20	0.70	2.22
5.31E-03	1.47E-02	2.095	0.25	0.75	2.78
4.98E-03	1.66E-02	2.096	0.30	0.80	3.33
4.42E-03	1.97E-02	2.098	0.40	0.90	4.44
3.98E-03	2.21E-02	2.099	0.50	1.00	5.56

Table 22: ZnTPP-Pyridine titration.

[ZnTPP] (M)	[Pyr] (M)	CH21	CH22	CH1	addition (mL)	tot. Vol (mL)	G/H
8.54E-03	0.00E+00	-	-	-	0.00	0.50	0.00
8.38E-03	8.96E-04	2.750	5.589	6.405	0.01	0.51	0.11
8.22E-03	1.76E-03	2.779	5.597	6.410	0.02	0.52	0.21
8.06E-03	2.59E-03	2.815	5.605	6.417	0.03	0.53	0.32
7.91E-03	3.39E-03	2.866	5.620	6.428	0.04	0.54	0.43
7.77E-03	4.16E-03	2.938	5.639	6.442	0.05	0.55	0.53
7.63E-03	4.90E-03	3.027	5.666	6.462	0.06	0.56	0.64
7.50E-03	5.61E-03	3.158	5.703	6.490	0.07	0.57	0.75
7.37E-03	6.30E-03	3.340	5.756	6.529	0.08	0.58	0.86
7.24E-03	6.97E-03	3.568	5.822	6.577	0.09	0.59	0.96
7.12E-03	7.62E-03	3.831	5.899	6.635	0.10	0.60	1.07
6.89E-03	8.85E-03	4.414	6.068	6.762	0.12	0.62	1.28
6.68E-03	1.00E-02	4.938	6.218	6.876	0.14	0.64	1.50
6.47E-03	1.11E-02	5.356	6.342	6.968	0.16	0.66	1.71
6.28E-03	1.21E-02	5.701	6.441	7.043	0.18	0.68	1.93
6.10E-03	1.31E-02	5.984	6.524	7.107	0.20	0.70	2.14
5.34E-03	1.71E-02	6.855	6.776	7.294	0.30	0.80	3.21

Table 23: ZnTPFPP-MeOH titration.

[ZnTPFPP] (M)	[MeOH] (M)	δ CH_3 (ppm)	addition (mL)	tot. Vol (mL)	G/H
2.08E-03	0.00E+00	-	0.00	0.50	0.00
2.04E-03	5.67E-04	2.718	0.01	0.51	0.28
2.00E-03	1.11E-03	2.744	0.02	0.52	0.56
1.96E-03	1.64E-03	2.767	0.03	0.53	0.83
1.93E-03	2.14E-03	2.788	0.04	0.54	1.11
1.89E-03	2.63E-03	2.809	0.05	0.55	1.39
1.86E-03	3.10E-03	2.828	0.06	0.56	1.67
1.83E-03	3.55E-03	2.846	0.07	0.57	1.94
1.80E-03	3.99E-03	2.863	0.08	0.58	2.22
1.76E-03	4.41E-03	2.879	0.09	0.59	2.50
1.74E-03	4.82E-03	2.896	0.10	0.60	2.78
1.68E-03	5.59E-03	2.924	0.12	0.62	3.33

1.63E-03	6.32E-03	2.950	0.14	0.64	3.89
1.58E-03	7.01E-03	2.975	0.16	0.66	4.44
1.53E-03	7.65E-03	2.996	0.18	0.68	5.00
1.49E-03	8.26E-03	3.017	0.20	0.70	5.55
1.39E-03	9.63E-03	3.063	0.25	0.75	6.94
1.30E-03	1.08E-02	3.102	0.30	0.80	8.33
1.16E-03	1.28E-02	3.159	0.40	0.90	11.10
1.04E-03	1.45E-02	3.202	0.50	1.00	13.88
8.68E-04	1.69E-02	3.258	0.70	1.20	19.43
7.44E-04	1.86E-02	3.289	0.90	1.40	24.98

Table 24: ZnTPFPP-AcOH titration.

[ZnTPFPP] (M)	[AcOH] (M)	δ CH_3 (ppm)	addition (mL)	tot. Vol (mL)	G/H
4.59E-03	0.00E+00	-	0.00	0.50	0.00
4.50E-03	5.67E-04	2.021	0.01	0.51	0.13
4.41E-03	1.11E-03	2.026	0.02	0.52	0.25
4.33E-03	1.64E-03	2.031	0.03	0.53	0.38
4.25E-03	2.14E-03	2.034	0.04	0.54	0.50
4.17E-03	2.63E-03	2.037	0.05	0.55	0.63
4.10E-03	3.10E-03	2.040	0.06	0.56	0.76
4.02E-03	3.55E-03	2.042	0.07	0.57	0.88
3.96E-03	3.99E-03	2.044	0.08	0.58	1.01
3.89E-03	4.41E-03	2.046	0.09	0.59	1.13
3.82E-03	4.82E-03	2.048	0.10	0.60	1.26
3.70E-03	5.59E-03	2.051	0.12	0.62	1.51
3.58E-03	6.32E-03	2.053	0.14	0.64	1.76
3.48E-03	7.01E-03	2.056	0.16	0.66	2.02
3.37E-03	7.65E-03	2.058	0.18	0.68	2.27
3.28E-03	8.26E-03	2.060	0.20	0.70	2.52
3.06E-03	9.63E-03	2.063	0.25	0.75	3.15
2.87E-03	1.08E-02	2.068	0.30	0.80	3.78
2.55E-03	1.28E-02	2.071	0.40	0.90	5.04
2.29E-03	1.45E-02	2.074	0.50	1.00	6.30
1.91E-03	1.69E-02	2.079	0.70	1.20	8.82
1.64E-03	1.86E-02	2.081	0.90	1.40	11.34

Table 25: ZnTPFPP-Acetone titration.

[ZnTPFPP] (M)	[CH_3OCH_3] (M)	δ CH_3 (ppm)	addition (mL)	tot. Vol (mL)	G/H
1.68E-03	0.00E+00	-	0.00	0.50	0.00
1.65E-03	5.67E-04	2.073	0.01	0.51	0.34
1.61E-03	1.11E-03	2.075	0.02	0.52	0.69
1.58E-03	1.64E-03	2.077	0.03	0.53	1.03

1.55E-03	2.14E-03	2.079	0.04	0.54	1.38
1.53E-03	2.63E-03	2.081	0.05	0.55	1.72
1.50E-03	3.10E-03	2.083	0.06	0.56	2.07
1.47E-03	3.55E-03	2.085	0.07	0.57	2.41
1.45E-03	3.99E-03	2.086	0.08	0.58	2.75
1.42E-03	4.41E-03	2.088	0.09	0.59	3.10
1.40E-03	4.82E-03	2.090	0.10	0.60	3.44
1.35E-03	5.59E-03	2.093	0.12	0.62	4.13
1.31E-03	6.32E-03	2.096	0.14	0.64	4.82
1.27E-03	7.01E-03	2.098	0.16	0.66	5.51
1.23E-03	7.65E-03	2.101	0.18	0.68	6.20
1.20E-03	8.26E-03	2.103	0.20	0.70	6.88
1.12E-03	9.63E-03	2.109	0.25	0.75	8.61
1.05E-03	1.08E-02	2.113	0.30	0.80	10.33
9.33E-04	1.28E-02	2.121	0.40	0.90	13.77
8.40E-04	1.45E-02	2.126	0.50	1.00	17.21
7.00E-04	1.69E-02	2.133	0.70	1.20	24.10
6.00E-04	1.86E-02	2.139	0.90	1.40	30.98

Table 26: ZnTPFPP-Pyridine titration.

[ZnTPFPP] (M)	[Pyr] (M)	CH21	CH22	CH1	addition (mL)	tot. Vol (mL)	G/H
4.94E-03	0.00E+00	-	-	-	0.00	0.50	0.00
4.84E-03	5.67E-04	2.376	5.504	6.358	0.01	0.51	0.12
4.75E-03	1.11E-03	2.379	5.505	6.359	0.02	0.52	0.23
4.66E-03	1.64E-03	2.384	5.506	6.359	0.03	0.53	0.35
4.57E-03	2.14E-03	2.389	5.508	6.360	0.04	0.54	0.47
4.49E-03	2.63E-03	2.403	5.511	6.362	0.05	0.55	0.59
4.41E-03	3.10E-03	2.430	5.519	6.368	0.06	0.56	0.70
4.33E-03	3.55E-03	2.536	5.549	6.389	0.07	0.57	0.82
4.26E-03	3.99E-03	2.969	5.673	6.479	0.08	0.58	0.94
4.19E-03	4.41E-03	3.531	5.835	6.601	0.09	0.59	1.05
4.12E-03	4.82E-03	4.032	5.977	6.705	0.10	0.60	1.17
3.98E-03	5.59E-03	4.786	6.193	6.868	0.12	0.62	1.40
3.86E-03	6.32E-03	5.333	6.350	6.983	0.14	0.64	1.64
3.74E-03	7.01E-03	5.743	6.466	7.069	0.16	0.66	1.87
3.63E-03	7.65E-03	6.061	6.557	7.138	0.18	0.68	2.11
3.53E-03	8.26E-03	6.320	6.633	7.193	0.20	0.70	2.34
3.29E-03	9.63E-03	6.803	6.781	7.298	0.25	0.75	2.93
3.09E-03	1.08E-02	7.130	6.870	7.368	0.30	0.80	3.51
2.74E-03	1.28E-02	7.514	6.976	7.447	0.40	0.90	4.68
2.47E-03	1.45E-02	7.734	7.040	7.495	0.50	1.00	5.85
2.06E-03	1.69E-02	7.964	7.104	7.543	0.70	1.20	8.19
1.76E-03	1.86E-02	8.105	7.143	7.572	0.90	1.40	10.53

Design of oxophilic metalloporphyrins: An experimental and DFT study of methanol binding
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Table 27: $ZnTPPBr_8$-MeOH titration.

$[ZnTPPBr_8]$ (M)	[MeOH] (M)	δ CH_3 (ppm)	addition (mL)	tot. Vol (mL)	G/H
5.02E-03	0.00E+00	-	0.00	0.50	0.00
4.92E-03	4.49E-04	2.670	0.01	0.51	0.09
4.82E-03	8.81E-04	2.694	0.02	0.52	0.18
4.73E-03	1.30E-03	2.719	0.03	0.53	0.27
4.65E-03	1.70E-03	2.741	0.04	0.54	0.37
4.56E-03	2.08E-03	2.763	0.05	0.55	0.46
4.48E-03	2.45E-03	2.784	0.06	0.56	0.55
4.40E-03	2.81E-03	2.802	0.07	0.57	0.64
4.33E-03	3.16E-03	2.820	0.08	0.58	0.73
4.25E-03	3.50E-03	2.838	0.09	0.59	0.82
4.18E-03	3.82E-03	2.852	0.10	0.60	0.91
4.05E-03	4.43E-03	2.884	0.12	0.62	1.10
3.92E-03	5.01E-03	2.912	0.14	0.64	1.28
3.80E-03	5.55E-03	2.938	0.16	0.66	1.46
3.69E-03	6.07E-03	2.961	0.18	0.68	1.64
3.58E-03	6.55E-03	2.982	0.20	0.70	1.83
3.34E-03	7.64E-03	3.035	0.25	0.75	2.28
3.14E-03	8.59E-03	3.079	0.30	0.80	2.74
2.79E-03	1.02E-02	3.140	0.40	0.90	3.65
2.28E-03	1.25E-02	3.209	0.60	1.10	5.48
1.93E-03	1.41E-02	3.263	0.80	1.30	7.31

Table 28: $ZnTPPBr_8$-Acetone titration.

$[ZnTPPBr_8]$ (M)	$[CH_3OCH_3]$ (M)	δ CH_3 (ppm)	addition (mL)	tot. Vol (mL)	G/H
2.29E-03	0.00E+00	-	0.00	0.50	0.00
2.25E-03	4.49E-04	2.1186	0.01	0.51	0.20
2.20E-03	8.81E-04	2.1204	0.02	0.52	0.40
2.16E-03	1.30E-03	2.1214	0.03	0.53	0.60
2.12E-03	1.70E-03	2.1238	0.04	0.54	0.80
2.08E-03	2.08E-03	2.1243	0.05	0.55	1.00
2.05E-03	2.45E-03	2.1247	0.06	0.56	1.20
2.01E-03	2.81E-03	2.1251	0.07	0.57	1.40
1.98E-03	3.16E-03	2.1257	0.08	0.58	1.60
1.94E-03	3.50E-03	2.1260	0.09	0.59	1.80
1.91E-03	3.82E-03	2.1263	0.10	0.60	2.00
1.85E-03	4.43E-03	2.1269	0.12	0.62	2.40
1.79E-03	5.01E-03	2.1273	0.14	0.64	2.80
1.74E-03	5.55E-03	2.1277	0.16	0.66	3.20
1.68E-03	6.07E-03	2.1280	0.18	0.68	3.60

1.64E-03	6.55E-03	2.1283	0.20	0.70	4.00
1.53E-03	7.64E-03	2.1287	0.25	0.75	5.00
1.43E-03	8.59E-03	2.1293	0.30	0.80	6.00
1.27E-03	1.02E-02	2.1304	0.40	0.90	8.00
1.15E-03	1.15E-02	2.1311	0.50	1.00	10.00
9.55E-04	1.34E-02	2.1320	0.70	1.20	14.00
8.18E-04	1.47E-02	2.1328	0.90	1.40	18.00

Table 29: $ZnTPPBr_8$-AcOH titration.

$[ZnTPPBr_8]$ (M)	[AcOH] (M)	δ CH_3 (ppm)	addition (mL)	tot. Vol (mL)	G/H
2.29E-03	0.00E+00	-	0.00	0.50	0.00
2.25E-03	4.49E-04	1.9901	0.01	0.51	0.20
2.20E-03	8.81E-04	2.0031	0.02	0.52	0.40
2.16E-03	1.30E-03	2.0099	0.03	0.53	0.60
2.12E-03	1.70E-03	2.0153	0.04	0.54	0.80
2.08E-03	2.08E-03	2.0181	0.05	0.55	1.00
2.05E-03	2.45E-03	2.0222	0.06	0.56	1.20
2.01E-03	2.81E-03	2.0242	0.07	0.57	1.40
1.98E-03	3.16E-03	2.0260	0.08	0.58	1.60
1.94E-03	3.50E-03	2.0262	0.09	0.59	1.80
1.91E-03	3.82E-03	2.0316	0.10	0.60	2.00
1.85E-03	4.43E-03	2.0316	0.12	0.62	2.40
1.79E-03	5.01E-03	2.0362	0.14	0.64	2.80
1.74E-03	5.55E-03	2.0379	0.16	0.66	3.20
1.68E-03	6.07E-03	2.0382	0.18	0.68	3.60
1.64E-03	6.55E-03	2.0395	0.20	0.70	4.00
1.53E-03	7.64E-03	2.0403	0.25	0.75	5.00
1.43E-03	8.59E-03	2.0456	0.30	0.80	6.00
1.27E-03	1.02E-02	2.0487	0.40	0.90	8.00
1.15E-03	1.15E-02	2.0530	0.50	1.00	10.00
9.55E-04	1.34E-02	2.0566	0.70	1.20	14.00
8.18E-04	1.47E-02	2.0593	0.90	1.40	18.00

Table 30: $ZnTPPBr_8$-Pyridine titration.

$[ZnTPPBr_8]$ (M)	[Pyr] (M)	CH21	CH22	CH1	addition (mL)	tot. Vol (mL)	G/H
5.12E-03	0.00E+00	-	-	-	0.00	0.50	0.00
3.05E-03	4.49E-04	6.6592	5.8735	3.2899	0.01	0.51	0.15
2.99E-03	8.81E-04	6.6592	5.8735	3.2907	0.02	0.52	0.30
2.93E-03	1.30E-03	6.6592	5.8735	3.2919	0.03	0.53	0.44
2.88E-03	1.70E-03	6.6592	5.8735	3.2928	0.04	0.54	0.59
2.82E-03	2.08E-03	6.6592	5.8735	3.2936	0.05	0.55	0.74
2.77E-03	2.45E-03	6.6592	5.8735	3.2936	0.06	0.56	0.89

2.73E-03	2.81E-03	6.6592	5.8735	3.2944	0.07	0.57	1.03
2.68E-03	3.16E-03	6.6592	5.8735	3.2953	0.08	0.58	1.18
2.63E-03	3.50E-03	6.6592	5.8735	3.2961	0.09	0.59	1.33
2.59E-03	3.82E-03	6.6599	5.8745	3.2981	0.10	0.60	1.48
2.51E-03	4.43E-03	6.6637	5.8813	3.3201	0.12	0.62	1.77
2.43E-03	5.01E-03	6.6808	5.9038	3.4065	0.14	0.64	2.07
2.35E-03	5.55E-03	6.7385	5.9827	3.6946	0.16	0.66	2.36
2.28E-03	6.07E-03	6.8231	6.0997	4.1328	0.18	0.68	2.66
2.22E-03	6.55E-03	6.9043	6.2109	4.5503	0.20	0.70	2.95
2.07E-03	7.64E-03	7.0645	6.4324	5.3639	0.25	0.75	3.69
1.94E-03	8.59E-03	7.1738	6.5839	5.9176	0.30	0.80	4.43
1.73E-03	1.02E-02	7.3040	6.7688	6.5773	0.40	0.90	5.90
1.55E-03	1.15E-02	7.4133	6.9370	6.9408	0.50	1.00	7.38
1.29E-03	1.34E-02	7.5014	7.0755	-	0.70	1.20	10.33
1.11E-03	1.47E-02	7.5526	7.1711	-	0.90	1.40	13.28

3: Experimental binding constants and errors

Table 31: Binding constants, calculated from the titration data. Standard errors in brackets.

	K_a (M^{-1}), standard error in brackets							
Porphyrin	**Methanol**		**Acetic acid**		**Acetone**		**Pyridine**	
Al(TPP)Cl	$3.8x10^{-3}$	$(2.2x10^{-2})$[a]	$2.8x10^{1}$	$(2.6x10^{-4})$	nb	-	nb	-
Co(TPP)Cl	$3.2x10^{-3}$	$(1.5x10^{-4})$	$1.7x10^{2}$	$(4.9x10^{-3})$	nb	-	cc	-
Co(TPFPP)Cl	$5.4x10^{1}$	$(8.9x10^{-3})$	$1.8x10^{4}$	$(3.6x10^{-4})$	nb	-	cc	-
Fe(TPP)	nb	-	nb	-	nb	-	nb	-
Mg(TPP)	$5.7x10^{1}$	$(3.0x10^{-2})$	D	-	7.4	$(1.4x10^{-3})$	$1.7x10^{1}$	(0.2)
Mg(TPFPP)	$1.5x10^{2}$	$(8.6x10^{-2})$	$2.3x10^{3}$	$(8.0x10^{-2})$	$3.1x10^{2}$	$(2.9x10^{-2})$	$1.3x10^{4}$	$(1.9x10^{-2})$
Mg(TPP)Br_8	$1.6x10^{2}$	$(4.6x10^{-2})$	$8.2x10^{2}$	$(1.0x10^{-1})$	$3.8x10^{2}$	$(2.2x10^{-2})$	1.3	$(9.3x10^{-2})$
Mn(TPP)	nb	-	nb	-	nb	-	nb	-
Ni(TPP)	nb	-	nb	-	nb	-	nb	-
Sn(TPP)OH_2	nb	-	nm	-	nm	-	$1.3x10^{4}$	$(6.6x10^{-3})$
O=Ti(TPP)	nb	-	$4.8x10^{2}$	$(8.1x10^{-4})$	nb	-	nb	-
Zn(TPP)	$2.4x10^{-3}$	$(3.8x10^{-3})$[a]	$3.6x10^{2}$	$(1.0x10^{-3})$	nb	-	$6.8x10^{3}$	(0.2)[b]
Zn(TPFPP)	$1.5x10^{1}$	$(1.0x10^{-2})$	$1.2x10^{3}$	$(1.1x10^{-3})$	$1.1x10^{-2}$	$(1.4x10^{-3})$	$2.7x10^{4}$	(0.5)[b]
Zn(TPP)Br_8	$2.0x10^{1}$	$(1.1x10^{-2})$	$2.5x10^{2}$	$(3.1x10^{-3})$	$6.0x10^{-3}$	$(1.4x10^{-3})$	$3.2x10^{2}$	$(6.0x10^{-2})$[b]

nb = no binding; nm = not measured; nc = cannot calculate, binding to weak; cc = cannot calculate, binding to strong; D = demetallation; [a] Very broad signals; [b] Binding 1:2.

Design of oxophilic metalloporphyrins: An experimental and DFT study of methanol binding
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4: DFT, Optimized geometries

The geometries and spin states for the structures used in the study are presented here, the rest can be sent upon request.

4.1: Free porphyrins

AlPCl (Singlet)

Al	-0.00051300	0.00053800	0.22010900
C	1.11061300	2.82830800	-0.25890000
N	0.00993700	1.99589100	-0.22187300
C	-1.08262100	2.83898600	-0.25891000
C	-0.65989400	4.21225200	-0.32148800
C	0.70130000	4.20562800	-0.32149500
N	-1.99603500	0.00966600	-0.22137300
C	-2.82839300	1.11043600	-0.25792600
C	-4.20580000	0.70119600	-0.31942200
C	-4.21249300	-0.65999800	-0.31946800
C	-2.83920000	-1.08278300	-0.25791000
C	-2.40772100	2.43143100	-0.25989900
C	-2.43145600	-2.40784200	-0.25975600
C	-1.11037500	-2.82828700	-0.25869600
N	-0.00965800	-1.99600900	-0.22173300
C	1.08273100	-2.83909500	-0.25883700
C	0.65997800	-4.21244800	-0.32139000
C	-0.70117700	-4.20575300	-0.32127200
C	2.40787400	-2.43158000	-0.25987600
C	2.82850600	-1.11054100	-0.25784500
N	1.99615300	-0.00993700	-0.22122600
C	2.83918600	1.08255500	-0.25768600
C	4.21262100	0.65988000	-0.31923400
C	4.20599700	-0.70127700	-0.31930500
C	2.43164200	2.40766600	-0.25974500
H	-1.38024100	-5.04664200	-0.36591700
H	1.33075500	-5.05995700	-0.36615000
H	5.04694100	-1.38030300	-0.36346400
H	5.06014200	1.33068900	-0.36330000
H	-5.04677100	1.38019200	-0.36354300
H	-5.06008100	-1.33071200	-0.36363100
H	1.38026800	5.04658800	-0.36623800
H	-1.33064100	5.05978600	-0.36620800
H	3.20220700	3.17063700	-0.28717600
H	-3.17070200	3.20198600	-0.28730800
H	-3.20187100	-3.17096600	-0.28718800
H	3.17085400	-3.20213200	-0.28743600
Cl	-0.00028700	0.00024500	2.43670100

$CoPBr_8Cl$ (Quintet)

Co	-0.00001100	-0.00001000	0.46133700
C	2.81583300	-1.19870500	-0.07576100
N	2.03594100	-0.06881600	-0.05689100
C	2.89033300	1.00589500	-0.07560900
C	4.25829500	0.53670600	-0.11083200
C	4.21233900	-0.82311300	-0.11114700
N	0.06882200	2.03593700	-0.05690400
C	1.19871000	2.81583000	-0.07575300
C	0.82311800	4.21233500	-0.11117300
C	-0.53670100	4.25829100	-0.11089100
C	-1.00589000	2.89032800	-0.07566000
C	2.50561100	2.34184300	-0.07755200
C	-2.34183900	2.50560900	-0.07761900
C	-2.81583000	1.19871000	-0.07580700
N	-2.03593700	0.06882100	-0.05694500
C	-2.89032800	-1.00589100	-0.07570500
C	-4.25829000	-0.53670200	-0.11094900
C	-4.21233500	0.82311700	-0.11123500
C	-2.50560600	-2.34183800	-0.07766800
C	-1.19870600	-2.81582700	-0.07584700
N	-0.06881600	-2.03593400	-0.05695500
C	1.00589600	-2.89032600	-0.07570100
C	0.53670700	-4.25828700	-0.11097300
C	-0.82311300	-4.21233100	-0.11128600
C	2.34184400	-2.50560500	-0.07761600
H	3.08169000	-3.29724400	-0.09266900
H	3.29724900	3.08169000	-0.09258700
H	-3.08168300	3.29724900	-0.09267300
H	-3.29724400	-3.08168500	-0.09273600
Cl	-0.00005400	-0.00004700	2.67725000
Br	2.03753300	5.68525500	-0.16205400
Br	-1.64886600	5.80990600	-0.16056500
Br	-5.68525300	2.03753300	-0.16213300
Br	-5.80990500	-1.64886700	-0.16062800
Br	-2.03752600	-5.68524900	-0.16222600
Br	1.64887200	-5.80990100	-0.16065200
Br	5.68525900	-2.03752700	-0.16203500
Br	5.80991200	1.64887200	-0.16045400

$CoPCl_8Cl$ (Quintet)

Co	-0.00001000	-0.00000900	0.39100400
C	2.83369300	-1.14660300	-0.14654700
N	2.03328100	-0.03186600	-0.12686400
C	2.86826200	1.05727500	-0.14646200
C	4.24592400	0.61598800	-0.18285000
C	4.22442400	-0.74883000	-0.18306500
N	0.03187400	2.03327500	-0.12688100
C	1.14661100	2.83368900	-0.14654800
C	0.74883700	4.22441800	-0.18312300
C	-0.61598000	4.24591800	-0.18292600
C	-1.05726800	2.86825600	-0.14652600
C	2.46284800	2.38685800	-0.14902600
C	-2.38685200	2.46284600	-0.14909400
C	-2.83368800	1.14661100	-0.14659400
N	-2.03327500	0.03187300	-0.12691900
C	-2.86825600	-1.05726800	-0.14656200
C	-4.24591600	-0.61598000	-0.18296400
C	-4.22441700	0.74883700	-0.18315900
C	-2.46284100	-2.38685100	-0.14914600
C	-1.14660400	-2.83368300	-0.14664600
N	-0.03186600	-2.03327000	-0.12693400
C	1.05727600	-2.86825100	-0.14656900
C	0.61598800	-4.24591100	-0.18301400
C	-0.74883000	-4.22441100	-0.18323500
C	2.38686000	-2.46283900	-0.14909100
H	3.14117200	-3.24160500	-0.16592600
H	3.24161300	3.14117200	-0.16584500
H	-3.14116200	3.24161400	-0.16593000
H	-3.24160500	-3.14116400	-0.16599700
Cl	-0.00005200	-0.00004700	2.60873100
Cl	1.81835900	5.56971800	-0.23038700
Cl	-1.64248300	5.62436200	-0.22972600
Cl	-5.56971600	1.81835900	-0.23042000
Cl	-5.62436100	-1.64248400	-0.22976100
Cl	-1.81835000	-5.56971000	-0.23054800
Cl	1.64249200	-5.62435500	-0.22982100
Cl	5.56972500	-1.81835100	-0.23031300
Cl	5.62436900	1.64249200	-0.22959800

$CoPF_8Cl$ (Quintet)

Co	0.00000800	0.00000800	0.33033800
C	-2.82834900	1.14145600	-0.20419800
N	-2.02209600	0.02785600	-0.18498300
C	-2.85904000	-1.06296500	-0.20418400
C	-4.22920700	-0.62132000	-0.23950100
C	-4.21023300	0.73818800	-0.23943900
N	-0.02786500	-2.02208800	-0.18500300
C	-1.14146500	-2.82834200	-0.20420700
C	-0.73819700	-4.21022500	-0.23950700
C	0.62131100	-4.22919800	-0.23960400
C	1.06295600	-2.85903200	-0.20425700
C	-2.46121000	-2.39413800	-0.20795200
C	2.39413100	-2.46120800	-0.20802300
C	2.82834200	-1.14146500	-0.20424500
N	2.02208900	-0.02786400	-0.18503900
C	2.85903200	1.06295700	-0.20428500
C	4.22919800	0.62131200	-0.23962300
C	4.21022500	-0.73819700	-0.23953200
C	2.46120100	2.39413000	-0.20807500
C	1.14145600	2.82833500	-0.20430600
N	0.02785600	2.02208200	-0.18505600
C	-1.06296600	2.85902600	-0.20430000
C	-0.62132000	4.22919000	-0.23969000
C	0.73818800	4.21021700	-0.23962500
C	-2.39414000	2.46119900	-0.20802000
H	-3.15070300	3.23869000	-0.22636600
H	-3.23869800	-3.15070400	-0.22627800
H	3.15069200	-3.23870000	-0.22637100
H	3.23868900	3.15069600	-0.22643600
Cl	0.00004600	0.00004200	2.54907000
F	-5.23651500	1.58683200	-0.27577400
F	-5.27886200	-1.44083900	-0.27597800
F	-1.58684200	-5.23650600	-0.27585100
F	1.44082900	-5.27885200	-0.27613300
F	5.23650700	-1.58684100	-0.27587300
F	5.27885300	1.44082900	-0.27614300
F	1.58683100	5.23649700	-0.27601000
F	-1.44083900	5.27884400	-0.27622200

CoPCl (Quintet)

Co	0.00000300	0.00000500	0.25186000
C	1.02903600	2.88013500	-0.29437900
N	-0.04774000	2.02789600	-0.27184200
C	-1.16339100	2.82841600	-0.29440000
C	-0.78096500	4.22016000	-0.33488300
C	0.58126100	4.25239200	-0.33470700
N	-2.02788900	-0.04779300	-0.27184900
C	-2.88012000	1.02898800	-0.29439200
C	-4.25238000	0.58122100	-0.33476500
C	-4.22016200	-0.78100600	-0.33475100
C	-2.82841700	-1.16343800	-0.29436500
C	-2.47684300	2.36298200	-0.29844300
C	-2.36297600	-2.47689000	-0.29838900
C	-1.02897700	-2.88015900	-0.29434600

N	0.04780500	-2.02793300	-0.27178600
C	1.16344800	-2.82845800	-0.29432900
C	0.78101500	-4.22020500	-0.33473600
C	-0.58121200	-4.25242100	-0.33474300
C	2.47690400	-2.36302400	-0.29834800
C	2.88017900	-1.02902500	-0.29430700
N	2.02794300	0.04774900	-0.27177300
C	2.82846000	1.16340000	-0.29430800
C	4.22021000	0.78097500	-0.33470500
C	4.25243900	-0.58125100	-0.33464200
C	2.36303000	2.47685600	-0.29837400
H	-1.23205000	-5.11640300	-0.36409400
H	1.47208200	-5.05239000	-0.36394500
H	5.11642600	-1.23208300	-0.36394300
H	5.05239100	1.47204800	-0.36392000
H	-5.11636300	1.23205600	-0.36410200
H	-5.05234800	-1.47207300	-0.36394100
H	1.23209200	5.11638100	-0.36398500
H	-1.47203600	5.05234000	-0.36416500
H	3.11254500	3.26256100	-0.31806900
H	-3.26255200	3.11249200	-0.31818300
H	-3.11247900	-3.26260600	-0.31809900
H	3.26261500	-3.11253300	-0.31804900
Cl	-0.00026400	0.00016300	2.49134800

CoP(Doublet)

Co	0.00000000	0.00000000	0.00012000
N	1.41010800	1.40891100	0.00001500
N	-1.41010700	1.40891200	0.00005600
N	1.41010700	-1.40891200	0.00004800
N	-1.41010800	-1.40891100	0.00000800
C	2.77586700	1.22701000	-0.00002800
C	3.45816700	2.49662500	-0.00017800
C	2.49626900	3.45788300	-0.00017700
C	1.22716800	2.77466100	-0.00014100
H	4.53365100	2.61543700	-0.00023500
H	2.61439200	4.53350600	-0.00024700
C	0.00000100	3.41805600	-0.00012800
C	3.41979000	-0.00000100	0.00006000
C	-2.49626700	3.45788400	0.00003100
C	-3.45816600	2.49662700	0.00017600
C	-2.77586600	1.22701100	0.00009700
C	-1.22716600	2.77466200	-0.00000600
H	-2.61439000	4.53350700	-0.00001000
H	-4.53365000	2.61544000	0.00026100
C	-3.41979000	0.00000100	0.00006000
C	1.22716600	-2.77466200	-0.00001500
C	2.49626700	-3.45788400	0.00003300
C	3.45816600	-2.49662700	0.00019400
C	2.77586600	-1.22701100	0.00009900
H	2.61439000	-4.53350700	-0.00000600
H	4.53365000	-2.61544000	0.00029400
C	-3.45816700	-2.49662500	-0.00015900
C	-2.49626900	-3.45788300	-0.00017500
C	-1.22716800	-2.77466100	-0.00015100
C	-2.77586700	-1.22701000	-0.00002800
H	-4.53365100	-2.61543800	-0.00019900
H	-2.61439200	-4.53350600	-0.00024400
C	-0.00000100	-3.41805600	-0.00014300
H	-4.50491200	0.00000200	0.00007600
H	-0.00000100	-4.50322100	-0.00021700
H	4.50491200	-0.00000200	0.00007600
H	0.00000200	4.50322100	-0.00020200

CoTPFPPCl(Quintet)

Co	0.00000700	-0.00000600	-0.41351100
C	2.76648900	-1.30565500	0.11365400
N	1.40053100	-1.46516100	0.09810400
C	1.18022400	-2.82261800	0.11151200
C	2.43721400	-3.53219500	0.13901400
C	3.41886000	-2.59327800	0.14683900
N	-1.46516500	-1.40053100	0.09805300
C	-1.30566000	-2.76648900	0.11360200
C	-2.59328300	-3.41886000	0.14674400
C	-3.53220000	-2.43721400	0.13889200
C	-2.82262200	-1.18022400	0.11141700
C	-0.07740500	-3.44170300	0.11186700
C	-3.44170600	0.07740500	0.11175500
C	-2.76649300	1.30565900	0.11351700
N	-1.40053500	1.46516400	0.09801300
C	-1.18022900	2.82262100	0.11139000
C	-2.43722000	3.53219900	0.13882700
C	-3.41886600	2.59328200	0.14664200
C	0.07740000	3.44170600	0.11177300
C	1.30565500	2.76649300	0.11357100
N	1.46516000	1.40053500	0.09806600
C	2.82261800	1.18022800	0.11148600
C	3.53219400	2.43721900	0.13895200
C	2.59327600	3.41886500	0.14674200
C	3.44170200	-0.07740100	0.11188300
H	-4.48580200	2.75548500	0.18014700
H	-2.55169200	4.60571700	0.15129300
H	2.75547900	4.48580200	0.18025800
H	4.60571200	2.55169200	0.15145500
H	-2.75548700	-4.48579600	0.18028300
H	-4.60571800	-2.55168600	0.15135800
H	4.48579600	-2.75548000	0.18038800
H	2.55168600	-4.60571300	0.15151500
Cl	0.00004700	-0.00003500	-2.63151400
C	4.93693000	-0.11214300	0.11432600
C	5.65595900	-0.47365000	-1.02985400
C	5.67308500	0.21440100	1.25765900
C	7.04871500	-0.51100700	-1.04102200
C	7.06574600	0.18720700	1.26868800
C	7.75422300	-0.17838900	0.11365700
C	0.11214300	4.93693400	0.11416600
C	0.47365500	5.65592300	-1.03003700
C	-0.21440700	5.67312700	1.25747300
C	0.51101300	7.04867900	-1.04125100
C	-0.18721300	7.06578800	1.26845500
C	0.17838800	7.75422600	0.11340200
C	-0.11214800	-4.93693100	0.11430100
C	-0.47361900	-5.65595300	-1.02989400
C	0.21436100	-5.67309200	1.25764100
C	-0.51097500	-7.04871000	-1.04107000
C	0.18716800	-7.06575200	1.26866100
C	-0.17839100	-7.75422400	0.11361500
C	-4.93693400	0.11214800	0.11413900
C	-5.65591700	0.47362100	-1.03008000
C	-5.67313400	-0.21436400	1.25745200
C	-7.04867300	0.51097700	-1.04130500
C	-7.06579500	-0.18717100	1.26842500
C	-7.75422700	0.17839100	0.11335600
F	0.79644900	5.00501000	-2.15339100
F	0.85880500	7.70979800	-2.14907700
F	0.20916900	9.08782000	0.11291900
F	-0.50415700	7.74282300	2.37647300
F	-0.56914800	5.03788600	2.38211400
F	-5.00499700	0.79637700	-2.15344100
F	-7.70978500	0.85873200	-2.14914600
F	-9.08782000	0.20917000	0.11286300
F	-7.74283700	-0.50407800	2.37645000
F	-5.03790000	-0.56906600	2.38210900
F	-0.79637200	-5.00507300	-2.15327900
F	-0.85872800	-7.70986000	-2.14889000
F	-0.20917100	-9.08781700	0.11316900
F	0.50407300	-7.74275600	2.37671100
F	0.56906200	-5.03781800	2.38227700
F	5.03780600	0.56913700	2.38228100
F	7.74274300	0.50414600	2.37673200
F	9.08781600	-0.20916900	0.11321900
F	7.70987200	-0.85879500	-2.14882700
F	5.00508400	-0.79643800	-2.15323200

CoTPPBr$_8$Cl(Quintet)

Co	-0.00001800	0.00000000	0.51539200
C	1.11352300	2.68382500	-0.55607900
N	0.00040000	1.97455500	-0.17350400
C	-1.11242300	2.68430200	-0.55605700
C	-0.68326400	3.79782800	-1.37615600
C	0.68482900	3.79755100	-1.37614500
N	-2.05463900	0.00043700	0.01986100
C	-2.76967200	1.11150100	0.38920800
C	-3.91253000	0.68576600	1.17086900
C	-3.91283800	-0.68411700	1.17083500
C	-2.77014700	-1.11032600	0.38918900
C	-2.41738900	2.39852600	-0.07762200
C	-2.41841000	-2.39749300	-0.07766000
C	-1.11356200	-2.68382200	-0.55607400
N	-0.00043900	-1.97455700	-0.17349900
C	1.11238300	-2.68430700	-0.55605200
C	0.68322000	-3.79783700	-1.37614500
C	-0.68487400	-3.79754600	-1.37614300
C	2.41734900	-2.39852700	-0.07761700
C	2.76963400	-1.11149900	0.38919400
N	2.05459800	-0.00043800	0.01984500
C	2.77010700	1.11032400	0.38917200
C	3.91284200	0.68412000	1.17075100
C	3.91253100	-0.68576300	1.17079500
C	2.41836800	2.39749200	-0.07766000
Cl	-0.00001400	0.00000400	2.75873800
C	3.43542900	3.47781300	-0.07198700
C	3.19627900	4.67229900	0.62603700
C	4.64760400	3.31982600	-0.76259000
C	4.15565100	5.68206000	0.64276400
H	2.26477000	4.79594200	1.16980700
C	5.59379900	4.34142200	-0.76727000
H	4.83478600	2.40104100	-1.30997900
C	5.35310100	5.52222300	-0.05935600
H	3.96750000	6.59516000	1.19949800
H	6.52091000	4.21526200	-1.31837600
H	6.09608300	6.31439500	-0.05479500
C	3.43393900	-3.47928900	-0.07189200
C	3.19434100	-4.67357100	0.62632700
C	4.64611500	-3.32192800	-0.76263700
C	4.15327500	-5.68374700	0.64310400
H	2.26283600	-4.79673000	1.17021400
C	5.59185900	-4.34394200	-0.76727600
H	4.83364400	-2.40330400	-1.31017600
C	5.35071900	-5.52453600	-0.05916800
H	3.96478400	-6.59668400	1.19999000
H	6.51896800	-4.21826500	-1.31849600
H	6.09335500	-6.31703200	-0.05457100
C	-3.43397500	3.47929300	-0.07195000
C	-3.19442400	4.67355800	0.62631500
C	-4.64608000	3.32197500	-0.76283000

C	-4.15334400	5.68374800	0.64302300
H	-2.26296900	4.79669000	1.17029300
C	-5.59180600	4.34400400	-0.76753900
H	-4.83356600	2.40337200	-1.31041900
C	-5.35072000	5.52457400	-0.05937200
H	-3.96489200	6.59666900	1.19994900
H	-6.51886000	4.21835900	-1.31885900
H	-6.09334400	6.31708300	-0.05483100
C	-3.43546600	-3.47781900	-0.07204900
C	-3.19637700	-4.67227900	0.62603700
C	-4.64755300	-3.31988600	-0.76282000
C	-4.15573200	-5.68205800	0.64268300
H	-2.26493100	-4.79588800	1.16992300
C	-5.59372600	-4.34150200	-0.76758500
H	-4.83468000	-2.40113000	-1.31027500
C	-5.35309700	-5.52226900	-0.05959200
H	-3.96763200	-6.59513500	1.19947100
H	-6.52076800	-4.21538200	-1.31881700
H	-6.09606400	-6.31445700	-0.05509800
Br	5.08865900	1.76149700	2.23295300
Br	5.08784100	-1.76360000	2.23309300
Br	1.76026400	-4.91913000	-2.49882400
Br	-1.76241400	-4.91840300	-2.49877900
Br	-5.08853700	-1.76146100	2.23320100
Br	-5.08773100	1.76358100	2.23331100
Br	-1.76031500	4.91911300	-2.49883600
Br	1.76236000	4.91841000	-2.49878700

CoTPPCl(Quintet)

Co	0.00370900	-0.00001000	0.38304100
C	1.09834700	2.85978500	-0.15544200
N	-0.00068300	2.03192100	-0.14526500
C	-1.09876600	2.86041200	-0.16875400
C	-0.67963900	4.24205400	-0.19306100
C	0.68028000	4.24131100	-0.19661400
N	-2.03156200	-0.00039400	-0.11788900
C	-2.85814900	1.09796100	-0.17114900
C	-4.23616300	0.67910800	-0.27702000
C	-4.23591800	-0.68069900	-0.27719700
C	-2.85774800	-1.09907500	-0.17114200
C	-2.44043800	2.44044100	-0.17503200
C	-2.43952100	-2.44138200	-0.17499000
C	-1.09762400	-2.86081500	-0.16870700
N	0.00012800	-2.03189300	-0.14526800
C	1.09950400	-2.85932300	-0.15556400
C	0.68194500	-4.24099500	-0.19682700
C	-0.67796800	-4.24228700	-0.19248300
C	2.44159800	-2.44007700	-0.14995300
C	2.86049600	-1.09786700	-0.15314100
N	2.03175000	0.00037500	-0.17358200
C	2.86001100	1.09900500	-0.15304800
C	4.24143900	0.68084900	-0.11093100
C	4.24174400	-0.67915100	-0.11062900
C	2.44059300	2.44101300	-0.14976100
H	-1.33955800	-5.09497600	-0.20859800
H	1.34489200	-5.09228400	-0.22712300
H	5.09327800	-1.34136400	-0.07185000
H	5.09270800	1.34340300	-0.07231900
H	-5.08412300	1.34177400	-0.36091400
H	-5.08370200	-1.34357600	-0.36114500
H	1.34302200	5.09276400	-0.22683300
H	-1.34158600	5.09445700	-0.20955700
Cl	0.03409800	-0.00008600	2.64130100
C	3.49849000	3.50062000	-0.13847400
C	3.69589900	4.29868800	0.99926100
C	4.31039100	3.71443100	-1.26319800
C	4.68357200	5.28438400	1.01151800
H	3.07702500	4.13536100	1.87652300
C	5.29372700	4.70454000	-1.25143500
H	4.16144600	3.10527900	-2.14995400
C	5.48389200	5.49123900	-0.11378000
H	4.82857800	5.88866100	1.90244500
H	5.90933700	4.86185400	-2.13253900
H	6.25097300	6.26017300	-0.10408200
C	3.49997000	-3.49913100	-0.13879200
C	4.31206400	-3.71228900	-1.26350100
C	3.69795200	-4.29723600	0.99886000
C	5.29601200	-4.70179300	-1.25188100
H	4.16276700	-3.10310700	-2.15017500
C	4.68621900	-5.28230700	1.01097900
H	3.07907900	-4.13434300	1.87620400
C	5.48668100	-5.48852800	-0.11435700
H	5.91174000	-4.85854900	-2.13300400
H	4.83160800	-5.88660300	1.90182900
H	6.25427100	-6.25695400	-0.10476300
C	-3.50287900	3.49529600	-0.20027700
C	-4.31979500	3.70746600	0.92124500
C	-3.70404200	4.28614900	-1.34223800
C	-5.31017700	4.69034300	0.90188100
H	-4.16779800	3.10340700	1.81081600
C	-4.69874400	5.26469200	-1.36210500
H	-3.08172200	4.12445200	-2.21751700
C	-5.50333300	5.47060700	-0.23974500
H	-5.92910400	4.84698100	1.78070900
H	-4.84593300	5.86399800	-2.25609500
H	-6.27591300	6.23392400	-0.25484200
C	-3.50139600	-3.49673400	-0.20013500
C	-3.70231600	-4.28767900	-1.34207900
C	-4.31796100	-3.70958400	0.92155900
C	-4.69644400	-5.26680600	-1.36184300
H	-3.08028100	-4.12555600	-2.21747900
C	-5.30773400	-4.69304700	0.90231200
H	-4.16607900	-3.10562000	1.81121400
C	-5.50067600	-5.47332700	-0.23935900
H	-4.84340400	-5.86613600	-2.25585500
H	-5.92637000	-4.85015400	1.78126000
H	-6.27275700	-6.23715000	-0.25436200

FePCl(Sextet)

Fe	-0.00002100	-0.00054300	0.25218900
C	2.75772000	-1.33295400	-0.29024100
N	1.39033200	-1.48498000	-0.25857900
C	1.14869400	-2.83942100	-0.29024600
C	2.39785000	-3.55862400	-0.34152100
C	3.39323600	-2.62667800	-0.34147500
N	-1.48518400	-1.39012000	-0.25857300
C	-1.33310000	-2.75751700	-0.29023200
C	-2.62681500	-3.39307200	-0.34144100
C	-3.55878400	-2.39770800	-0.34154100
C	-2.83962000	-1.14854100	-0.29024100
C	-0.11299500	-3.42913500	-0.29422800
C	-3.42927400	0.11316600	-0.29412800
C	-2.75756100	1.33322000	-0.29001900
N	-1.39024100	1.48530200	-0.25826200
C	-1.14866400	2.83966100	-0.29001300
C	-2.39785700	3.55891300	-0.34138800
C	-3.39319800	2.62696800	-0.34130300
C	0.11299800	3.42941300	-0.29400700
C	1.33307400	2.75776100	-0.29001300
N	1.48510200	1.39045000	-0.25826700
C	2.83946400	1.14881700	-0.29003700
C	3.55875300	2.39800100	-0.34138500
C	2.62683000	3.39336200	-0.34133500
C	3.42927800	-0.11282700	-0.29413600
H	-4.46248800	2.78824300	-0.37983000
H	-2.48855500	4.63648700	-0.37995600
H	2.78812300	4.46264800	-0.37988900
H	4.63633000	2.48867900	-0.37993000
H	-2.78813600	-4.46235700	-0.37991900
H	-4.63635600	-2.48845500	-0.38007400
H	4.46251700	-2.78802000	-0.37998800
H	2.48857600	-4.63619800	-0.38001900
H	4.51386200	-0.14857200	-0.31980900
H	-0.14882100	-4.51371700	-0.31983400
H	-4.51385300	0.14907100	-0.31980200
H	0.14882200	4.51399400	-0.31973600
Cl	0.00001700	-0.00053400	2.49242600

FeP(Triplet)

Fe	0.00000000	0.00000000	0.00012700
N	1.41849900	1.41853100	0.00005800
N	-1.41850700	1.41852300	0.00003200
N	1.41850700	-1.41852300	0.00001100
N	-1.41849900	-1.41853100	0.00003800
C	2.78513400	1.23205000	0.00001700
C	3.46635600	2.50202500	-0.00004900
C	2.50298700	3.46390700	-0.00007900
C	1.23201400	2.78310400	-0.00006000
H	4.54151400	2.62404200	-0.00007700
H	2.62463100	4.53925200	-0.00011700
C	-0.00001000	3.42317700	-0.00006400
C	3.42439700	0.00001000	0.00000200
C	-2.50300900	3.46389300	-0.00001900
C	-3.46637100	2.50200400	-0.00003100
C	-2.78514000	1.23203300	-0.00002000
C	-1.23203100	2.78309800	-0.00001400
H	-2.62466000	4.53923600	-0.00004200
H	-4.54153000	2.62401300	-0.00004100
C	-3.42439700	-0.00001000	0.00000200
C	1.23203100	-2.78309800	-0.00003400
C	2.50300800	-3.46389300	-0.00001400
C	3.46637100	-2.50200400	0.00001300
C	2.78514000	-1.23203300	-0.00001400
H	2.62465900	-4.53923600	-0.00003700
H	4.54153000	-2.62401400	0.00003900
C	-3.46635600	-2.50202500	-0.00000300
C	-2.50298700	-3.46390700	-0.00007500
C	-1.23201400	-2.78310400	-0.00008300
C	-2.78513400	-1.23204900	0.00002300
H	-4.54151400	-2.62404200	0.00000700
H	-2.62463100	-4.53925200	-0.00011200
C	0.00001000	-3.42317700	-0.00010000
H	-4.50975700	-0.00001200	-0.00000900
H	0.00001200	-4.50853300	-0.00015200
H	4.50975700	0.00001200	-0.00001000
H	-0.00001200	4.50853300	-0.00011100

$MgPBr_8$(Singlet)

C	-1.82664600	-2.47415000	0.00013300
N	-0.54308400	-1.98313000	-0.00001800
C	0.31145200	-3.05944700	-0.00014500
C	-0.46588000	-4.28064500	-0.00009600
C	-1.77975600	-3.92102000	0.00014100
Mg	0.00002500	-0.00006400	0.00007800
N	1.98315800	-0.54295200	-0.00009400
C	2.47411700	-1.82655900	-0.00007200

C	3.92100100	-1.77972600	-0.00000500
C	4.28066800	-0.46585700	-0.00010700
C	3.05950200	0.31151600	-0.00009000
C	1.82661200	2.47416000	-0.00005300
N	0.54306000	1.98314500	-0.00008500
C	-0.31146700	3.05946800	-0.00006300
C	0.46587500	4.28066300	-0.00001600
C	1.77973200	3.92103600	-0.00002300
C	-2.47412100	1.82657900	-0.00018100
N	-1.98315300	0.54300400	-0.00006300
C	-3.05949700	-0.31148800	0.00005700
C	-4.28067500	0.46589500	0.00000600
C	-3.92100800	1.77974900	-0.00015700
Br	5.08025300	-3.30005800	0.00006800
Br	6.05255000	0.25255700	-0.00000200
Br	3.30009200	5.08025700	0.00015000
Br	-0.25264300	6.05250400	0.00009600
Br	-5.08024800	3.30009000	-0.00026600
Br	-6.05252500	-0.25258900	0.00012400
Br	-3.30007400	-5.08030800	0.00031300
Br	0.25261000	-6.05248800	-0.00028500
C	-1.70426500	2.98940100	-0.00022000
C	2.98944800	1.70432300	-0.00009300
C	1.70425700	-2.98936700	-0.00015200
C	-2.98946200	-1.70428700	0.00016800
H	-3.93068800	-2.24089500	0.00033700
H	2.24087800	-3.93058800	-0.00018100
H	3.93067100	2.24093000	-0.00011700
H	-2.24087900	3.93062500	-0.00027500

$MgPCl_8$(Singlet)

C	3.07628900	-0.18317500	-0.00025100
N	1.88217500	-0.85876000	-0.00011300
C	2.15437400	-2.20352700	-0.00012400
C	3.59143000	-2.39037100	-0.00027500
C	4.15912100	-1.14611200	-0.00036100
Mg	-0.00000100	-0.00001200	-0.00010600
N	-0.85890200	-1.88207100	0.00012200
C	-0.18322000	-3.07616200	0.00014700
C	-1.14607900	-4.15904200	0.00028900
C	-2.39038500	-3.59142700	0.00035200
C	-2.20364100	-2.15438800	0.00022800
C	-3.07625700	0.18317900	0.00009800
N	-1.88215100	0.85878700	0.00035200
C	-2.15438500	2.20355500	0.00000800
C	-3.59143900	2.39036700	-0.00031200
C	-4.15910400	1.14609500	-0.00027300
C	0.18321200	3.07616800	0.00036700
N	0.85888400	1.88207200	0.00004600
C	2.20363000	2.15437500	-0.00005500
C	2.39038000	3.59142600	0.00021900
C	1.14608900	4.15904800	0.00051000
Cl	-0.76510100	-5.83776400	0.00042300
Cl	-3.90764900	-4.40448500	0.00046200
Cl	-5.83783800	0.76516400	-0.00060300
Cl	-4.40439800	3.90766400	-0.00091900
Cl	0.76508000	5.83777300	0.00096000
Cl	3.90765300	4.40446700	0.00011700
Cl	5.83785000	-0.76515400	-0.00051900
Cl	4.40439100	-3.90768400	-0.00036000
C	3.22785800	1.20505800	-0.00021900
C	1.20501600	-3.22771200	0.00000400
C	-3.22785100	-1.20504800	0.00023100
C	-1.20501900	3.22773200	0.00033200
H	4.24369100	1.58440100	-0.00034800
H	1.58433300	-4.24355400	0.00003300
H	-4.24369100	-1.58437100	0.00027100
H	-1.58432300	4.24358000	0.00039900

$MgPF_8$(Singlet)

C	2.82198100	-1.22812400	0.00044500
N	2.05939600	-0.08495900	0.00077000
C	2.91342200	0.99143200	0.00062600
C	4.27143400	0.50565500	0.00066600
C	4.21546700	-0.85547900	0.00054200
Mg	-0.00000600	-0.00000100	0.00002100
N	0.08495200	2.05940100	0.00005300
C	1.22811600	2.82195300	0.00023000
C	0.85547700	4.21542200	0.00018700
C	-0.50564200	4.27140700	-0.00028800
C	-0.99145700	2.91343200	-0.00026000
C	-2.82198900	1.22812900	-0.00053200
N	-2.05940800	0.08496200	-0.00048000
C	-2.91342900	-0.99143700	-0.00067200
C	-4.27142700	-0.50566000	-0.00055000
C	-4.21546300	0.85547900	-0.00042800
C	-1.22812400	-2.82195900	-0.00047200
N	-0.08496900	-2.05939900	-0.00043200
C	0.99145000	-2.91342100	-0.00006300
C	0.50564500	-4.27140000	0.00027800
C	-0.85547500	-4.21542700	-0.00016900
F	-5.22839200	1.72391000	-0.00012000
F	-5.35205300	-1.28828400	-0.00040900
F	-1.72394100	-5.22832000	-0.00015500
F	1.28828300	-5.35200700	0.00081600
F	1.72395100	5.22830900	0.00041400
F	-1.28827400	5.35201800	-0.00063900
F	5.22840600	-1.72389800	0.00026900
F	5.35207000	1.28826500	0.00057400
C	-2.53754100	-2.33632700	-0.00078400
C	2.33633800	-2.53754300	0.00025200
C	2.53753300	2.33632200	0.00057200
C	-2.33634600	2.53755100	-0.00054400
H	-3.33604700	-3.07115600	-0.00082800
H	3.07116300	-3.33605200	0.00032100
H	3.33603600	3.07115200	0.00058100
H	-3.07117200	3.33606100	-0.00067300

MgP(Singlet)

Mg	0.00000000	0.00000000	0.00002000
N	-1.68168700	1.19737300	0.00004000
N	-1.19737400	-1.68168600	-0.00003300
N	1.19737400	1.68168600	-0.00002500
N	1.68168800	-1.19737200	0.00005000
C	-1.70447200	2.56985500	0.00001300
C	-3.07694100	3.02866800	0.00000700
C	-3.86869200	1.91667200	0.00004200
C	-2.98608400	0.76985700	-0.00000200
H	-3.38618600	4.06595100	0.00003100
H	-4.95006300	1.86952000	0.00002800
C	-3.39197300	-0.57059500	0.00000200
C	-0.57059500	3.39197200	-0.00002100
C	-3.02866800	-3.07694100	-0.00000400
C	-1.91667200	-3.86869200	-0.00007200
C	-0.76985700	-2.98608400	-0.00004000
C	-2.56985500	-1.70447200	0.00000200
H	-4.06595100	-3.38618600	0.00005100
H	-1.86951700	-4.95006300	-0.00014400
C	0.57059500	-3.39197100	-0.00002300
C	2.56985400	1.70447200	-0.00000400
C	3.02866800	3.07694000	-0.00007200
C	1.91667200	3.86869200	0.00004300
C	0.76985700	2.98608400	-0.00004000
H	4.06595100	3.38618600	-0.00007700
H	1.86951900	4.95006300	0.00005900
C	3.07694100	-3.02866800	0.00011700
C	3.86869200	-1.91667200	-0.00001700
C	2.98608500	-0.76985700	-0.00000900
C	1.70447200	-2.56985400	0.00001200
H	3.38618400	-4.06595200	0.00022600
H	4.95006400	-1.86952000	-0.00008300
C	3.39197300	0.57059500	-0.00002000
H	0.75078900	-4.46317700	-0.00001700
H	4.46317800	0.75079000	-0.00003800
H	-0.75078900	4.46317700	-0.00001400
H	-4.46317800	-0.75078900	0.00001200

MgTPFPP(Singlet)

N	-0.08726400	2.06073900	0.16222700
N	-2.08937500	0.08243600	-0.60949100
N	2.00951800	0.04972700	-0.12009000
N	0.00739600	-1.92853800	-0.89166500
C	0.99400300	2.84905600	0.47162000
C	0.54844100	4.20295100	0.72038400
C	-0.80301200	4.21329400	0.56082300
C	-1.19879600	2.86615300	0.21098400
C	-2.52042700	2.45431500	-0.05437300
C	2.33403100	2.41581400	0.52463600
C	-4.28942200	0.75781500	-0.70069500
C	-4.25862300	-0.55882300	-1.04312500
C	-2.87594100	-0.98054300	-0.98070400
C	-2.92481400	1.15836800	-0.43323100
C	-2.41388400	-2.28355500	-1.25436800
C	2.84496100	-1.02626700	-0.29581400
C	4.20951000	-0.62569700	-0.02813600
C	4.17862700	0.69089600	0.31444800
C	2.79599900	1.11274600	0.25128000
C	-0.62823500	-4.07059700	-1.45046500
C	0.72318500	-4.08099000	-1.29071100
C	1.11892600	-2.73388900	-0.94046900
C	-1.07381100	-2.71670400	-1.20142500
C	2.44054900	-2.32218700	-0.67481000
C	-3.59189100	3.49073200	0.07332700
C	-4.00240000	3.96667100	1.32313700
C	-4.22796700	4.02687000	-1.05138700
C	-4.99714000	4.93306200	1.45486900
C	-5.22867600	4.99001900	-0.94486200
C	-5.61308900	5.44460100	0.31476900
C	3.36138400	3.43596500	0.90216400
C	4.23991400	3.97333000	-0.04444400
C	3.48350200	3.89664200	2.21730300
C	5.19996500	4.92385500	0.29506200
C	4.43255900	4.84963400	2.58027700
C	5.29408900	5.36384900	1.61364000
C	3.51203100	-3.35862400	-0.80230800
C	3.92297100	-3.83444800	-2.05203400
C	4.14777000	-3.89479000	0.32256900
C	4.91777700	-4.80080700	-2.18350200
C	5.14854500	-4.85790600	0.21630400
C	5.53335800	-5.31240600	-1.04322400
C	-3.44118600	-3.30367500	-1.63209800
C	-4.31967500	-3.84141800	-0.68565100
C	-3.56331400	-3.76395300	-2.94737800
C	-5.27967800	-4.79189100	-1.02545400
C	-4.51230600	-4.71689000	-3.31064900
C	-5.37378300	-5.23148100	-2.34417400

Mg	-0.03994600	0.06632800	-0.36463600
H	1.18450100	5.03901300	0.97127800
H	-1.46688000	5.05963500	0.65810400
H	-5.15839000	1.39538900	-0.63162200
H	-5.09581700	-1.18371900	-1.31714800
H	-1.26427600	-4.90658600	-1.70163600
H	1.38706500	-4.92730500	-1.38807900
H	5.07846500	-1.26331500	-0.09692400
H	5.01575300	1.31575500	0.58877300
F	2.67166700	3.42089600	3.17063800
F	4.52516100	5.26872900	3.84660900
F	6.20783700	6.27633300	1.95020200
F	6.02450200	5.41907500	-0.63394900
F	4.17210900	3.57433000	-1.32164300
F	-3.87974400	3.61300100	-2.27725600
F	-5.81683200	5.48337000	-2.03974000
F	-6.56954000	6.36834800	0.42865700
F	-5.36695300	5.36697800	2.66434400
F	-3.43379500	3.49230200	2.43929700
F	3.35469500	-3.36001900	-3.16832900
F	5.28800600	-5.23465100	-3.39287300
F	6.48986000	-6.23614100	-1.15684500
F	5.73637000	-5.35131600	1.31133600
F	3.79914200	-3.48101200	1.54835500
F	-2.75155800	-3.28783000	-3.90060000
F	-4.60488800	-5.13558100	-4.57712200
F	-6.28747500	-6.14391900	-2.68101600
F	-6.10415600	-5.28747200	-0.09659000
F	-4.25186400	-3.44284800	0.59168300

MgTPPBr$_8$(Singlet)

N	-0.07273100	2.03768300	-0.09373500
N	2.03773200	0.07270000	0.09408600
N	-2.03775500	-0.07271600	0.09400700
N	0.07266400	-2.03768800	-0.09373900
C	-1.21721500	2.72826600	-0.42703100
C	-0.82443000	3.91721300	-1.15898600
C	0.54362300	3.96609100	-1.15843200
C	1.01971800	2.80805900	-0.42636600
C	2.33797900	2.51096700	0.00056000
C	-2.51104000	2.33792100	-0.00045900
C	3.91749400	0.82437300	1.15892700
C	3.96630900	-0.54367700	1.15845600
C	2.80813600	-1.01977100	0.42658300
C	2.72836400	1.21717100	0.42723800
C	2.51092500	-2.33801000	-0.00038100
C	-2.72839500	-1.21716300	0.42714100
C	-3.91737800	-0.82443200	1.15904600
C	-3.96626600	0.54363400	1.15850600
C	-2.80819800	1.01970600	0.42646700
C	0.82435200	-3.91718600	-1.15903400
C	-0.54370600	-3.96603300	-1.15856300
C	-1.01980100	-2.80805400	-0.42640000
C	1.21711800	-2.72828300	-0.42701100
C	-2.33805200	-2.51092500	0.00052000
C	3.35249700	3.60122100	0.00044500
C	4.50550200	3.50064500	-0.79271500
C	3.16945700	4.74425500	0.79333200
C	5.44948600	4.52517500	-0.80085500
H	4.65044200	2.62150800	-1.41338600
C	4.12319800	5.75977800	0.80060000
H	2.28239000	4.82559400	1.41432200
C	5.26329600	5.65522000	-0.00041100
H	6.33184300	4.44099400	-1.42844900
H	3.97584100	6.63402300	1.42788300
H	6.00312000	6.45047200	-0.00077500
C	-3.60132000	3.35242800	-0.00052100
C	-3.50154100	4.50472600	0.79375100
C	-4.74351300	3.17010800	-0.79477200
C	-4.52607600	5.44871100	0.80167000
H	-2.62303500	4.64910600	1.41544800
C	-5.75901000	4.12388300	-0.80227500
H	-4.82419500	2.28360300	-1.41665300
C	-5.65527800	5.26325900	-0.00013100
H	-4.44254400	6.33050700	1.43014100
H	-6.63259100	3.97710600	-1.43061800
H	-6.45051400	6.00310100	0.00005300
C	-3.35272900	-3.60105500	0.00044400
C	-3.17072500	-4.74326300	0.79474100
C	-4.50473300	-3.50123600	-0.79424200
C	-4.12458300	-5.75868500	0.80196900
H	-2.28440200	-4.82401900	1.41687400
C	-5.44880100	-4.52569900	-0.80243500
H	-4.64881700	-2.62276500	-1.41605900
C	-5.26370200	-5.65488500	-0.00052800
H	-3.97806100	-6.63227100	1.43036500
H	-6.33037900	-4.44212200	-1.43120400
H	-6.00359600	-6.45007100	-0.00093400
C	3.60101900	-3.35270900	-0.00039000
C	4.74354900	-3.17033500	-0.79415200
C	3.50077700	-4.50521000	0.79353000
C	5.75890000	-4.12425900	-0.80154500
H	4.82461000	-2.28366100	-1.41574100
C	4.52515700	-5.44936400	0.80155000
H	2.62202800	-4.64962600	1.41487500
C	5.65468900	-5.26385500	0.00022400
H	6.63274100	-3.97743200	-1.42951400
H	4.44125300	-6.33132800	1.42973500
H	6.44981100	-6.00381900	0.00049500
Mg	-0.00002900	-0.00001200	0.00034300
Br	-1.92997200	5.10255100	-2.18772700
Br	1.56285700	5.22717400	-2.18607300
Br	5.10300200	1.92983800	2.18755200
Br	5.22744300	-1.56282900	2.18610300
Br	-5.22701700	1.56290400	2.18650100
Br	-5.10235600	-1.93004400	2.18811200
Br	-1.56292000	-5.22695100	-2.18641600
Br	1.92995500	-5.10238300	-2.18787300

MgTPP(Singlet)

Mg	0.00000000	0.00000100	0.00000000
N	-2.06495100	-0.00014400	0.03453600
N	-0.00014500	2.06513700	0.00000500
N	0.00014500	-2.06513600	-0.00000500
N	2.06495100	0.00014500	-0.03453600
C	-2.88139800	-1.10712200	-0.00755100
C	-4.26160700	-0.68148400	-0.08792100
C	-4.26170100	0.68088300	-0.08796100
C	-2.88155500	1.10671900	-0.00753900
H	-5.11540900	-1.33920500	-0.15350600
H	-5.11559500	1.33848100	-0.15357700
C	-2.45193000	2.45181500	-0.01222000
C	-2.45158500	-2.45215800	-0.01223900
C	-0.68149500	4.26496900	0.00226600
C	0.68089500	4.26506500	-0.00225300
C	1.10681100	2.88267400	0.00634300
C	-1.10721600	2.88251800	-0.00632500
H	-1.33890800	5.12142900	0.00951200
H	1.33818600	5.12161800	-0.00949900
C	2.45158500	2.45215900	0.01224000
C	1.10721600	-2.88251700	0.00632500
C	0.68149500	-4.26496800	-0.00225900
C	-0.68089500	-4.26506400	0.00225300
C	-1.10681100	-2.88267300	-0.00634200
H	1.33890800	-5.12142800	-0.00950000
H	-1.33818600	-5.12161700	0.00949800
C	4.26160700	0.68148500	0.08791100
C	4.26170100	-0.68088100	0.08796500
C	2.88155500	-1.10671800	0.00753800
C	2.88139800	1.10712300	0.00755100
H	5.11541000	1.33920700	0.15348900
H	5.11559500	-1.33848000	0.15358300
C	2.45193000	-2.45181400	0.01222000
C	-3.51357500	3.50999800	-0.03267900
C	-3.70232500	4.31864900	-1.16480700
C	-4.34428700	3.71373700	1.08068200
C	-4.69205000	5.30238300	-1.18305400
H	-3.07108200	4.16631400	-2.03536500
C	-5.33348100	4.69803200	1.06350100
H	-4.20494800	3.09813300	1.96453900
C	-5.51067200	5.49560900	-0.06863700
H	-4.82574400	5.91485000	-2.07039300
H	-5.96307800	4.84363500	1.93687500
H	-6.28085200	6.26148200	-0.08251300
C	-3.51308600	-3.51048500	-0.03268600
C	-4.34378100	-3.71431200	1.08067200
C	-3.70172600	-4.31917500	-1.16480400
C	-5.33284600	-4.69873600	1.06350100
H	-4.20453100	-3.09867300	1.96451800
C	-4.69132200	-5.30303900	-1.18304100
H	-3.07050000	-4.16676800	-2.03536300
C	-5.50992500	-5.49635500	-0.06862600
H	-5.96243100	-4.84440600	1.93687200
H	-4.82493200	-5.91553600	-2.07037300
H	-6.28000600	-6.26232800	-0.08249500
C	3.51357400	-3.50999800	0.03268100
C	3.70232500	-4.31864400	1.16481300
C	4.34428400	-3.71374300	-1.08068000
C	4.69204800	-5.30237900	1.18306200
H	3.07108300	-4.16630400	2.03537100
C	5.33347700	-4.69803900	-1.06349700
H	4.20494400	-3.09814300	-1.96454000
C	5.51066900	-5.49561100	0.06864500
H	4.82574300	-5.91484200	2.07040400
H	5.96307200	-4.84364700	-1.93687100
H	6.28084800	-6.26148500	0.08252300
C	3.51308700	3.51048500	0.03268300
C	4.34378000	3.71431100	-1.08067600
C	3.70173100	4.31917500	1.16480100
C	5.33284500	4.69873400	-1.06350800
H	4.20452700	3.09867100	-1.96452100
C	4.69132800	5.30303800	1.18303500
H	3.07050700	4.16676900	2.03536100
C	5.50992800	5.49635300	0.06861800
H	5.96242900	4.84440300	-1.93688100
H	4.82494100	5.91553500	2.07036600
H	6.28001000	6.26232500	0.08248500

MnPCl(Quintet)

Mn	0.00003700	0.00002500	0.06669000
C	2.85007100	-1.08616300	-0.25950800
N	2.01738600	0.01065900	-0.24925500
C	2.83838500	1.11627700	-0.25956900
C	4.21716200	0.70351600	-0.28629000
C	4.22437000	-0.65881300	-0.28625600
N	-0.01074800	2.01728800	-0.24921200

C	1.08611200	2.84997200	-0.25887000
C	0.65878000	4.22429300	-0.28453200
C	-0.70355000	4.21711700	-0.28452700
C	-1.11634800	2.83834400	-0.25884300
C	2.41151200	2.43721800	-0.25758900
C	-2.43729600	2.41148400	-0.25749700
C	-2.85004700	1.08608300	-0.25946400
N	-2.01740600	-0.01076300	-0.24917700
C	-2.83842200	-1.11634500	-0.25951400
C	-4.21720500	-0.70355600	-0.28626300
C	-4.22437900	0.65876400	-0.28621900
C	-2.41156400	-2.43729400	-0.25752300
C	-1.08615500	-2.85002900	-0.25878600
N	0.01067200	-2.01733000	-0.24908900
C	1.11629400	-2.83834600	-0.25874600
C	0.70352500	-4.21714900	-0.28444300
C	-0.65879600	-4.22435500	-0.28447100
C	2.43725700	-2.41155100	-0.25746600
H	-5.07447000	1.32760900	-0.30576600
H	-5.06021400	-1.38129800	-0.30585300
H	-1.32762200	-5.07447400	-0.30343800
H	1.38128300	-5.06016100	-0.30337600
H	1.32760600	5.07441200	-0.30347400
H	-1.38127700	5.06015400	-0.30346200
H	5.07448800	-1.32762300	-0.30580100
H	5.06017100	1.38126000	-0.30586200
H	3.20828300	-3.17455400	-0.26393200
H	3.17445500	3.20830300	-0.26406800
H	-3.20837600	3.17443200	-0.26396400
H	-3.17450500	-3.20838000	-0.26403800
Cl	0.00009900	0.00023100	2.41889200

NiP(Singlet)

Ni	0.00000000	0.00000000	0.00004500
N	1.40328300	-1.40182000	-0.00000700
N	1.40250900	1.40259400	0.00003500
N	-1.40250900	-1.40259400	0.00003100
N	-1.40328300	1.40182000	-0.00001100
C	1.22356500	-2.76796300	0.00007800
C	2.49158100	-3.45120900	-0.00004500
C	3.45265900	-2.48992100	-0.00022900
C	2.76921600	-1.22193600	-0.00019100
H	2.60784500	-4.52693600	-0.00000600
H	4.52841800	-2.60603800	-0.00036600
C	3.41659200	0.00093500	-0.00024100
C	0.00093500	-3.41574800	0.00022400
C	3.45129500	2.49180500	0.00001300
C	2.48969700	3.45257200	0.00018300
C	1.22205300	2.76864000	0.00018000
C	2.76853900	1.22344800	-0.00008900
H	4.52699200	2.60850500	-0.00004300
H	2.60537800	4.52836300	0.00029000
C	-0.00093500	3.41574800	0.00022400
C	-2.76853800	-1.22344800	-0.00008900
C	-3.45129500	-2.49180500	0.00000600
C	-2.48969700	-3.45257200	0.00019900
C	-1.22205200	-2.76864000	0.00018400
H	-4.52699100	-2.60850500	-0.00005900
H	-2.60537700	-4.52836200	0.00031800
C	-2.49158100	3.45120900	-0.00002900
C	-3.45265900	2.48992100	-0.00023700
C	-2.76921600	1.22193600	-0.00019100
C	-1.22356500	2.76796300	0.00008300
H	-2.60784500	4.52693600	0.00002000
H	-4.52841900	2.60603800	-0.00038300
C	-3.41659200	-0.00093500	-0.00024500
H	-0.00124000	4.50058300	0.00031300
H	-4.50142500	-0.00124000	-0.00036900
H	0.00123900	-4.50058300	0.00031300
H	4.50142500	0.00124000	-0.00035800

O=TiP(Singlet)

Ti	0.00004300	0.00013400	0.47325800
C	3.05435400	0.31173100	-0.14701900
N	1.82260100	0.92495500	-0.10103400
C	2.05468800	2.28119300	-0.14730400
C	3.47424300	2.52798400	-0.22067000
C	4.09151600	1.31185000	-0.22047700
N	-0.92508600	1.82250100	-0.10109100
C	-0.31178700	3.05424900	-0.14685300
C	-1.31187200	4.09147200	-0.21994200
C	-2.52803900	3.47426300	-0.22007100
C	-2.28130600	2.05468100	-0.14709800
C	1.06673100	3.26549300	-0.15397100
C	-3.26559400	1.06670200	-0.15389300
C	-3.05427000	-0.31180700	-0.14691900
N	-1.82253300	-0.92510200	-0.10083600
C	-2.05470600	-2.28130900	-0.14720600
C	-3.47427700	-2.52804000	-0.22066200
C	-4.09148400	-1.31188400	-0.22048900
C	-1.06678100	-3.26565400	-0.15388400
C	0.31173700	-3.05435600	-0.14675000
N	0.92494800	-1.82258000	-0.10088000
C	2.28119700	-2.05469300	-0.14699000
C	2.52799600	-3.47427200	-0.22008400
C	1.31187000	-4.09153700	-0.21993300
C	3.26556300	-1.06680200	-0.15388900
H	-5.15104400	-1.09944600	-0.27601300
H	-3.92838500	-3.50862800	-0.27635600
H	1.09949200	-5.15112100	-0.27524100
H	3.50861200	-3.92834900	-0.27553800
H	-1.09947400	5.15105400	-0.27518200
H	-3.50862300	3.92841900	-0.27544100
H	5.15109600	1.09949400	-0.27592200
H	3.92833500	3.50858300	-0.27630100
H	4.29665400	-1.40374000	-0.19411600
H	1.40359400	4.29661100	-0.19417800
H	-4.29672600	1.40351600	-0.19411700
H	-1.40364300	-4.29676800	-0.19416800
O	0.00012300	0.00042700	2.09030200

O=VP(Doublet)

V	0.00008000	0.00005600	0.42321400
C	-2.59763900	1.60823000	-0.14186300
N	-1.98733800	0.37352900	-0.10524200
C	-3.00464100	-0.55486200	-0.14240700
C	-4.28107000	0.11182500	-0.20202500
C	-4.02908800	1.45108600	-0.20154900
N	-0.37372200	-1.98731100	-0.10527400
C	-1.60832900	-2.59769000	-0.14271300
C	-1.45108600	-4.02909700	-0.20279100
C	-0.11181000	-4.28100100	-0.20256400
C	0.55478400	-3.00454000	-0.14226600
C	-2.83091100	-1.93470800	-0.14706400
C	1.93462900	-2.83086800	-0.14630900
C	2.59768800	-1.60832600	-0.14199400
N	1.98726600	-0.37367200	-0.10530500
C	3.00456600	0.55481100	-0.14239900
C	4.28099500	-0.11182200	-0.20208000
C	4.02907900	-1.45110000	-0.20168500
C	2.83082100	1.93464500	-0.14699700
C	1.60825600	2.59763600	-0.14270700
N	0.37356400	1.98729300	-0.10534600
C	-0.55485500	3.00461700	-0.14240300
C	0.11179400	4.28099600	-0.20269900
C	1.45106200	4.02902400	-0.20284300
C	-1.93469800	2.83082000	-0.14631300
H	4.73764900	-2.26763300	-0.24670000
H	5.23785900	0.39136800	-0.24750000
H	2.26760500	4.73755500	-0.24843700
H	-0.39138400	5.23785500	-0.24818000
H	-2.26761500	-4.73763300	-0.24841600
H	0.39143900	-5.23783100	-0.24798400
H	-4.73760400	2.26767500	-0.24649900
H	-5.23793400	-0.39135000	-0.24747300
H	-2.54702100	3.72635100	-0.17747100
H	-3.72647900	-2.54696000	-0.17860100
H	2.54682200	-3.72648900	-0.17746800
H	3.72638900	2.54689700	-0.17844100
O	0.00034800	0.00024900	1.99618300

$ZnPBr_8$(Singlet)

C	-2.86831600	-1.10945000	-0.00010900
N	-2.05979800	0.00032300	-0.00004300
C	-2.86791600	1.11040800	-0.00007400
C	-4.25074000	0.68163200	-0.00016500
C	-4.25099100	-0.68017200	-0.00018300
N	0.00035000	2.05979200	0.00007800
C	-1.10943400	2.86829800	0.00006100
C	-0.68017100	4.25097700	0.00012000
C	0.68163400	4.25074100	0.00014900
C	1.11042500	2.86792400	0.00012300
C	2.86831400	1.10944700	0.00006900
N	2.05979800	-0.00032800	0.00013700
C	2.86791900	-1.11041000	0.00007000
C	4.25074200	-0.68163300	-0.00005200
C	4.25099000	0.68017200	-0.00003600
C	1.10943500	-2.86829900	0.00011700
N	-0.00034900	-2.05979100	0.00004500
C	-1.11042300	-2.86792300	0.00001400
C	-0.68163400	-4.25074100	0.00008900
C	0.68017100	-4.25097900	0.00014200
C	-2.43349600	-2.43266900	-0.00007500
C	-2.43265200	2.43347500	-0.00001400
C	2.43349600	2.43266700	0.00011000
C	2.43265300	-2.43347800	0.00011300
H	-3.19981500	-3.19870800	-0.00011200
H	-3.19868800	3.19979800	-0.00002900
H	3.19981800	3.19870400	0.00010700
H	3.19868800	-3.19980200	0.00011600
Zn	-0.00000200	0.00000700	0.00003600
Br	-1.84055800	5.77012100	0.00013500
Br	1.84255200	5.76949200	0.00022200
Br	5.77014100	1.84055000	-0.00014300
Br	5.76948400	-1.84256300	-0.00018500
Br	1.84055800	-5.77012200	0.00025200
Br	-1.84255200	-5.76949200	0.00008400
Br	-5.77014100	-1.84055100	-0.00028800
Br	-5.76948200	1.84256200	-0.00023300

$ZnPCl_8$(Singlet)

C	-3.06704700	-0.18134600	-0.00017800
N	-1.95954500	0.62810000	-0.00004100
C	-2.39014800	1.93054600	-0.00009400
C	-3.83823300	1.94771800	-0.00026700
C	-4.25536800	0.64641000	-0.00032000

N	0.62818700	1.95949500	0.00017400
C	-0.18131200	3.06697400	0.00014300
C	0.64639700	4.25532100	0.00022900
C	1.94772600	3.83823500	0.00027500
C	1.93061200	2.39016100	0.00023600
C	3.06703300	0.18133900	0.00012200
N	1.95953700	-0.62811700	0.00030900
C	2.39015500	-1.93056000	0.00009300
C	3.83823800	-1.94772100	-0.00024200
C	4.25536100	-0.64640700	-0.00020600
C	0.18131400	-3.06697600	0.00027900
N	-0.62817900	-1.95949500	0.00011600
C	-1.93060600	-2.39015500	0.00002600
C	-1.94772500	-3.83823400	0.00018100
C	-0.64640200	-4.25532300	0.00034100
Cl	0.06912000	5.87668600	0.00024800
Cl	3.35986400	4.82200100	0.00035000
Cl	5.87673800	-0.06916300	-0.00050100
Cl	4.82195100	-3.35989200	-0.00064600
Cl	-0.06911400	-5.87668700	0.00058400
Cl	-3.35986900	-4.82199400	0.00012200
Cl	-5.87674100	0.06915700	-0.00050800
Cl	-4.82194800	3.35989200	-0.00037800
C	-3.05859100	-1.57371300	-0.00013500
C	-1.57367900	3.05850600	0.00001400
C	3.05859000	1.57370600	0.00021400
C	1.57368000	-3.05851600	0.00024600
H	-4.02292800	-2.06941000	-0.00024100
H	-2.06936300	4.02284900	-0.00001800
H	4.02293300	2.06939000	0.00017700
H	2.06935700	-4.02286400	0.00023400
Zn	0.00000000	0.00001200	0.00008600

ZnPF$_8$(Singlet)

C	-2.81460600	-1.22126500	-0.00038600
N	-2.04796800	-0.08073400	-0.00048500
C	-2.90241200	0.99566800	-0.00045200
C	-4.26097400	0.51267300	-0.00053300
C	-4.20699600	-0.84737700	-0.00048900
N	-0.08073300	2.04796400	-0.00008900
C	-1.22126300	2.81460100	-0.00021200
C	-0.84737700	4.20699500	-0.00017300
C	0.51267200	4.26097300	0.00013300
C	0.99567000	2.90241200	0.00016300
C	2.81460600	1.22126600	0.00048600
N	2.04796700	0.08073500	0.00036600
C	2.90241200	-0.99566800	0.00054000
C	4.26097300	-0.51267300	0.00063100
C	4.20699600	0.84737700	0.00058200
C	1.22126500	-2.81460200	0.00027300
N	0.08073500	-2.04796400	0.00012600
C	-0.99566800	-2.90241100	-0.00008800
C	-0.51267100	-4.26097200	-0.00020200
C	0.84737800	-4.20699500	0.00010700
F	5.21858500	1.71685500	0.00061700
F	5.33844800	-1.29901800	0.00073200
F	1.71686100	-5.21857900	0.00019700
F	-1.29902100	-5.33844400	-0.00049100
F	-1.71686100	5.21857800	-0.00034100
F	1.29902100	5.33844500	0.00034200
F	-5.21858600	-1.71685400	-0.00050600
F	-5.33844900	1.29901600	-0.00061000
C	2.52987800	-2.33778000	0.00051200
C	-2.33778000	-2.52987700	-0.00027500
C	-2.52987700	2.33778000	-0.00039300
C	2.33778100	2.52987800	0.00041300
H	3.32653500	-3.07444400	0.00061400
H	-3.07444300	-3.32653600	-0.00036500
H	-3.32653400	3.07444600	-0.00047200
H	3.07444500	3.32653600	0.00053500
Zn	-0.00000100	-0.00000100	-0.00010000

ZnP(Singlet)

Zn	0.00000000	-0.00000100	0.00006100
N	-1.38714400	1.51395400	0.00000700
N	-1.51395600	-1.38714100	0.00000000
N	1.51395500	1.38714200	0.00003100
N	1.38714400	-1.51395300	0.00003800
C	-1.12503100	2.86175200	-0.00002700
C	-2.37029100	3.59676100	-0.00005900
C	-3.37612700	2.67523600	-0.00004900
C	-2.75268800	1.37054900	-0.00004100
H	-2.45330200	4.67592000	-0.00005500
H	-4.44391800	2.85216900	-0.00008800
C	-3.43202300	0.15007500	-0.00002800
C	0.15007500	3.43202100	-0.00004200
C	-3.59676100	-2.37029100	0.00006200
C	-2.67523500	-3.37612600	0.00002500
C	-1.37054900	-2.75268600	-0.00003000
C	-2.86175300	-1.12503000	0.00000200
H	-4.67592000	-2.45330400	0.00013400
H	-2.85216600	-4.44391800	0.00001000
C	-0.15007500	-3.43201900	-0.00004700
C	2.86175200	1.12503000	0.00000000
C	3.59676200	2.37029000	0.00002400
C	2.67523600	3.37612700	0.00007100
C	1.37055000	2.75268800	-0.00002600
H	4.67592100	2.45330300	0.00006000
H	2.85216900	4.44391800	0.00009000
C	2.37029000	-3.59676000	-0.00001200
C	3.37612700	-2.67523600	-0.00007700
C	2.75268800	-1.37054900	-0.00004500
C	1.12503000	-2.86175100	-0.00002900
H	2.45329900	-4.67592000	0.00002600
H	4.44391800	-2.85217000	-0.00014300
C	3.43202300	-0.15007500	-0.00004200
H	-0.19745000	-4.51705300	-0.00005100
H	4.51705700	-0.19744900	-0.00005800
H	0.19745000	4.51705500	-0.00004800
H	-4.51705700	0.19745100	-0.00002900

ZnTPFPP(Singlet)

Zn	0.00009500	0.00015600	-0.00005500
N	1.93970100	0.67280000	-0.00680600
N	0.67274200	-1.93944500	0.00752300
N	-0.67257700	1.93975300	0.00675700
N	-1.93950300	-0.67249600	-0.00766600
C	2.35118800	1.98343700	0.02184200
C	3.79481000	2.03615400	0.08235900
C	4.24058800	0.75138300	0.08250900
C	3.07449700	-0.10129200	0.02192600
H	4.38876500	2.93680100	0.13111700
H	5.26482900	0.41232000	0.13134700
C	3.10707200	-1.50641900	-0.00048900
C	1.50669900	3.10705400	-0.00024000
C	2.03602800	-3.79431000	-0.08713200
C	0.75126700	-4.24008500	-0.08737900
C	-0.10138900	-3.07417300	-0.02336000
C	1.98336600	-2.35084800	-0.02330200
H	2.93662200	-4.38815500	-0.13807700
H	0.41221400	-5.26421800	-0.13834500
C	-1.50657000	-3.10685300	-0.00010300
C	-1.98319600	2.35132200	-0.02205700
C	-2.03577500	3.79494200	-0.08294900
C	-0.75097400	4.24063900	-0.08290500
C	0.10158400	3.07448600	-0.02213400
H	-2.93634200	4.38897200	-0.13214900
H	-0.41178100	5.26484600	-0.13167200
C	-3.79444000	-2.03562300	0.08765100
C	-4.24014500	-0.75083800	0.08755400
C	-3.07416900	0.10169200	0.02341000
C	-2.35098000	-1.98310800	0.02334000
H	-4.38837000	-2.93613400	0.13892400
H	-5.26423800	-0.41164700	0.13858200
C	-3.10684400	1.50685400	0.00068500
C	-4.45279900	2.15932200	0.00123200
C	-5.28175700	2.12401700	-1.12518800
C	-4.93864700	2.83183700	1.12767200
C	-6.53807800	2.72568000	-1.13629200
C	-6.18927900	3.44524700	1.13887400
C	-6.99173900	3.38988500	0.00129500
C	2.15933500	4.45299000	-0.00057300
C	2.82817800	4.94043700	-1.12845700
C	2.12793800	5.28002800	1.12731300
C	3.44180400	6.19097400	-1.13969000
C	2.72993800	6.53619500	1.13847600
C	3.39043100	6.99155800	-0.00060100
C	4.45287700	-2.15922100	-0.00030200
C	5.28165500	-2.12489400	-1.12685700
C	4.93853700	-2.83141600	1.12642200
C	6.53772200	-2.72709700	-1.13780500
C	6.18892200	-3.44534000	1.13779400
C	6.99124500	-3.39091300	0.00007500
C	-2.15920700	-4.45268000	-0.00039000
C	-2.12090000	-5.28332700	1.12471800
C	-2.83515700	-4.93680600	-1.12558200
C	-2.72280900	-6.53952600	1.13572900
C	-3.44881800	-6.18730700	-1.13683300
C	-3.39036500	-6.99143000	-0.00059100
F	4.19395100	-2.89845800	2.23782600
F	6.62453500	-4.07923100	2.23149800
F	8.19209200	-3.97327900	0.00018200
F	7.30561400	-2.67700600	-2.23128200
F	4.87373600	-1.49865400	-2.23840800
F	-2.90616400	-4.19061300	-2.23567300
F	-4.08636700	-6.62130800	-2.22904900
F	-3.97248200	-8.19239500	-0.00061800
F	-2.66880400	-7.30912700	2.22781500
F	-1.49109900	-4.87710600	2.23487000
F	-4.87374500	1.49737200	-2.23645800
F	-7.30609200	2.67466800	-2.22964000
F	-8.19283000	3.97175300	0.00127000
F	-6.62502800	4.07950700	2.23231500
F	-4.19398500	2.89974100	2.23899800
F	2.89219700	4.19744500	-2.24111900
F	4.07249100	6.62838900	-2.23453400
F	3.97255000	8.19253200	-0.00055700
F	2.68275900	7.30244400	2.23323800
F	1.50478500	4.87026700	2.23991100

ZnTPPBr$_8$(Singlet)

Zn	-0.00041400	0.00021700	-0.00007600
N	-0.98526400	1.78641400	-0.10793500
N	1.78549100	0.98501700	0.10904700
N	-1.78660300	-0.98460400	0.10789900
N	0.98428200	-1.78585500	-0.10931000

C	-2.31843100	1.88180600	-0.43449800
C	-2.50501700	3.12319000	-1.16185800
C	-1.30583800	3.78385700	-1.16383100
C	-0.35460000	2.96405100	-0.43732400
C	0.95204800	3.29344900	-0.00200500
C	-3.29357300	0.95280400	0.00292500
C	3.12318300	2.50507900	1.16148300
C	3.78387600	1.30601800	1.16312700
C	2.96344600	0.35438300	0.43758600
C	1.88109300	2.31830300	0.43524400
C	3.29265800	-0.95236000	0.00250000
C	-1.88197600	-2.31782300	0.43406300
C	-3.12344500	-2.50475400	1.16117500
C	-3.78381600	-1.30541700	1.16423700
C	-2.96414700	-0.35392500	0.43789200
C	2.50480900	-3.12381500	-1.16074300
C	1.30545600	-3.78404600	-1.16371100
C	0.35364100	-2.96361400	-0.43861900
C	2.31772000	-1.88161200	-0.43466100
C	-0.95302500	-3.29291700	-0.00365800
C	-1.36757400	-4.72352300	-0.00622200
C	-0.69074700	-5.66194900	0.78697700
C	-2.44123300	-5.15137200	-0.80140800
C	-1.08581400	-6.99793100	0.79288100
H	0.13707400	-5.33581700	1.40950600
C	-2.82314800	-6.49119100	-0.81126100
H	-2.96561400	-4.43073200	-1.42184800
C	-2.14975500	-7.41698800	-0.01013000
H	-0.56180200	-7.71283700	1.42040800
H	-3.64821000	-6.81250800	-1.44013000
H	-2.45259800	-8.46006900	-0.01162600
C	-4.72415900	1.36725000	0.00583400
C	-5.15236400	2.43939100	0.80289500
C	-5.66240700	0.69148800	-0.78850300
C	-6.49225600	2.82098900	0.81328400
H	-4.43193200	2.96279300	1.42439600
C	-6.99844500	1.08636200	-0.79395800
H	-5.33606700	-0.13523700	-1.41237700
C	-7.41780900	2.14885000	0.01081700
H	-6.81381700	3.64486300	1.44358200
H	-7.71317100	0.56328700	-1.42247100
H	-8.46095000	2.45148200	0.01270700
C	1.36617400	4.72415200	-0.00453400
C	2.43818200	5.15287600	-0.80149200
C	0.69019200	5.66197500	0.79011400
C	2.81943400	6.49287000	-0.81146900
H	2.96178500	4.43276300	-1.42319300
C	1.08469500	6.99812400	0.79594800
H	-0.13642600	5.33521600	1.41391200
C	2.14705500	7.41800800	-0.00872200
H	3.64322400	6.81483800	-1.44166900
H	0.56143800	7.71252500	1.42467900
H	2.44941300	8.46123000	-0.01030400
C	4.72364600	-1.36650100	0.00485100
C	5.65953500	-0.69639300	-0.79700700
C	5.15410000	-2.43232800	0.80906500
C	6.99594500	-1.09016100	-0.80185500
H	5.33115900	0.12426000	-1.42780700
C	6.49427600	-2.81307400	0.81932500
H	4.43567100	-2.95065700	1.43712400
C	7.41772000	-2.14622400	0.01005500
H	7.70898100	-0.57158000	-1.43599600
H	6.81778500	-3.63184700	1.45525600
H	8.46110900	-2.44799900	0.01218300
Br	-3.68796500	-4.03222300	2.17687300
Br	-5.37263200	-0.96887800	2.18700400
Br	-4.03135500	3.68689700	-2.17973500
Br	-0.96891700	5.37294900	-2.18603800
Br	3.68817000	4.03158100	2.17836000
Br	5.37509800	0.96986800	2.18214400
Br	0.96924300	-5.37366100	-2.18533400
Br	4.03304800	-3.69028900	-2.17415600

ZnTPP(Singlet)

Zn	0.00000100	0.00000200	-0.00000100
N	2.05382600	-0.00574400	-0.03265600
N	-0.00583200	-2.05381100	-0.00036300
N	0.00582000	2.05380400	0.00037000
N	-2.05384100	0.00574600	0.03266300
C	2.87560700	1.09790400	0.00801300
C	4.25378200	0.66871800	0.08538000
C	4.24994100	-0.69263100	0.08535900
C	2.86935100	-1.11404500	0.00794200
H	5.10792600	1.32612800	0.14875900
H	5.10046500	-1.35474300	0.14855900
C	2.44174600	-2.45560000	0.01230800
C	2.45555400	2.44190400	0.01250800
C	0.66873200	-4.25664900	-0.00166200
C	-0.69264400	-4.25285200	0.00161600
C	-1.11422300	-2.87023600	-0.00693400
C	1.09798400	-2.87641600	0.00653000
H	1.32587300	-5.11325800	-0.00835300
H	-1.35443200	-5.10588500	0.00848500
C	-2.45556700	-2.44192400	-0.01263300
C	-1.09798500	2.87643000	-0.00628100
C	-0.66870600	4.25665700	0.00217100
C	0.69267200	4.25283400	-0.00121000
C	1.11421800	2.87021600	0.00704400
H	-1.32581100	5.11329200	0.00913800
H	1.35448000	5.10585400	-0.00795400
C	-4.25376900	-0.66869800	-0.08589400
C	-4.24992400	0.69264900	-0.08574400
C	-2.86935200	1.11405400	-0.00801200
C	-2.87561200	-1.09790600	-0.00826100
H	-5.10790900	-1.32608600	-0.14952700
H	-5.10043700	1.35476000	-0.14910100
C	-2.44174900	2.45562500	-0.01215900
C	-3.50015200	3.51703400	-0.03207900
C	-4.32146100	3.73072100	1.08619500
C	-3.69418000	4.31803900	-1.16854700
C	-5.30743300	4.71828500	1.06945400
H	-4.17758500	3.12048600	1.97305700
C	-4.68087500	5.30485700	-1.18617900
H	-3.06956900	4.15766200	-2.04245300
C	-5.49033800	5.50846800	-0.06694200
H	-5.93008200	4.87208700	1.94637400
H	-4.81915100	5.91174100	-2.07662500
H	-6.25802200	6.27684100	-0.08036800
C	3.52006100	3.49718600	0.03206900
C	4.34233000	3.70601100	-1.08641100
C	3.71917000	4.29698000	1.16851600
C	5.33417900	4.68767000	-1.06992900
H	4.19465800	3.09657900	-1.97320300
C	4.71172900	5.27790600	1.18588100
H	3.09393700	4.14022800	2.04263500
C	5.52212000	5.47669800	0.06645100
H	5.95754600	4.83770300	-1.94699300
H	4.85391100	5.88388800	2.07632700
H	6.29445000	6.24040100	0.07974600
C	3.50015600	-3.51701900	0.03231400
C	4.32115100	-3.73110000	-1.08610600
C	3.69447700	-4.31761300	1.16901800
C	5.30713000	-4.71866000	-1.06927900
H	4.17704400	-3.12116900	-1.97313900
C	4.68117200	-5.30443200	1.18673200
H	3.07010100	-4.15691800	2.04303300
C	5.49033300	-5.50844000	0.06734800
H	5.92954800	-4.87277500	-1.94630800
H	4.81968500	-5.91100800	2.07735200
H	6.25801500	-6.27681300	0.08083900
C	-3.52006800	-3.49720100	-0.03229400
C	-3.71877500	-4.29729600	-1.16860900
C	-4.34273800	-3.70576300	1.08594700
C	-4.71133600	-5.27821400	-1.18608700
H	-3.09324700	-4.14075200	-2.04255100
C	-5.33457600	-4.68742700	1.06935800
H	-4.19537000	-3.09612600	1.97264700
C	-5.52212500	-5.47672900	-0.06689700
H	-4.85321700	-5.88440600	-2.07643800
H	-5.95824300	-4.83725700	1.94624300
H	-6.29445000	-6.24043600	-0.08027500

4.2: Porphyrin-Methanol complexes

AlPCl(Singlet)-MeOH

Al	-0.04202700	-0.01601400	-0.25540600
C	2.64886500	-1.45443200	-0.09446500
N	1.27654500	-1.53940300	-0.03147600
C	0.97847700	-2.88222500	-0.00444600
C	2.19213400	-3.65909100	-0.03306500
C	3.22700400	-2.77477400	-0.09096900
N	-1.57729900	-1.32081600	0.03066600
C	-1.48794200	-2.69135400	0.05670200
C	-2.80661300	-3.27467000	0.11406400
C	-3.69362100	-2.24227100	0.12016900
C	-2.91836400	-1.02616800	0.06986200
C	-0.30360800	-3.42003700	0.03870600
C	-3.45897000	0.25548400	0.08321700
C	-2.73044400	1.44035300	0.08257000
N	-1.35402700	1.52581700	0.07499100
C	-1.05750200	2.87293600	0.05775300
C	-2.27175500	3.64629800	0.08327800
C	-3.30724400	2.75955300	0.09704800
C	0.22486200	3.41019600	0.01495800
C	1.40833700	2.68032200	-0.03858400
N	1.49553000	1.30721500	-0.05165200
C	2.83822500	1.01238100	-0.11415000
C	3.61295600	2.22805400	-0.13146100
C	2.72698100	3.26167400	-0.08317800
C	3.37739100	-0.26991000	-0.13793500
H	-4.36890200	2.96761800	0.11086100
H	-2.31383400	4.72743300	0.08296300
H	2.93266600	4.32388200	-0.08083500
H	4.69314800	2.27015300	-0.17629300
H	-3.00997800	-4.33682700	0.14493500
H	-4.77406300	-2.28338600	0.15844700
H	4.28796400	-2.98321200	-0.12947300
H	2.23223100	-4.74011800	-0.01584700
H	4.45811000	-0.35342200	-0.18986600
H	-0.38655000	-4.50190700	0.05626500
H	-4.54080100	0.33851000	0.10020000
H	0.30885200	4.49212000	0.00984300
Cl	-0.11973500	0.01035100	-2.51542700
C	1.04304600	0.01827600	2.91541400
H	1.66099200	0.91367700	2.79163200

H	0.70417800	-0.06125700	3.95395700
H	1.63567900	-0.86048400	2.66304600
O	-0.07995000	0.02150900	2.02666800
H	-0.63676000	0.79412200	2.19873600

$CoPBr_8Cl$(Singlet)-MeOH

Co	-0.01189600	-0.01095800	-0.01274100
C	-0.27185800	3.00812800	0.04987000
N	-0.89310900	1.78874600	-0.06429900
C	-2.24307600	2.03599900	-0.08305100
C	-2.47828700	3.46119900	-0.01490200
C	-1.26398100	4.05948400	0.07670100
N	-1.80968700	-0.90438100	-0.05476700
C	-3.02900700	-0.27954900	-0.09143100
C	-4.08602000	-1.26794900	-0.05471700
C	-3.48858700	-2.48210700	0.02645500
C	-2.05989400	-2.24981900	0.02469100
C	-3.24595000	1.08520200	-0.12433300
C	-1.11125600	-3.25514700	0.06882800
C	0.25318000	-3.04158200	0.01259200
N	0.87561500	-1.81935700	-0.10289400
C	2.22950500	-2.06829100	-0.10735500
C	2.46137800	-3.49195400	-0.03910500
C	1.24516000	-4.09039600	0.04404700
C	3.23119500	-1.11561600	-0.13730500
C	3.01327500	0.24991800	-0.09593700
N	1.79145600	0.87620100	-0.06777700
C	2.04280300	2.22189600	0.04153500
C	3.46999800	2.45165900	0.05651100
C	4.06816300	1.23745700	-0.03799200
C	1.09277000	3.22442800	0.10244300
H	1.43986100	4.24536700	0.19212700
H	-4.27042900	1.43310000	-0.14019200
H	-1.46004600	-4.27645400	0.14662100
H	4.25621900	-1.46228600	-0.14394900
Cl	0.00306100	-0.01975700	2.19295500
C	0.41885700	0.92895500	-2.98344700
H	1.48226700	1.12380900	-2.82188600
H	0.23777400	0.63840700	-4.02203200
H	-0.15727200	1.82274000	-2.75022700
O	-0.06493100	-0.10926000	-2.10849500
H	0.41582400	-0.93314000	-2.27890100
Br	4.17740800	-4.33199100	-0.05432900
Br	0.87099600	-5.95949700	0.16929700
Br	5.94043000	0.85755300	-0.07882100
Br	4.31122000	4.16296300	0.17526500
Br	-0.88846800	5.92840000	0.20632200
Br	-4.19479100	4.29939200	-0.04088700
Br	-5.95721900	-0.88651800	-0.10623200
Br	-4.32802600	-4.19617900	0.11149100

$CoPCl_8Cl$(Singlet)-MeOH

Co	-0.02147000	0.00784400	0.00500700
C	2.62572700	1.47683500	0.05534700
N	1.25845100	1.54549800	-0.04493400
C	0.93217700	2.87809600	-0.04280100
C	2.13551500	3.67796200	0.02418200
C	3.18268500	2.81107600	0.09100800
N	-1.57038300	1.28104500	-0.04136500
C	-1.49916500	2.64900100	-0.05451200
C	-2.83285300	3.21225000	-0.02584200
C	-3.70032500	2.16609900	0.02174100
C	-2.90094600	0.95886500	0.01316800
C	-0.34425900	3.40826600	-0.07059200
C	-3.43450300	-0.31661100	0.03942400
C	-2.67803800	-1.47268800	-0.00014900
N	-1.30685200	-1.54139800	-0.09146300
C	-0.98121500	-2.87828000	-0.07263100
C	-2.18499800	-3.67423800	-0.01382200
C	-3.23326200	-2.80555400	0.03693300
C	0.29631600	-3.40669500	-0.08046500
C	1.45136500	-2.64625600	-0.04800300
N	1.52306900	-1.27551500	-0.04522000
C	2.85414300	-0.95404600	0.05207300
C	3.65011200	-2.16091100	0.08403300
C	2.78288400	-3.20779000	0.01600500
C	3.38447500	0.32178900	0.09879600
H	4.45975400	0.42251100	0.17863100
H	-0.44535000	4.48646600	-0.06932500
H	-4.51130800	-0.41566900	0.09744300
H	0.39845900	-4.48474600	-0.06828200
Cl	-0.02905500	-0.00966800	2.21292800
C	1.01444200	0.00599200	-2.96575100
H	1.64859800	-0.86647600	-2.78821700
H	0.67579300	0.02592700	-4.00547300
H	1.57247700	0.91496300	-2.74793200
O	-0.13142400	0.01039200	-2.09214400
H	-0.66881600	-0.78033400	-2.25066300
Cl	-2.24301900	-5.39357700	-0.00538000
Cl	-4.90860900	-3.18497100	0.12134300
Cl	3.15807100	-4.88663500	0.01060300
Cl	5.36664400	-2.22041200	0.18059300
Cl	4.85791400	3.18902800	0.19017600
Cl	2.19097600	5.39717900	0.02298200
Cl	-3.20643800	4.89090300	-0.04739100
Cl	-5.41884800	2.22262500	0.07107400

$CoPF_8Cl$(Singlet)-MeOH

Co	-0.02685100	0.01042200	0.01174300
C	2.68057800	1.35108000	0.06216000
N	1.31631200	1.48116900	-0.03407700
C	1.05424300	2.82890200	-0.00798400
C	2.28974600	3.56490700	0.07084800
C	3.29230400	2.65358700	0.11719100
N	-1.50715800	1.34708900	-0.04456000
C	-1.37576700	2.71156700	-0.03322500
C	-2.67819000	3.32949400	-0.01023400
C	-3.59003300	2.32809300	0.00575400
C	-2.85351600	1.08866100	-0.01157300
C	-0.19250100	3.42639600	-0.02643700
C	-3.45479300	-0.15674000	-0.00030600
C	-2.74362500	-1.34204600	-0.02384900
N	-1.37446800	-1.47299200	-0.09748700
C	-1.11398800	-2.82493900	-0.04687500
C	-2.35055200	-3.55609300	0.01448500
C	-3.35410600	-2.64264000	0.03124500
C	0.13393600	-3.42013600	-0.02918700
C	1.31750200	-2.70414100	-0.00802700
N	1.45037200	-1.33695700	-0.03283500
C	2.79671400	-1.07904000	0.06188800
C	3.52878200	-2.31774200	0.11758400
C	2.61686600	-3.31989000	0.07143700
C	3.39437200	0.16731000	0.09963200
H	4.47406800	0.21981200	0.17815100
H	-0.24576300	4.50868300	-0.00498500
H	-4.53653600	-0.20691600	0.04359000
H	0.18797100	-4.50197700	0.00843400
Cl	-0.04748100	-0.00872100	2.22344900
C	1.02140000	-0.05371100	-2.95388200
H	1.61155400	-0.95363900	-2.76179600
H	0.69440300	-0.02792500	-3.99744700
H	1.62122400	0.82902900	-2.73889400
O	-0.12924900	0.01524200	-2.09131400
H	-0.69427600	-0.75947400	-2.23318400
F	-2.42485000	-4.88664200	0.04950600
F	-4.67086100	-2.84226700	0.08517000
F	4.85773500	-2.39087600	0.19458500
F	2.81142400	-4.63883300	0.09404600
F	4.60871000	2.85092000	0.19411000
F	2.35975200	4.89584000	0.09346400
F	-2.87161200	4.64850200	-0.00663200
F	-4.92120300	2.39801000	0.02684000

CoPCl(Singlet)-MeOH

C	-2.77439000	-3.19600600	-0.14203800
C	-1.44860000	-2.63698600	-0.04352500
N	-1.50703400	-1.26417200	-0.04007400
C	-2.83874100	-0.94801000	-0.16303500
C	-3.63680400	-2.14738400	-0.22143700
C	-0.29057000	-3.39726800	0.01742800
C	0.99397200	-2.87789400	0.04679600
N	1.31291700	-1.53775300	0.07964100
C	2.68838500	-1.48197300	0.02670700
C	3.24216800	-2.81078700	-0.00013700
C	2.19184700	-3.67650200	0.01733900
C	3.44404200	-0.32093300	0.00883000
C	2.91789600	0.96131600	0.02163600
N	1.58364800	1.27775900	0.04455800
C	1.52557900	2.64756800	0.06123700
C	2.85573900	3.20860900	0.06340800
C	3.72063800	2.16117500	0.03386000
Co	0.03771400	0.01311100	-0.04883800
O	0.10187600	-0.01102500	2.05612300
C	-1.07642800	-0.06007000	2.87904600
C	0.36630600	3.40610400	0.05902900
C	-0.91625500	2.88450800	0.00328400
N	-1.23616100	1.54920800	-0.01197400
C	-2.60336900	1.49445800	-0.13728800
C	-3.15793900	2.82522000	-0.17157300
C	-2.11091000	3.68805700	-0.07927700
C	-3.35995100	0.33526200	-0.20643300
Cl	0.09911600	0.00627100	-2.26417600
H	4.30057800	-3.03314700	-0.03327400
H	2.20726200	-4.75826200	-0.00136000
H	-2.99342500	-4.25551600	-0.15848000
H	-4.71475900	-2.16308000	-0.31395600
H	3.07427800	4.26817300	0.07886000
H	4.80246100	2.17528400	0.02245100
H	-4.21320800	3.04774900	-0.25912600
H	-2.12332400	4.76997400	-0.07721400
H	-4.43521200	0.44004500	-0.30618400
H	0.47062300	4.48597400	0.06737600
H	4.52371000	-0.42288500	-0.02155100
H	-0.39616200	-4.47691600	-0.00156500
H	-1.69416200	-0.93008600	2.64147900
H	-0.78346500	-0.07544000	3.93351500
H	-1.63559500	0.85040900	2.66907100
H	0.62285000	-0.82074500	2.17238500

CoP(Doublet)-MeOH

Co	0.04826300	-0.01707000	-0.16265000
N	-1.57333400	1.15453100	-0.30166600
N	-1.11777900	-1.63693800	-0.26009400
N	1.21867000	1.61351700	-0.19378600
N	1.67381400	-1.17988000	-0.19791000
C	-1.61058000	2.53053100	-0.31518300

C	-2.97269800	3.00039200	-0.39372600
C	-3.76579100	1.89573400	-0.43224100
C	-2.88760500	0.75233300	-0.37402800
H	-3.26350100	4.04245400	-0.42198500
H	-4.84464300	1.84043300	-0.49743700
C	-3.32231000	-0.56542400	-0.38297200
C	-0.50165800	3.36393300	-0.26881700
C	-2.96040800	-3.04022300	-0.35020000
C	-1.85700700	-3.83310600	-0.29123900
C	-0.71522200	-2.95172800	-0.23985300
C	-2.49121300	-1.67528800	-0.33192800
H	-4.00089600	-3.33254700	-0.40626400
H	-1.80050400	-4.91381400	-0.28916200
C	0.60166700	-3.38581800	-0.19537800
C	2.59574000	1.65097100	-0.18976400
C	3.06485200	3.01439300	-0.20830200
C	1.96029600	3.80939000	-0.22913900
C	0.81639300	2.93128200	-0.22642200
H	4.10692900	3.30640800	-0.21098700
H	1.90640000	4.88999900	-0.25373900
C	3.07599800	-3.02519900	-0.16615700
C	3.86969400	-1.92173500	-0.16606700
C	2.98817900	-0.77792100	-0.18227100
C	1.71124800	-2.55347000	-0.18511500
H	3.36662000	-4.06758700	-0.15763400
H	4.95036800	-1.86558100	-0.15693200
C	3.42533200	0.53878400	-0.17711300
H	0.77698400	-4.45687200	-0.18337100
H	4.49677500	0.71204000	-0.16969600
H	-0.67759300	4.43482200	-0.28931900
H	-4.39188500	-0.74097200	-0.44071200
O	0.10805300	0.09503400	2.16062500
C	-1.10087400	0.08313600	2.92328400
H	-0.89651900	0.24965600	3.98819900
H	-1.81660800	0.83039800	2.56328900
H	-1.53700900	-0.90870500	2.79765500
H	0.50374800	0.97608900	2.20463700

CoTPFPPCl(Singlet)-MeOH

C	-3.97580500	-1.46619300	-0.09646700
C	-2.54745900	-1.60166100	0.06096700
N	-1.93941100	-0.37633800	-0.04851900
C	-2.94916000	0.52453800	-0.28952200
C	-4.22039900	-0.15468100	-0.34342900
C	-1.89984400	-2.82809900	0.22437500
C	-0.51628000	-2.98544300	0.13160300
N	0.40017000	-1.96565800	0.00736700
C	1.61503800	-2.57716300	-0.20784100
C	1.45776800	-4.00947900	-0.19978500
C	0.14669800	-4.26254500	0.04575700
C	2.83997200	-1.92131200	-0.33344800
C	2.98510200	-0.54190500	-0.17667900
N	1.96646600	0.35272400	0.03897800
C	2.56933500	1.56963500	0.23292500
C	4.00464600	1.43285600	0.16065800
C	4.26101400	0.12998800	-0.11571900
Co	0.01350800	-0.00638900	-0.04960200
O	0.08562100	-0.05468100	2.04791700
C	-1.06895900	0.09369500	2.89857600
C	1.91522400	2.79063400	0.40042000
C	0.53635000	2.94754700	0.25736400
N	-0.36815300	1.93836600	0.03659500
C	-1.57692500	2.55468500	-0.17033000
C	-1.43322200	3.98596900	-0.05656300
C	-0.13049000	4.22750000	0.23443700
C	-2.79720100	1.90837600	-0.37417800
Cl	0.05134200	0.02041300	-2.26374100
H	2.25230500	-4.72422100	-0.35284200
H	-0.33753900	-5.22358600	0.13271100
H	-4.68557500	-2.27901700	-0.05669900
H	-5.17142900	0.31848200	-0.53691500
H	4.71256000	2.23907500	0.28207600
H	5.22130000	-0.34635800	-0.24551700
H	-2.23477300	4.70159900	-0.16326400
H	0.34661700	5.18102000	0.40421200
H	-1.77040900	-0.73504500	2.77175300
H	-0.73990800	0.15762400	3.94005200
H	-1.54865600	1.02812500	2.61136000
H	0.49552600	-0.91804200	2.20575800
C	2.74805500	4.00037900	0.67524600
C	3.27088300	4.23489600	1.95093000
C	3.05062800	4.93373000	-0.32150400
C	4.05923600	5.34834400	2.23189400
C	3.83453400	6.05658200	-0.06354000
C	4.34076000	6.26196300	1.21831300
C	4.06558700	-2.73740900	-0.58235500
C	4.64049900	-3.52307600	0.42153800
C	4.69336300	-2.73884400	-1.83279700
C	5.78331100	-4.28690700	0.19879400
C	5.84038800	-3.49172100	-2.07809100
C	6.38501800	-4.26873200	-1.05795900
C	-2.74618700	-4.03593800	0.45999600
C	-3.30449000	-4.26982400	1.72057700
C	-3.03140600	-4.96309900	-0.54688200
C	-4.10920900	-5.37594900	1.97998000
C	-3.83150300	-6.07986100	-0.31152000
C	-4.37243900	-6.28426000	0.95629600
C	-4.00617600	2.74797800	-0.62675900
C	-4.22274300	3.35236600	-1.86980600
C	-4.96158100	2.97422500	0.36895700
C	-5.34266000	4.14487000	-2.11597600
C	-6.08985700	3.75904000	0.14539900
C	-6.27844500	4.34716300	-1.10378500
F	-3.06605800	-3.41146400	2.72618300
F	-4.62539400	-5.57285900	3.19751200
F	-5.14109200	-7.34939000	1.19030400
F	-4.08764300	-6.95043400	-1.29259400
F	-2.53069600	-4.79157000	-1.77558900
F	4.19520900	-2.00377700	-2.83172700
F	6.41768800	-3.47624500	-3.28323100
F	7.48185400	-4.99455700	-1.28343200
F	6.30776300	-5.02883700	1.18034300
F	4.08736900	-3.55579700	1.64364700
F	-4.80276200	2.42768900	1.58413600
F	-6.98524200	3.95673200	1.11912100
F	-7.35437200	5.10371600	-1.32908800
F	-5.52560300	4.70821400	-3.31392900
F	-3.34313700	3.17745300	-2.86063200
F	3.01569100	3.37417400	2.94620700
F	4.54234500	5.54672300	3.46300400
F	5.09397100	7.33329800	1.47484700
F	4.10804300	6.93229300	-1.03573700
F	2.58297000	4.76157700	-1.56318000

CoTPPBr$_8$Cl(Singlet)-MeOH

C	-3.83933600	-0.68435000	1.30495300
C	-2.67712100	-1.13112000	0.56587200
N	-1.95544700	-0.02045200	0.18602500
C	-2.70708700	1.09514600	0.47158300
C	-3.86464800	0.67974600	1.23739600
C	-2.37729900	-2.43005100	0.10794800
C	-1.09276000	-2.72898000	-0.37680100
N	0.02853200	-2.01436500	0.00525600
C	1.13757400	-2.70645400	-0.45062100
C	0.68953700	-3.80909300	-1.26611700
C	-0.67693600	-3.82724600	-1.21551600
C	2.44039000	-2.39681700	-0.02852700
C	2.73274800	-1.11090500	0.46874400
N	1.99518300	0.00098400	0.14333800
C	2.70562500	1.11130600	0.53533500
C	3.85260100	0.67261000	1.30445500
C	3.87413900	-0.69045100	1.25620900
Co	0.01558000	-0.00908200	-0.00521600
O	0.13990000	-0.13721400	2.09722700
C	-0.52387600	0.71325600	3.04967900
C	2.40337300	2.40823200	0.07979600
C	1.11720800	2.70237500	-0.40606200
N	0.00068500	1.98600600	-0.02860100
C	-1.10968700	2.67931400	-0.47358300
C	-0.66529000	3.78941000	-1.28603600
C	0.69973300	3.80715200	-1.23906900
C	-2.41100300	2.37346700	-0.04455400
Cl	-0.01704000	-0.01847000	-2.22294700
H	-1.60249600	0.53622900	3.06580800
H	-0.09919400	0.54520000	4.04373800
H	-0.32477600	1.73639900	2.73359400
H	-0.07934600	-1.06828900	2.25194000
C	3.45500100	3.45857600	0.08456100
C	3.26458800	4.65148700	0.79850600
C	4.65053400	3.27311800	-0.62654300
C	4.25338800	5.63282900	0.81143100
H	2.34295300	4.80008900	1.35338700
C	5.63030300	4.26340700	-0.63014400
H	4.79904700	2.35697500	-1.18995400
C	5.43690800	5.44324700	0.09315100
H	4.09958200	6.54673300	1.37764900
H	6.54556600	4.11421200	-1.19529100
H	6.20433100	6.21185700	0.09617300
C	3.52125300	-3.41292500	-0.11700500
C	3.40750700	-4.63848700	0.55680700
C	4.67347400	-3.15626300	-0.87587400
C	4.42913200	-5.58255900	0.48307900
H	2.52027800	-4.84153500	1.14921000
C	5.68592600	-4.10921500	-0.96595800
H	4.76180100	-2.21420900	-1.40843200
C	5.56893300	-5.32222000	-0.28243500
H	4.33513900	-6.52268400	1.01862900
H	6.56674300	-3.90503600	-1.56747800
H	6.36177200	-6.06183000	-0.34654600
C	-3.43734300	-3.47273200	0.09927900
C	-3.26436400	-4.66791500	0.81361000
C	-4.62191200	-3.27848000	-0.62762100
C	-4.25966900	-5.64291400	0.81185200
H	-2.35031700	-4.82466400	1.37889300
C	-5.60821600	-4.26210400	-0.64553400
H	-4.75655700	-2.36094700	-1.19225600
C	-5.43233600	-5.44428600	0.07846100
H	-4.11900700	-6.55903600	1.37788700
H	-6.51466800	-4.10616300	-1.22291300
H	-6.20470600	-6.20786400	0.06993600
C	-3.49365600	3.38782900	-0.14723600
C	-4.63214700	3.13148300	-0.92620800
C	-3.39396500	4.61037700	0.53381100
C	-5.64570900	4.08213800	-1.02843300
H	-4.70895700	2.19175700	-1.46466800
C	-4.41715900	5.55191300	0.44808400

H	-2.51608600	4.81414300	1.13979300
C	-5.54355100	5.29201500	-0.33705300
H	-6.51582800	3.87856800	-1.64552700
H	-4.33424300	6.49000600	0.98900600
H	-6.33731600	6.02974700	-0.41069100
Br	-5.00790200	-1.73704900	2.40545600
Br	-5.08678400	1.78484300	2.22148600
Br	-1.77426500	-4.98569900	-2.27667400
Br	1.73806200	-4.92763700	-2.41525000
Br	5.06561100	-1.79148800	2.28020500
Br	4.99982100	1.73560300	2.41567200
Br	1.79724300	4.96689700	-2.29868800
Br	-1.71508300	4.91404100	-2.42869200

CoTPPCl(Singlet)-MeOH

C	3.95100300	-1.51644800	0.17823000
C	2.96953000	-0.45919500	0.20282200
N	1.70603700	-0.98491400	0.04345300
C	1.87955800	-2.33844900	-0.13291300
C	3.27956600	-2.67356600	-0.05480100
C	3.29046600	0.89617700	0.33077300
C	2.33624500	1.91313400	0.22819400
N	0.97125400	1.74143500	0.10880500
C	0.45128800	3.00192800	-0.10507700
C	1.50578700	3.98161800	-0.08374700
C	2.66783600	3.31159200	0.13502200
C	-0.90111700	3.31904600	-0.25425300
C	-1.91603400	2.36586600	-0.13860300
N	-1.74034300	1.01678600	0.06387000
C	-3.00204600	0.48467900	0.17480900
C	-3.99404500	1.52659100	0.05282300
C	-3.32318500	2.68533600	-0.16631000
Co	-0.02261300	0.00818700	-0.00151000
O	-0.05803000	0.09490400	2.10463500
C	0.47220100	-0.94801300	2.94057800
C	-3.32466700	-0.87056100	0.28452500
C	-2.37171500	-1.88739900	0.17841600
N	-1.01089100	-1.71788300	0.06057100
C	-0.48862200	-2.97701600	-0.13568700
C	-1.54529200	-3.95821300	-0.12827300
C	-2.70395800	-3.28902200	0.10217200
C	0.86640400	-3.29273400	-0.26296000
Cl	-0.02109400	0.03122300	-2.22116800
H	1.36223100	5.04374300	-0.21256900
H	3.66724400	3.71350900	0.20475000
H	5.01275700	-1.37737300	0.31318600
H	3.67955800	-3.67259600	-0.14000800
H	-5.06111300	1.36967600	0.09682300
H	-3.72909600	3.67219700	-0.32830700
H	-1.40410900	-5.01916300	-0.26740400
H	-3.70107200	-3.69265100	0.18912300
H	1.53419700	-1.11878600	2.74594800
H	0.31328600	-0.68790400	3.99195500
H	-0.08988000	-1.84890900	2.69865100
H	0.44696100	0.91326400	2.22881700
C	-4.76708200	-1.24366200	0.43982100
C	-5.48582000	-1.81475400	-0.62214900
C	-5.43135000	-1.01326700	1.65427000
C	-6.83139500	-2.15248100	-0.47042600
H	-4.98421000	-1.98466700	-1.57025200
C	-6.77702600	-1.35133800	1.80605700
H	-4.88440200	-0.56919500	2.48109800
C	-7.48058800	-1.92312100	0.74440500
H	-7.37343500	-2.58990000	-1.30413900
H	-7.27443900	-1.16944400	2.75466700
H	-8.52800300	-2.18590600	0.86193800
C	-1.27049200	4.74538700	-0.52088400
C	-0.99227100	5.32376300	-1.76916700
C	-1.89011400	5.53218400	0.46233600
C	-1.32719500	6.65373900	-2.02751400
H	-0.51780700	4.72006900	-2.53714300
C	-2.22513600	6.86216700	0.20352100
H	-2.10429000	5.09633200	1.43400700
C	-1.94456700	7.42674800	-1.04219600
H	-1.10881900	7.08383900	-3.00089100
H	-2.70167900	7.45785000	0.97714000
H	-2.20547400	8.46181300	-1.24351300
C	4.72605700	1.28748100	0.49914100
C	5.17708100	1.84309900	1.70647400
C	5.64703000	1.12018400	-0.54730800
C	6.51270000	2.21489700	1.86724700
H	4.47373700	1.98019200	2.52305200
C	6.98245900	1.49208300	-0.38717500
H	5.30606000	0.70376900	-1.49045900
C	7.41980900	2.03928800	0.82077200
H	6.84409000	2.63926500	2.81085900
H	7.67985900	1.35927900	-1.20947100
H	8.45933600	2.32887500	0.94469700
C	1.26078000	-4.71474500	-0.51599400
C	1.78891400	-5.08642200	-1.76234000
C	1.12236800	-5.69832700	0.47570200
C	2.16335200	-6.40760900	-2.01110000
H	1.89607500	-4.33265900	-2.53671100
C	1.49764900	-7.01944300	0.22699800
H	0.72267900	-5.42113700	1.44697700
C	2.01872700	-7.37799000	-1.01767500
H	2.56498900	-6.67858300	-2.98342700
H	1.38670000	-7.76694700	1.00758300
H	2.31051300	-8.40616700	-1.21166900

FePCl(Singlet)-MeOH

Fe	-0.04419000	-0.01913700	0.22296000
C	1.73231900	2.46066100	0.08387500
N	1.64230400	1.08751000	0.07648600
C	2.93594800	0.62369800	0.14104900
C	3.85873700	1.72839200	0.17983500
C	3.11254300	2.86745300	0.14283200
N	1.06429700	-1.69225200	0.03006700
C	2.43488700	-1.78393100	0.09852200
C	2.84112300	-3.16596300	0.09497900
C	1.70314700	-3.91120100	0.03051600
C	0.59978200	-2.98589300	-0.00264900
C	3.31314200	-0.71148900	0.15371100
C	-0.73412900	-3.36285500	-0.05385200
C	-1.80650600	-2.48350200	-0.07253000
N	-1.71693400	-1.11322500	-0.04296700
C	-3.00946000	-0.64853600	-0.08075700
C	-3.93388500	-1.75301300	-0.13474800
C	-3.18757300	-2.89122400	-0.13134900
C	-3.38978500	0.68570400	-0.08339300
C	-2.51337900	1.76102700	-0.06584200
N	-1.13858200	1.66958800	-0.05413600
C	-0.67441300	2.96704900	-0.01470100
C	-1.77892800	3.88906800	-0.03066600
C	-2.91837500	3.14167900	-0.06071400
C	0.66060600	3.34149200	0.03892100
H	-3.52374200	-3.91904300	-0.16575700
H	-5.01038800	-1.65142700	-0.17303100
H	-3.94584200	3.48061100	-0.07428200
H	-1.68012800	4.96644500	-0.01352500
H	3.86784500	-3.50468800	0.13799600
H	1.60218500	-4.98826900	0.01024100
H	3.45003100	3.89541400	0.15634200
H	4.93500000	1.62845300	0.22909700
H	0.88309300	4.40312000	0.06164800
H	4.37367200	-0.93318600	0.20957200
H	-0.95509500	-4.42474700	-0.07546500
H	-4.45219300	0.90461400	-0.10077000
Cl	-0.12684100	-0.00664000	2.53800000
O	-0.09929300	0.08591700	-2.37277800
C	1.07414200	0.09761900	-3.18366900
H	1.82638500	0.80121700	-2.80760400
H	1.49026500	-0.91058700	-3.14542500
H	0.83730200	0.34052300	-4.22757300
H	-0.47608600	0.97589400	-2.34458500

FeP(Quintet)-MeOH

C	-3.13050100	-0.15866900	-0.18577000
N	-2.01171200	0.63315800	-0.15105000
C	-2.42845500	1.93590000	-0.24575700
C	-3.87778900	1.97355800	-0.30774300
C	-4.31087900	0.68094900	-0.27091600
Fe	-0.02862500	-0.04094400	-0.00677300
O	-0.15379700	0.10812000	2.21954000
C	0.91418100	0.62937700	3.02285000
C	-1.57426800	3.04285500	-0.31427900
C	-0.17204600	3.03509300	-0.35526500
N	0.61776100	1.91225300	-0.30830300
C	1.92576100	2.32388100	-0.39116200
C	1.96481500	3.76524400	-0.48966600
C	0.67027500	4.20404500	-0.46809700
C	3.04491700	1.47794700	-0.39531500
C	3.05511900	0.07992800	-0.34096600
N	1.93884800	-0.70726000	-0.22800100
C	2.35127000	-2.01272400	-0.27442400
C	3.79777900	-2.05624600	-0.38966900
C	4.23232500	-0.76494300	-0.43070500
C	1.49769900	-3.12105000	-0.25187600
C	0.09549100	-3.11437800	-0.22625300
N	-0.69138900	-1.99101800	-0.20652500
C	-2.00058500	-2.40350600	-0.19429000
C	-2.04365900	-3.84880600	-0.21033000
C	-0.74991400	-4.28747600	-0.22982300
C	-3.11937400	-1.55822100	-0.18081800
H	5.24919400	-0.40678100	-0.52902100
H	4.39021500	-2.96048500	-0.44767800
H	-0.39444200	-5.30982300	-0.24946100
H	-2.94794200	-4.44387400	-0.21128800
H	0.31304800	5.22416100	-0.53017900
H	2.86643100	4.35850700	-0.57412600
H	-5.33004900	0.31859100	-0.31542000
H	-4.47418900	2.87353800	-0.38783900
H	-4.08896200	-2.04832600	-0.19502100
H	-2.05018600	4.01755100	-0.37764900
H	4.01236000	1.96523800	-0.47981800
H	1.97235700	-4.09782800	-0.28303700
H	0.68616800	0.51527000	4.08827300
H	1.79694000	0.03924500	2.77705400
H	1.11223800	1.68126100	2.79216800
H	-0.96609900	0.60685800	2.38163100

$MgPBr_8$(Singlet)-MeOH

C	2.89438500	-1.09696300	0.00326700
N	2.08339200	0.00851800	0.06363600
C	2.88488100	1.12089200	0.00318600
C	4.26936300	0.69918700	-0.06519900

C	4.27520100	-0.66340000	-0.06511700
Mg	0.01337900	0.00008400	0.32207500
O	0.11128200	0.00072600	2.39859800
C	-0.90844500	0.00225200	3.41305200
C	1.11065400	2.87457400	-0.03283500
N	0.00626300	2.06341400	0.00505000
C	-1.10405800	2.86552900	-0.04265000
C	-0.68281500	4.25179200	-0.10650900
C	0.67856500	4.25734700	-0.10055500
C	-2.86297000	1.09681200	-0.02373800
N	-2.05244100	-0.00863300	0.04332900
C	-2.85349100	-1.12094000	-0.02355000
C	-4.23750900	-0.69923100	-0.10341700
C	-4.24334000	0.66324300	-0.10348700
C	-1.07969100	-2.87482500	-0.04217900
N	0.02396600	-2.06350100	0.00554900
C	1.13504300	-2.86547900	-0.03252000
C	0.71448800	-4.25177400	-0.10028000
C	-0.64689900	-4.25752800	-0.10609800
H	-0.84612400	-0.90160400	4.02648200
H	-0.82534400	0.89210600	4.04418800
H	-1.86375800	0.01855500	2.88936500
H	0.98858000	-0.00832300	2.80074400
Br	1.88204600	-5.76634300	-0.17612200
Br	-1.80099500	-5.78181600	-0.19149100
Br	-5.75104500	-1.86578400	-0.20854900
Br	-5.76680700	1.81681300	-0.20854100
Br	-1.84956900	5.76639400	-0.19212000
Br	1.83348300	5.78158900	-0.17599900
Br	5.78389000	1.86555300	-0.15806900
Br	5.79966100	-1.81679500	-0.15758500
C	-2.42871300	2.42380200	-0.04276200
C	2.43897000	2.44406200	-0.02073700
C	2.45971300	-2.42388600	-0.02051300
C	-2.40800700	-2.44419100	-0.04240800
H	-3.19672300	3.18679600	-0.09188400
H	3.20072300	3.21369000	-0.06364600
H	3.22793800	-3.18705100	-0.06344600
H	-3.16953200	-3.21365800	-0.09151600

$MgPCl_8$(Singlet)-MeOH

C	-1.37562600	2.76556500	-0.08037500
N	-1.54792700	1.40728400	-0.01219800
C	-2.89203600	1.14502600	-0.06926500
C	-3.61209100	2.40136700	-0.14804800
C	-2.67764300	3.40005700	-0.15477000
Mg	-0.02635100	-0.01103300	0.26734500
O	-0.06587900	0.08438600	2.39299100
C	1.08361800	0.12217700	3.25861100
C	-2.80410000	-1.35091700	-0.08420700
N	-1.44599500	-1.51955700	-0.04814200
C	-1.18271200	-2.86215000	-0.09183200
C	-2.43927200	-3.58653800	-0.15029200
C	-3.43890600	-2.65480500	-0.14580000
C	1.31436100	-2.77991100	-0.10046800
N	1.48820800	-1.42226100	-0.04338800
C	2.83100100	-1.16079400	-0.12306100
C	3.54951900	-2.41799400	-0.20858900
C	2.61484800	-3.41590400	-0.19484700
C	2.74381200	1.33538800	-0.14266200
N	1.38634300	1.50449100	-0.07457400
C	1.12179500	2.84763700	-0.12291400
C	2.37649700	3.57068300	-0.21439000
C	3.37639900	2.63848100	-0.22665700
H	1.50010700	1.13231300	3.31979000
H	0.81853800	-0.23801500	4.25681800
H	1.82226900	-0.54676100	2.81799100
H	-0.76187600	0.65643600	2.74149600
Cl	-2.96439000	5.09633200	-0.25199400
Cl	-5.32428500	2.57350300	-0.23503400
Cl	-5.13610700	-2.94328600	-0.21189100
Cl	-2.60821800	-5.29945400	-0.22365900
Cl	2.89886500	-5.11233500	-0.29059600
Cl	5.26009100	-2.59049700	-0.32382900
Cl	5.07175300	2.92730000	-0.33349900
Cl	2.54458700	5.28342300	-0.30253700
C	0.08637300	-3.44736600	-0.10246200
C	-3.47567300	-0.12515500	-0.08153100
C	-0.14764600	3.43290700	-0.10933900
C	3.41495400	0.10898400	-0.14915300
H	0.12168000	-4.53026100	-0.14792200
H	-4.55864300	-0.16279000	-0.12329100
H	-0.18399600	4.51550400	-0.16169900
H	4.49687800	0.14598000	-0.21317700

$MgPF_8$(Singlet)-MeOH

C	-1.28266400	2.80535400	-0.14319700
N	-1.50053700	1.45205300	-0.05990500
C	-2.85573300	1.23905900	-0.11729000
C	-3.52304700	2.51547800	-0.21081600
C	-2.55769500	3.47666700	-0.22659700
Mg	-0.03364900	-0.01526100	0.21107800
O	-0.06036100	0.11004200	2.34144200
C	1.10671900	0.13614600	3.18216500
C	-2.85566900	-1.25155100	-0.12773100
N	-1.50177000	-1.46633100	-0.09548400
C	-1.28920800	-2.81993700	-0.14437300
C	-2.56728200	-3.49109600	-0.20202800
C	-3.52913300	-2.52803200	-0.19198000
C	1.20196400	-2.82689800	-0.16861600
N	1.42255200	-1.47402100	-0.10733100
C	2.77528700	-1.26245700	-0.20401400
C	3.43962800	-2.54041000	-0.30455800
C	2.47394800	-3.50055400	-0.28287800
C	2.77593000	1.22827200	-0.22981800
N	1.42360200	1.44381300	-0.14643800
C	1.20875900	2.79782300	-0.20430300
C	2.48344000	3.46711000	-0.31770700
C	3.44556200	2.50357500	-0.33319800
F	2.62330400	-4.82495400	-0.36781400
F	4.76146800	-2.69876000	-0.41451100
F	4.76872400	2.65705500	-0.43481900
F	2.63742700	4.79153800	-0.40070600
F	-4.85506100	-2.68111600	-0.24186300
F	-2.72296500	-4.81604700	-0.26463400
F	-2.71091400	4.80045500	-0.31943400
F	-4.84732200	2.67320100	-0.28472800
H	1.58863800	1.11854500	3.16244300
H	0.84149300	-0.13338100	4.20876900
H	1.79224100	-0.60865700	2.77875800
H	-0.70621200	0.75792300	2.65241200
C	-0.04552800	-3.45695900	-0.16576200
C	-3.49034300	-0.00642800	-0.12650400
C	-0.03540400	3.43497100	-0.18739800
C	3.40995600	-0.01761800	-0.24091500
H	-0.04912400	-4.54100100	-0.21779700
H	-4.57476800	-0.00631900	-0.16986400
H	-0.03371300	4.51835800	-0.25269300
H	4.49233300	-0.01870900	-0.32069200

MgP(Singlet)-MeOH

Mg	-0.05155000	0.02400100	0.06351200
N	1.13957200	1.70792300	-0.23222500
N	-1.74783400	1.21405900	-0.17387700
N	1.62473400	-1.17501200	-0.30499900
N	-1.26006700	-1.67067100	-0.16651300
C	2.50558200	1.73261000	-0.34532900
C	2.95822700	3.10662100	-0.42716300
C	1.84472900	3.89467800	-0.37622500
C	0.70500500	3.00726400	-0.26320300
H	3.99020500	3.41842000	-0.52609500
H	1.79129400	4.97480800	-0.42522600
C	-0.63809600	3.40772300	-0.23005500
C	3.32716700	0.59803500	-0.40579700
C	-3.14597400	3.04314700	-0.22458200
C	-3.93601200	1.93091500	-0.21131600
C	-3.04847300	0.78502300	-0.18081500
C	-1.77134800	2.58305000	-0.20301100
H	-3.45603600	4.07989000	-0.25520900
H	-5.01730600	1.88178300	-0.22879400
C	-3.45354900	-0.55704000	-0.17878600
C	1.64521900	-2.54447700	-0.36647200
C	3.01375100	-3.00193200	-0.49934400
C	3.80367000	-1.88876800	-0.52269400
C	2.92243000	-0.74468300	-0.40382400
H	3.32049200	-4.03732500	-0.57647000
H	4.88055100	-1.83888000	-0.62218500
C	-3.08969500	-3.06377500	-0.28188400
C	-1.97624300	-3.85364900	-0.32276100
C	-0.83027700	-2.97032200	-0.26140100
C	-2.63146900	-1.69280700	-0.19483800
H	-4.12628600	-3.37326000	-0.32338000
H	-1.92863800	-4.93214400	-0.40420600
C	0.51217000	-3.36995900	-0.32923300
H	-4.52485100	-0.73726600	-0.19713900
H	0.69310700	-4.43922000	-0.39704600
H	4.39469900	0.77962800	-0.49510900
H	-0.82201200	4.47816700	-0.25845700
O	-0.02585600	-0.18252900	2.20457700
C	1.18011200	-0.12628900	2.98346500
H	0.94294500	-0.09229200	4.05170000
H	1.83397800	-0.97706200	2.76811400
H	1.68788900	0.79465700	2.69722400
H	-0.51097400	-0.99398100	2.40843900

MgTPFPP(Singlet)-MeOH

Mg	0.00688800	-0.01419300	-0.23909800
N	-0.25200300	2.03388400	0.11768600
N	2.06663600	0.24680400	0.01447100
N	-2.03986200	-0.27801000	0.05865100
N	0.27897600	-2.06436600	0.06418100
C	-1.44871700	2.70263000	0.13296600
C	-1.20648200	4.13138900	0.13630500
C	0.14321000	4.30416700	0.13043000
C	0.73812200	2.98252900	0.12159600
H	-1.96442100	4.90106100	0.14102800
H	0.68245700	5.24013600	0.12864700
C	2.12391600	2.71850900	0.11784000
C	-2.72271900	2.09665400	0.14274800
C	4.15242700	1.20090800	0.23025500
C	4.32714000	-0.14904800	0.21557100
C	3.01318400	-0.74354800	0.08405200
C	2.72993000	1.44412200	0.10861500
H	4.91462000	1.95843300	0.34060000
H	5.25740200	-0.68969800	0.31192100
C	2.74994200	-2.12965400	0.06039000

C	-2.70205000	-1.47603700	0.12948200
C	-4.12416000	-1.23564200	0.26730700
C	-4.29953400	0.11387000	0.27699700
C	-2.98546900	0.71047400	0.14914800
H	-4.88532800	-1.99545200	0.36799400
H	-5.22921900	0.65293500	0.38725800
C	1.23205400	-4.16222700	0.02082500
C	-0.11689900	-4.33435700	0.03053000
C	-0.71104900	-3.01235900	0.06319400
C	1.47511600	-2.73337200	0.04746200
H	1.98961100	-4.93168200	-0.00669900
H	-0.65708900	-5.26949700	0.01195900
C	-2.09645800	-2.74995800	0.09659600
O	0.07001500	0.07504900	-2.36800200
C	-0.82364100	0.82970300	-3.20655100
H	-0.53102400	1.88351200	-3.24874500
H	-0.84611900	0.40510100	-4.21465200
H	-1.81427400	0.75023700	-2.75952200
H	0.97197400	0.13560300	-2.70915000
C	3.04252700	3.89889100	0.13399600
C	3.20181200	4.69738600	1.27165500
C	3.78902300	4.24960200	-0.99592100
C	4.05975400	5.79527500	1.28879700
C	4.65665700	5.33880600	-1.00226000
C	4.79098500	6.11490800	0.14687300
C	-3.91030500	3.00534200	0.13725300
C	-4.28206700	3.75029500	1.26107600
C	-4.70297900	3.14381600	-1.00698100
C	-5.38823800	4.59773100	1.25121300
C	-5.81576900	3.98019400	-1.04054300
C	-6.15790200	4.71079600	0.09551600
C	-3.01371300	-3.93153400	0.11160400
C	-3.13824000	-4.75398800	1.23657600
C	-3.79310000	-4.25944300	-1.00315200
C	-3.99315000	-5.85398600	1.25634600
C	-4.65848200	-5.35080900	-1.00575100
C	-4.75705100	-6.15141100	0.12999200
C	3.93574000	-3.04100800	0.06319200
C	4.76001300	-3.16342600	-1.06051100
C	4.27491400	-3.80613900	1.18447600
C	5.87022100	-4.00414000	-1.07656500
C	5.37741500	-4.65801400	1.19125700
C	6.17824500	-4.75537100	0.05553700
F	-3.71855900	-3.51371300	-2.11458500
F	-5.38852200	-5.63754800	-2.08947300
F	-5.58181500	-7.20121500	0.13880200
F	-4.09067100	-6.61967700	2.34856200
F	-2.42298500	-4.49413700	2.33862900
F	4.48851500	-2.45924200	-2.16950100
F	6.63572800	-4.09991300	-2.16946300
F	7.23813300	-5.56702500	0.05169000
F	5.67524700	-5.37545200	2.27980300
F	3.53092700	-3.73199600	2.29537000
F	3.67692600	3.52821400	-2.12178000
F	5.35375500	5.64739200	-2.10154200
F	5.61786300	7.16289700	0.15302300
F	4.19111100	6.53790400	2.39306900
F	2.51861900	4.41585200	2.38831300
F	-4.39497500	2.46005500	-2.12060000
F	-6.55081300	4.09222800	-2.15255700
F	-7.22059600	5.51849100	0.07591800
F	-5.71883600	5.29639100	2.34237300
F	-3.56712200	3.66115000	2.38961800

MgTPPBr$_8$(Singlet)-MeOH

Mg	-0.00466100	-0.01213700	0.25631500
N	0.03926300	2.04183000	-0.08555100
N	-2.07209100	0.02934100	0.01342900
N	2.06487300	-0.05475600	0.00705700
N	-0.04727600	-2.06966000	-0.06516100
C	1.17067000	2.71840900	-0.48199600
C	0.75897600	3.85464100	-1.28314400
C	-0.60914800	3.88225300	-1.28158400
C	-1.06475300	2.76365600	-0.47910100
C	-2.38663400	2.46007900	-0.06374600
C	2.47987900	2.36135300	-0.06917000
C	-3.94113800	0.75788800	1.11289900
C	-3.96979200	-0.61032500	1.11895900
C	-2.81409700	-1.06991800	0.37073100
C	-2.76710000	1.16165400	0.36079500
C	-2.48806100	-2.38688400	-0.04127400
C	2.76060300	-1.18455900	0.36250000
C	3.93591600	-0.77424100	1.10849800
C	3.96501600	0.59429000	1.10239600
C	2.80753000	1.04760000	0.35310300
C	-0.77070300	-3.89025100	-1.24832500
C	0.59749500	-3.91837800	-1.25028400
C	1.05546300	-2.79422300	-0.45730600
C	-1.17975800	-2.74832700	-0.45392200
C	2.37869700	-2.48690600	-0.04892800
O	0.00422100	-0.08192600	2.32080900
C	0.24962900	0.96090000	3.28262100
H	-0.54131600	0.97897900	4.03802800
H	1.22573800	0.82860100	3.75879400
H	0.24152900	1.89550200	2.72227500
H	0.00653100	-0.94830500	2.74581900
C	-3.41363400	3.53517500	-0.09056000
C	-4.58717900	3.38253500	-0.84588200
C	-3.22655600	4.72013900	0.63847200
C	-5.54538300	4.39300000	-0.87817400
H	-4.73525200	2.47303500	-1.42013200
C	-4.19355200	5.72280400	0.62197100
H	-2.32328000	4.84545400	1.22806900
C	-5.35389300	5.56403100	-0.14016000
H	-6.44245900	4.26676800	-1.47722300
H	-4.04104200	6.62953700	1.20009900
H	-6.10436000	6.34902900	-0.15959300
C	3.54887800	3.39473900	-0.09582100
C	4.71424900	3.19741700	-0.85343200
C	3.40953600	4.58525100	0.63494400
C	5.71085800	4.17001600	-0.88650400
H	4.82587800	2.28357100	-1.42901200
C	4.41457900	5.54979600	0.61754000
H	2.51264400	4.74512700	1.22600500
C	5.56635400	5.34690600	-0.14707400
H	6.60118200	4.00986200	-1.48751600
H	4.29829000	6.46122600	1.19669500
H	6.34656800	6.10231700	-0.16737800
C	3.40563800	-3.56216100	-0.06935800
C	4.57767400	-3.41569100	-0.82826600
C	3.21994700	-4.74135300	0.66939400
C	5.53573200	-4.42646900	-0.85438800
H	4.72455800	-2.51088200	-1.41017200
C	4.18676100	-5.74427500	0.65889200
H	2.31759300	-4.86214400	1.26141400
C	5.34561900	-5.59160700	-0.10674600
H	6.43160000	-4.30512500	-1.45624600
H	4.03522200	-6.64647800	1.24431100
H	6.09594900	-6.37683200	-0.12153900
C	-3.55777200	-3.41967600	-0.05849500
C	-3.41800300	-4.60528100	0.68006800
C	-4.72401100	-3.22679000	-0.81592800
C	-4.42344600	-5.56949900	0.67017300
H	-2.52063000	-4.76131600	1.27139800
C	-5.72103200	-4.19917000	-0.84139700
H	-4.83592100	-2.31672900	-1.39741900
C	-5.57600900	-5.37124600	-0.09449200
H	-4.30692200	-6.47707400	1.25530000
H	-6.61207200	-4.04256400	-1.44228700
H	-6.35652200	-6.12648700	-0.10893900
Br	1.84888500	4.97856700	-2.39581100
Br	-1.65429100	5.04990600	-2.39222400
Br	5.19198300	1.64305200	2.14773100
Br	5.11480700	-1.86572500	2.16498400
Br	1.63942600	-5.09494900	-2.35461800
Br	-1.86355100	-5.02220000	-2.34992200
Br	-5.11769900	1.85819200	2.16196500
Br	-5.19096100	-1.65098900	2.17811100

MgTPP(Singlet)-MeOH

Mg	0.02998200	-0.01592900	0.19782300
N	-1.01673300	-1.79538600	-0.06531500
N	1.81719200	-1.04821400	-0.08581300
N	-1.75658800	1.03321000	-0.10165100
N	1.07602600	1.78194200	-0.03671300
C	-2.38160800	-1.94178900	-0.12597100
C	-2.70977300	-3.35088300	-0.19874400
C	-1.53291000	-4.03686700	-0.17695300
C	-0.47002100	-3.05509500	-0.11022600
H	-3.70733000	-3.75863100	-0.26796800
H	-1.39519600	-5.10716000	-0.21723000
C	0.91044900	-3.35753100	-0.10542100
C	-3.32525500	-0.88943100	-0.15535500
C	3.37122000	-2.74734000	-0.14469600
C	4.05951700	-1.57256300	-0.14094300
C	3.07818900	-0.50594600	-0.11243200
C	1.96172100	-2.41320700	-0.10200300
H	3.77659000	-3.74775800	-0.17659600
H	5.13077400	-1.43825800	-0.16064600
C	3.38546200	0.87370200	-0.10368900
C	-1.90108500	2.39983800	-0.12557000
C	-3.30905300	2.73306300	-0.19566800
C	-3.99768900	1.55762800	-0.20391200
C	-3.01805100	0.49101500	-0.15650400
H	-3.71425000	3.73322100	-0.23850300
H	-5.06839400	1.42391800	-0.24623300
C	2.77214400	3.33469700	-0.16038900
C	1.59560100	4.02293200	-0.15597700
C	0.53087800	3.04361100	-0.09722700
C	2.44245800	1.92699500	-0.08504000
H	3.77094800	3.74097500	-0.22029200
H	1.46040700	5.09328100	-0.20403600
C	-0.85010100	3.34525600	-0.11426000
O	0.04778600	0.20951500	2.34194800
C	-1.11325900	-0.01094700	3.15842800
H	-0.85456800	0.06512000	4.21953900
H	-1.91350200	0.69410700	2.91246800
H	-1.45222400	-1.02412600	2.94232000
H	0.38991800	1.10201600	2.49136000
C	1.29542400	-4.80738200	-0.12705900
C	1.11304100	-5.58491200	-1.28155700
C	1.85059200	-5.41735400	1.00880500
C	1.47274700	-6.93343400	-1.29908500
H	0.69171200	-5.12288600	-2.16959400
C	2.21112700	-6.76562900	0.99203200
H	1.99456800	-4.82696100	1.90907200

C	2.02273000	-7.52832600	-0.16206000
H	1.32728400	-7.51755600	-2.20358900
H	2.63636200	-7.22043600	1.88247700
H	2.30322200	-8.57770600	-0.17556300
C	-4.77382500	-1.27183000	-0.21347400
C	-5.53525400	-1.03751500	-1.36990400
C	-5.40204900	-1.87734200	0.88649700
C	-6.88315800	-1.39519600	-1.42350900
H	-5.06000200	-0.57788100	-2.23144800
C	-6.74987500	-2.23567000	0.83413900
H	-4.82608300	-2.06310500	1.78847500
C	-7.49538200	-1.99517300	-0.32142900
H	-7.45343100	-1.20937700	-2.32944100
H	-7.21774800	-2.69985000	1.69795900
H	-8.54441900	-2.27401300	-0.36320800
C	-1.23498400	4.79494400	-0.15469700
C	-1.81167500	5.41682600	0.96377100
C	-1.03099600	5.56180800	-1.31290900
C	-2.17188900	6.76483400	0.92767600
H	-1.97470800	4.83607700	1.86722300
C	-1.38999900	6.91003600	-1.35027600
H	-0.59299900	5.09119400	-2.18820700
C	-1.96137500	7.51624600	-0.22985900
H	-2.61413100	7.22811200	1.80537300
H	-1.22729500	7.48526400	-2.25750900
H	-2.24133300	8.56541400	-0.25894400
C	4.83470800	1.25617800	-0.14035100
C	5.61058500	1.03002800	-1.28865100
C	5.44846700	1.85295000	0.97240700
C	6.95906400	1.38807300	-1.32247500
H	5.14648000	0.57614500	-2.15929900
C	6.79693400	2.21119400	0.93981500
H	4.86143300	2.02935800	1.86906400
C	7.55700800	1.97966100	-0.20811500
H	7.54100000	1.20863600	-2.22225900
H	7.25417700	2.66769300	1.81336500
H	8.60659000	2.25841600	-0.23423600

MnPCl(Quintet)-MeOH

Mn	-0.04430900	-0.02068100	0.22385100
C	0.69874100	-2.97894200	0.00144500
N	1.12927400	-1.67454400	0.03096600
C	2.50130600	-1.71491900	0.09853000
C	2.94833600	-3.08545900	0.09732800
C	1.83375600	-3.86691400	0.03581600
N	1.62146900	1.15019500	0.07589900
C	2.92611800	0.72038300	0.13802700
C	3.81155700	1.85665300	0.17684400
C	3.02924400	2.97219000	0.14332400
C	1.66048800	2.52479700	0.08561900
C	3.33969000	-0.60712600	0.15036700
C	0.55414500	3.36662300	0.04271200
C	-0.77328100	2.95630400	-0.01290800
N	-1.20240000	1.64819800	-0.05689900
C	-2.57864000	1.68811500	-0.06972300
C	-3.02497300	3.05722800	-0.06194500
C	-1.90948100	3.84093300	-0.02800700
C	-3.41628600	0.57868400	-0.09051400
C	-3.00083000	-0.74808500	-0.08708300
N	-1.69733500	-1.17782300	-0.04485700
C	-1.73488900	-2.54995600	-0.07276100
C	-3.10403800	-2.99884100	-0.13589500
C	-3.88701100	-1.88457500	-0.14346600
C	-0.62810300	-3.39048800	-0.04978900
H	-1.84795400	4.92097900	-0.00794000
H	-4.06193100	3.36573800	-0.07623100
H	-4.96619400	-1.82062900	-0.18584100
H	-3.40957900	-4.03613300	-0.17039900
H	4.89063800	1.79357900	0.22430900
H	3.33667300	4.00946900	0.15842600
H	1.76986600	-4.94681000	0.01805800
H	3.98444600	-3.39420500	0.13981100
H	-0.81580600	-4.45886400	-0.06949800
H	4.40704400	-0.79394000	0.20503900
H	0.74250000	4.43482100	0.06856200
H	-4.48507900	0.76403000	-0.11022800
Cl	-0.12787800	-0.00816700	2.60684700
O	-0.09534800	0.09200000	-2.41311100
C	1.07135400	0.12422900	-3.23341600
H	0.82257500	0.35377300	-4.27753700
H	1.81079800	0.84712600	-2.86808600
H	1.51020600	-0.87418000	-3.19108600
H	-0.50402700	0.96792500	-2.40794100

NiP(Triplet)-MeOH

Ni	-0.04378700	-0.02074400	-0.05945500
N	1.59966500	1.19251700	-0.28922100
N	-1.25817300	1.63943500	-0.17547500
N	1.15935500	-1.66409100	-0.24477500
N	-1.69957100	-1.21948000	-0.19266700
C	2.90822700	0.78766200	-0.36727300
C	3.77548800	1.94308400	-0.44795000
C	2.97091700	3.04344000	-0.42011100
C	1.60892000	2.56434000	-0.32345200
H	4.85461400	1.90476100	-0.52442800
H	3.25997700	4.08548000	-0.46951400
C	0.47487200	3.37848000	-0.28487200
C	3.33965800	-0.54043600	-0.37186500
C	-2.01005000	3.81841200	-0.26813300
C	-3.11034200	3.01263700	-0.23938700
C	-2.63142100	1.64918600	-0.18833000
C	-0.85362300	2.95080400	-0.23580400
H	-1.97364900	4.89908800	-0.31942000
H	-4.15280500	3.30341300	-0.26227800
C	-3.44142100	0.51190300	-0.17509700
C	0.75234900	-2.97337100	-0.24861400
C	1.90536400	-3.84510900	-0.32067600
C	3.00549900	-3.04170900	-0.36866300
C	2.52867700	-1.67585600	-0.32480800
H	1.86482800	-4.92659500	-0.34208500
H	4.04553400	-3.33397800	-0.43722900
C	-3.88067000	-1.97173600	-0.18431900
C	-3.07596500	-3.07088300	-0.19264900
C	-1.71016500	-2.58928800	-0.19712700
C	-3.00878600	-0.81534700	-0.18222600
H	-4.96242200	-1.93309300	-0.18377200
H	-3.36610800	-4.11369300	-0.20063900
C	-0.57559700	-3.40224000	-0.21335400
H	-4.51503100	0.67643500	-0.17776900
H	-0.74283000	-4.47541200	-0.21859400
H	4.41109800	-0.70641400	-0.43705700
H	0.64166500	4.45099700	-0.32606300
O	-0.10876300	0.10192200	2.08970800
C	1.10363900	0.11119500	2.85892800
H	1.77054500	0.91959000	2.54497300
H	0.87352900	0.20188100	3.92591600
H	1.59114300	-0.84576500	2.67436000
H	-0.56629600	0.94907700	2.19034400

O=TiP(Triplet)-MeOH

Ti	0.04947000	0.01705000	0.48109600
C	1.27349300	-2.82759900	0.04192100
N	1.49407000	-1.47090900	0.00962600
C	2.85398500	-1.27129000	0.00024000
C	3.51984500	-2.55515100	-0.00620200
C	2.54622800	-3.51407400	0.01926400
N	1.52381600	1.46647200	0.13766400
C	2.87566500	1.24410400	0.04911400
C	3.55875400	2.51492500	-0.03397600
C	2.59853000	3.48904800	-0.01583100
C	1.31980400	2.82292100	0.08049400
C	3.48459100	-0.01891700	0.00565700
C	0.06583300	3.45048300	0.07754700
C	-1.19620400	2.83972400	0.09977600
N	-1.42002200	1.48736300	0.12617700
C	-2.77670300	1.29080100	0.16100100
C	-3.44360600	2.57605900	0.14078600
C	-2.46855100	3.53139300	0.10247500
C	-3.40766600	0.03974000	0.20696200
C	-2.79663000	-1.22313500	0.21907600
N	-1.43969900	-1.44400800	0.20339600
C	-1.24001300	-2.80384200	0.16837400
C	-2.52143100	-3.46924300	0.18210200
C	-3.48160900	-2.49407900	0.21301800
C	0.01169100	-3.43565600	0.10262700
H	-2.59229000	4.60655900	0.08223300
H	-4.51614500	2.72136500	0.15774800
H	-4.55639100	-2.62258300	0.22538800
H	-2.66653700	-4.54183500	0.16461200
H	4.63113100	2.64214100	-0.10836300
H	2.74001200	4.56071900	-0.07240900
H	2.67381800	-4.58892900	0.03182500
H	4.59259500	-2.69934900	-0.01853400
H	0.00121400	-4.52185400	0.10415800
H	4.57007000	-0.02778800	-0.03396100
H	0.07291600	4.53621400	0.04411100
H	-4.49367600	0.04821700	0.22821400
O	0.14764400	0.01798500	2.34877400
O	0.10034400	-0.01295000	-1.97754900
C	-1.01019700	-0.12317000	-2.87118500
H	-0.66982600	-0.14624600	-3.91295400
H	-1.61429400	-1.01226700	-2.65914500
H	-1.62254300	0.76562000	-2.71679100
H	0.67570900	-0.78602900	-2.06753300

O=VP(Doublet)-MeOH

V	-0.05192600	-0.01439900	0.55292600
C	0.49253100	-3.02579000	0.11732200
N	1.01391200	-1.75624600	0.16735500
C	2.38088100	-1.88991500	0.18810600
C	2.73354300	-3.28997000	0.14999000
C	1.56573600	-3.99220400	0.10530800
N	1.70790900	1.04555800	0.18624000
C	2.97937300	0.52486800	0.21050500
C	3.94503800	1.59831600	0.20484200
C	3.24118100	2.76612600	0.17869200
C	1.84100300	2.41321800	0.16881400
C	3.29190100	-0.83438300	0.21822100
C	0.78552300	3.32507200	0.13338100
C	-0.57352300	3.01392900	0.09549300
N	-1.09476600	1.73845200	0.07649500
C	-2.46534700	1.87224300	0.04849500
C	-2.81515800	3.27114400	0.03122600
C	-1.64690900	3.97627000	0.05986700
C	-3.37487900	0.81524900	0.02727900
C	-3.06087300	-0.54361300	0.03696800

N	-1.79313700	-1.06383400	0.10427100
C	-1.92202900	-2.42847500	0.05282600
C	-3.31994100	-2.78327000	-0.04191700
C	-4.02470700	-1.61714100	-0.05066200
C	-0.86570700	-3.33823200	0.06980300
H	-1.51398500	5.05030300	0.05754300
H	-3.82666700	3.65466100	0.00050700
H	-5.09622400	-1.48180500	-0.11864900
H	-3.69817900	-3.79546200	-0.10066100
H	5.01882500	1.46386900	0.21567600
H	3.62381700	3.77833600	0.16399500
H	1.43054300	-5.06509800	0.06344300
H	3.74574800	-3.67285500	0.15192000
H	-1.12502100	-4.39168200	0.02874800
H	4.34552100	-1.09574600	0.23582400
H	1.04735800	4.37871100	0.13449900
H	-4.42804300	1.07586300	-0.01221200
O	-0.09780400	0.00462300	2.12715200
O	-0.11701900	0.06289200	-2.09560500
C	1.00209500	0.03129200	-2.97808900
H	1.79174800	0.72575300	-2.66711000
H	1.39910300	-0.98479600	-2.94394700
H	0.70447100	0.25697100	-4.01032400
H	-0.48193700	0.95810600	-2.06828400

ZnPBr$_8$(Triplet)-MeOH

C	-2.88930700	1.11104800	-0.03716800
N	-2.08572200	0.00066800	0.00283000
C	-2.88977100	-1.10937200	-0.03698000
C	-4.27311100	-0.68001300	-0.08175100
C	-4.27282300	0.68227600	-0.08187300
O	-0.07296000	-0.00114900	2.43021900
C	0.96213400	-0.00108800	3.42087100
C	-1.12654800	-2.87096600	-0.06886500
N	-0.01739300	-2.06798900	-0.04825100
C	1.09084700	-2.87166800	-0.08226800
C	0.66211000	-4.25653600	-0.12405000
C	-0.69918300	-4.25610700	-0.11619200
C	2.85485200	-1.11091600	-0.07297100
N	2.05164700	-0.00061200	-0.02893900
C	2.85534600	1.10933600	-0.07257300
C	4.23854700	0.68002200	-0.12651900
C	4.23824900	-0.68220200	-0.12675300
C	1.09224600	2.87106000	-0.08168100
N	-0.01649800	2.06802800	-0.04775000
C	-1.12518400	2.87168600	-0.06884800
C	-0.69697800	4.25654500	-0.11619000
C	0.66432900	4.25616000	-0.12379200
H	0.91977200	0.90378000	4.03656300
H	0.89748500	-0.88875200	4.05922300
H	1.90640500	-0.01972400	2.87695700
H	-0.94513400	0.01462400	2.84256300
Br	-1.85858600	5.77641800	-0.16389800
Br	1.82617400	5.77534200	-0.18435600
Br	5.75838700	1.84056000	-0.19612200
Br	5.75755900	-1.84340900	-0.19677700
Br	1.82307100	-5.77638600	-0.18459600
Br	-1.86169600	-5.77528800	-0.16343700
Br	-5.79346700	-1.84040000	-0.14320000
Br	-5.79267300	1.84333500	-0.14347000
C	2.41560400	-2.43488000	-0.08455800
C	-2.45103900	-2.43350000	-0.05494600
C	-2.44993700	2.43496900	-0.05517600
C	2.41675800	2.43351900	-0.08388000
H	3.18102600	-3.20128800	-0.11844400
H	-3.21711000	-3.19951900	-0.08250900
H	-3.21560200	3.20138500	-0.08298900
H	3.18258600	3.19952600	-0.11765000
Zn	-0.01365700	-0.00012500	0.19370800

ZnPCl$_8$(Triplet)-MeOH

C	1.32691200	-2.78338300	-0.10716000
N	1.51695000	-1.42654700	-0.05727800
C	2.86558100	-1.18486500	-0.09842800
C	3.56797000	-2.45181300	-0.15402600
C	2.61996000	-3.43672700	-0.15915400
O	0.11267600	-0.06723000	2.37605800
C	-1.06144000	-0.11837400	3.20213600
C	2.81542900	1.30482300	-0.11368000
N	1.46013400	1.49375000	-0.09599300
C	1.21875900	2.84035000	-0.12330400
C	2.48662800	3.54565200	-0.15636400
C	3.47097100	2.59901200	-0.15088500
C	-1.27118700	2.79464900	-0.13299900
N	-1.46284400	1.43890100	-0.09685400
C	-2.81026300	1.19822200	-0.15301000
C	-3.51175300	2.46617500	-0.21011800
C	-2.56341400	3.44998000	-0.19758400
C	-2.76126500	-1.29135900	-0.16521100
N	-1.40567700	-1.48028800	-0.10948100
C	-1.16340800	-2.82815100	-0.14384900
C	-2.42958700	-3.53198400	-0.21440300
C	-3.41441600	-2.58481800	-0.22766900
H	-1.64863000	-1.02253000	3.01118800
H	-0.78790800	-0.06648500	4.26084200
H	-1.65831600	0.75630800	2.94380600
H	0.68862400	-0.81493300	2.58546400
Cl	2.88128700	-5.13810800	-0.22747600
Cl	5.27820400	-2.64770400	-0.21518100
Cl	5.17309500	2.85943200	-0.18706600
Cl	2.68055600	5.25635500	-0.20169700
Cl	-2.82237100	5.15154500	-0.25938500
Cl	-5.22130900	2.66239900	-0.28988300
Cl	-5.11504300	-2.84626700	-0.31137800
Cl	-2.62337500	-5.24266000	-0.27733800
C	-0.03768000	3.44607800	-0.13185200
C	3.46955500	0.07278100	-0.10790500
C	0.09315200	-3.43452300	-0.12941100
C	-3.41503200	-0.05870700	-0.17263200
H	-0.05741700	4.52977400	-0.16056700
H	4.55328600	0.09425800	-0.13447500
H	0.11311600	-4.51797800	-0.16728400
H	-4.49802800	-0.07958300	-0.22093900
Zn	0.02444500	0.01551200	0.13185400

ZnPF$_8$(Triplet)-MeOH

C	1.28921500	-2.79730600	-0.16127300
N	1.49738100	-1.44140800	-0.09912000
C	2.85201500	-1.22161400	-0.13855600
C	3.52770400	-2.49498500	-0.20476400
C	2.56884500	-3.46176500	-0.21868000
O	0.11041900	-0.08122900	2.33510000
C	-1.07382700	-0.13862000	3.14389500
C	2.83879500	1.26166000	-0.15056400
N	1.48402500	1.46898800	-0.13892300
C	1.26542700	2.82153400	-0.16868400
C	2.54052400	3.49988400	-0.19690500
C	3.50653500	2.54213400	-0.18628700
C	-1.21781500	2.81401800	-0.19332500
N	-1.42834700	1.45908900	-0.15652200
C	-2.78106300	1.24083100	-0.22487700
C	-3.45507700	2.51580600	-0.29102200
C	-2.49575900	3.48123300	-0.27132800
C	-2.76893100	-1.24230200	-0.24184300
N	-1.41447800	-1.44993900	-0.17330800
C	-1.19431000	-2.80361600	-0.21486400
C	-2.46669300	-3.48005400	-0.30331400
C	-3.43316000	-2.52178500	-0.31965400
F	-2.65186200	4.80609500	-0.32455800
F	-4.78002100	2.66420600	-0.36691600
F	-4.75677000	-2.67997300	-0.39969300
F	-2.61237300	-4.80622600	-0.36324000
F	4.83225100	2.69922800	-0.20963600
F	2.68684100	4.82640400	-0.23401100
F	2.72812000	-4.78603200	-0.28482200
F	4.85372900	-2.64302700	-0.25477200
H	-1.68049900	-1.01935600	2.90872600
H	-0.81436500	-0.13691900	4.20774600
H	-1.64731700	0.75965000	2.91461100
H	0.66201600	-0.85490500	2.51373000
C	0.02196400	3.45346600	-0.18590300
C	3.48146600	0.02361200	-0.14427100
C	0.04929300	-3.43621800	-0.19642100
C	-3.41112900	-0.00351500	-0.25263100
H	0.01895100	4.53814100	-0.21741600
H	4.56630000	0.02932200	-0.16975000
H	0.05300000	-4.52034400	-0.24435700
H	-4.49461600	-0.00845600	-0.31255900
Zn	0.03065900	0.01883700	0.07866700

ZnP(Triplet)-MeOH

Zn	0.04694000	-0.02738500	-0.03736700
N	-1.64544200	1.14683800	-0.31058900
N	1.21839300	1.68695800	-0.18761100
N	-1.11417700	-1.71848000	-0.25382900
N	1.75282900	-1.18003000	-0.19210200
C	-2.93745500	0.69563100	-0.39348900
C	-3.83865900	1.82486900	-0.49046000
C	-3.06787000	2.95067100	-0.46961000
C	-1.69088000	2.51632900	-0.35998000
H	-4.91585600	1.75528400	-0.57251300
H	-3.39142800	3.98190700	-0.53123900
C	-0.57634700	3.36186400	-0.32486900
C	-3.32238800	-0.64980400	-0.39375800
C	1.90012800	3.88324100	-0.30263200
C	3.02540600	3.11142400	-0.26227300
C	2.58950200	1.73283400	-0.19874100
C	0.76890000	2.98127800	-0.26450200
H	1.83339200	4.96190500	-0.36563200
H	4.05773400	3.43647000	-0.28578900
C	3.43100900	0.61514700	-0.17904500
C	-0.66083000	-3.01150600	-0.26235900
C	-1.78783200	-3.91731400	-0.34182600
C	-2.91331800	-3.14757100	-0.39037800
C	-2.48112500	-1.76631700	-0.34020100
H	-1.71650600	-4.99715500	-0.36750900
H	-3.94265100	-3.47465500	-0.46350700
C	3.95210000	-1.86029300	-0.18933800
C	3.18134000	-2.98513800	-0.20172900
C	1.79986900	-2.54848500	-0.20407100
C	3.04604300	-0.72970300	-0.18302400
H	5.03236500	-1.79099800	-0.18893500
H	3.50692900	-4.01742400	-0.21393000
C	0.68471500	-3.39272100	-0.22714300
H	4.49911500	0.81321100	-0.18289200
H	0.88572700	-4.46020400	-0.23818200

H	-4.38800700	-0.84867100	-0.46477200
H	-0.77583300	4.42837500	-0.37925800
O	0.07254000	0.17460100	2.24518300
C	-1.14337500	0.12783000	3.00177200
H	-0.94677100	0.30761800	4.06491300
H	-1.87845700	0.84964200	2.63058100
H	-1.54482000	-0.87863600	2.87892400
H	0.46174400	1.05747300	2.31415600

ZnTPFPP(Triplet)-MeOH

Zn	-0.01954000	0.01259900	0.08355800
N	2.01694900	-0.17540300	-0.22766700
N	-0.21864500	-2.04790700	-0.13493700
N	0.15343000	2.05952500	-0.13570000
N	-2.08055400	0.18592000	-0.05242700
C	2.92465900	0.84928800	-0.29480400
C	4.26118900	0.30528500	-0.41531200
C	4.13950900	-1.04973900	-0.41059300
C	2.72725200	-1.34603500	-0.28878200
H	5.16924500	0.88270800	-0.51012100
H	4.93032600	-1.78009400	-0.50072200
C	2.17714600	-2.64130200	-0.24759200
C	2.61390600	2.22206600	-0.25447000
C	0.26247300	-4.29901500	-0.22675400
C	-1.09209800	-4.17871800	-0.18926800
C	-1.38892200	-2.76283600	-0.12661500
C	0.80621300	-2.95732800	-0.20051400
H	0.83818800	-5.21159000	-0.27585800
H	-1.82191400	-4.97469700	-0.21396900
C	-2.68292700	-2.21111700	-0.06172300
C	-0.87205600	2.96715000	-0.10091100
C	-0.33142200	4.31069600	-0.14554700
C	1.02198900	4.19202300	-0.19636500
C	1.32091000	2.77438400	-0.19577700
H	-0.91066200	5.22233000	-0.14784000
H	1.74918400	4.98977400	-0.23455600
C	-4.33234200	-0.29286900	0.03965100
C	-4.20892100	1.06111600	0.04880000
C	-2.79241800	1.35719900	-0.01473700
C	-2.99239100	-0.83821500	-0.02949500
H	-5.24515900	-0.86876700	0.08142300
H	-5.00323500	1.79125200	0.09896800
C	-2.24247300	2.65284000	-0.03436700
O	0.07395700	-0.08603200	2.34445000
C	1.32955000	-0.14703500	3.04356000
H	1.16418300	-0.11105200	4.12556500
H	1.89540700	-1.04735600	2.78173800
H	1.90036300	0.73095800	2.74066100
H	-0.46057700	-0.85245700	2.59130000
C	-3.20126300	3.80080300	0.01170200
C	-3.98859600	4.14131700	-1.09334600
C	-3.34841800	4.58303500	1.16200800
C	-4.88564100	5.20681900	-1.06071200
C	-4.23462900	5.65647700	1.21706200
C	-5.00681900	5.96753600	0.10003000
C	3.76637500	3.17517100	-0.24952100
C	4.10633700	3.93673500	-1.37166100
C	4.55456400	3.33980800	0.89418400
C	5.17894400	4.82625800	-1.36128100
C	5.63442600	4.21841900	0.92811500
C	5.94578400	4.96509200	-0.20646400
C	3.14351100	-3.78301000	-0.23300500
C	3.36329900	-4.58942700	-1.35374900
C	3.87331400	-4.08541900	0.92121600
C	4.26574700	-5.65115500	-1.33227300
C	4.78450700	-5.13736400	0.96655500
C	4.97971200	-5.92344900	-0.16732800
C	-3.82938400	-3.17136600	-0.02419800
C	-4.10807100	-3.92543300	1.12037700
C	-4.66838100	-3.35936500	-1.12768700
C	-5.16653500	-4.82892900	1.17257600
C	-5.73701600	-4.25311900	-1.09843600
C	-5.98475700	-4.99146900	0.05668100
F	-3.89361700	3.43306100	-2.22599700
F	-5.62450300	5.50657900	-2.13429500
F	-5.86133800	6.99233000	0.14195500
F	-4.35267200	6.38436600	2.33307700
F	-2.62290500	4.30933300	2.25473400
F	3.39098100	3.82412200	-2.49814800
F	5.47965000	5.54100500	-2.45060400
F	6.97693600	5.81249200	-0.18650500
F	6.36811500	4.35382500	2.03808800
F	4.27669500	2.63842000	2.00414400
F	-3.34234700	-3.78870900	2.21361600
F	-5.40527500	-5.53393700	2.28391900
F	-7.00396000	-5.85247500	0.09474100
F	-6.52049200	-4.41049000	-2.17035300
F	-4.45663000	-2.66824500	-2.25462400
F	2.69431500	-4.35323900	-2.48951600
F	4.45413100	-6.40473700	-2.42051400
F	5.84842200	-6.93633100	-0.13658300
F	5.46614900	-5.40055000	2.08670900
F	3.70345100	-3.35021100	2.03180400

ZnTPPBr$_8$(Triplet)-MeOH

Zn	-0.01547300	-0.00452800	0.17869600
N	2.06143800	-0.09924400	-0.00248400
N	-0.09993100	-2.06471000	-0.09934100
N	0.07859500	2.03855800	-0.12743600
N	-2.08548800	0.07852500	-0.00026200
C	2.82662400	0.98919800	0.33188600
C	3.97891300	0.51119100	1.07359200
C	3.91565300	-0.85726600	1.09066000
C	2.72648400	-1.24565200	0.35561700
C	2.31436600	-2.53845900	-0.05587800
C	2.52503200	2.30691700	-0.09725500
C	0.50531400	-3.93947700	-1.25461500
C	-0.86211200	-3.87838200	-1.25926100
C	-1.24901300	-2.71765800	-0.48066500
C	0.98882300	-2.81624200	-0.47525800
C	-2.54685500	-2.32718300	-0.06441500
C	-1.01224000	2.79114400	-0.49274300
C	-0.53279700	3.91741100	-1.27226400
C	0.83395900	3.85720600	-1.28388400
C	1.22556800	2.69388700	-0.50979000
C	-3.98979300	-0.52319100	1.10488700
C	-3.92886800	0.84422700	1.10727600
C	-2.74586800	1.22582800	0.35728500
C	-2.84472200	-1.00654200	0.35544900
C	-2.33528000	2.51524800	-0.06496900
O	-0.05796700	-0.13890400	2.39367200
C	0.63752600	0.73433900	3.29926700
H	0.22590200	0.64150100	4.30928100
H	1.71229600	0.52679800	3.31220800
H	0.47168400	1.74773300	2.93382900
H	0.09894600	-1.06154200	2.63498700
C	-3.33454700	3.61746700	-0.07098800
C	-3.11846800	4.77979100	0.68547200
C	-4.50914300	3.51165800	-0.83215200
C	-4.05919100	5.80730600	0.68942500
H	-2.21449000	4.86735800	1.28080600
C	-5.44050300	4.54740700	-0.84407800
H	-4.67933700	2.61916800	-1.42672600
C	-5.22069200	5.69604600	-0.07926200
H	-3.88525500	6.69622500	1.28876000
H	-6.33892000	4.45807100	-1.44774200
H	-5.95050900	6.50050500	-0.08278700
C	3.61828500	3.31593600	-0.12603500
C	3.51944200	4.49768100	0.62479600
C	4.76630400	3.10090600	-0.90453200
C	4.54793300	5.43722800	0.60586400
H	2.63610800	4.67034200	1.23248500
C	5.78612600	4.04921300	-0.93912600
H	4.84664200	2.19311100	-1.49485600
C	5.68221800	5.21777500	-0.18000000
H	4.46338000	6.34218800	1.20044000
H	6.66292300	3.87634200	-1.55629000
H	6.48057400	5.95395100	-0.20132400
C	3.31475100	-3.63960600	-0.06458300
C	4.48705300	-3.53356500	-0.82941500
C	3.10184900	-4.80245600	0.69218400
C	5.41924400	-4.56852100	-0.84360000
H	4.65465600	-2.64140600	-1.42518900
C	4.04323000	-5.82940100	0.69374300
H	2.19860100	-4.89218800	1.28848500
C	5.20268900	-5.71718700	-0.07787800
H	6.31569300	-4.47871700	-1.45009400
H	3.87115100	-6.71872800	1.29300200
H	5.93305700	-6.52111200	-0.08341300
C	-3.64005400	-3.33586000	-0.08295200
C	-4.79545400	-3.11976700	-0.85036100
C	-3.53374800	-4.51908300	0.66456600
C	-5.81488000	-4.06862600	-0.87772000
H	-4.88171500	-2.21075800	-1.43793400
C	-4.56176500	-5.45917600	0.65294200
H	-2.64538700	-4.69181700	1.26480000
C	-5.70320600	-5.23883000	-0.12227500
H	-6.69747100	-3.89483300	-1.48630300
H	-4.47156100	-6.36510400	1.24519800
H	-6.50129500	-5.97544000	-0.13789300
Br	-1.97647800	-4.99982000	-2.34926900
Br	1.52197400	-5.16065500	-2.33319800
Br	-5.23935300	-1.54009600	2.15171600
Br	-5.08356900	1.96408100	2.15746100
Br	-1.55476900	5.13904400	-2.34504300
Br	1.94215100	4.98258800	-2.37623500
Br	5.24759300	1.53341100	2.09413800
Br	5.07990300	-1.96894700	2.14182900

ZnTPP(Triplet)-MeOH

Zn	0.03208800	-0.00904000	0.08356900
N	-1.98655400	0.45409700	-0.09999300
N	0.47782600	2.01514100	-0.10058700
N	-0.42620200	-2.01012300	-0.12606200
N	2.03973300	-0.44922500	-0.09906500
C	-3.02034900	-0.44644800	-0.19771300
C	-4.26641600	0.26975100	-0.37011700
C	-3.96815100	1.59831700	-0.36252200
C	-2.53584700	1.71128300	-0.18595500
H	-5.23604100	-0.18667200	-0.50242700
H	-4.64953200	2.42671500	-0.48720900
C	-1.82772000	2.93114100	-0.13730100
C	-2.90092100	-1.85220900	-0.16012700
C	0.29549000	4.30836300	0.00100200
C	1.62462100	4.00876400	0.00461100
C	1.73680400	2.56857200	-0.07527700

C	-0.42279800	3.05509700	-0.08207000
H	-0.15815700	5.28670400	0.05566900
H	2.45378900	4.69804400	0.06253800
C	2.95383200	1.85570800	-0.12012800
C	0.47488900	-3.04669700	-0.08957700
C	-0.24187900	-4.30126000	-0.00508500
C	-1.57088500	-4.00420900	-0.01454600
C	-1.68366600	-2.56387900	-0.10469900
H	0.21366900	-5.27794000	0.06119200
H	-2.39961700	-4.69401100	0.04282700
C	4.32515000	-0.26474400	-0.30743500
C	4.02687200	-1.59254400	-0.30933700
C	2.58965000	-1.70481000	-0.16811100
C	3.07393000	0.45090100	-0.16468100
H	5.29787800	0.19238200	-0.41101100
H	4.71079200	-2.42140300	-0.41518000
C	1.87982400	-2.92331200	-0.12904500
O	0.05254600	0.20639100	2.37631600
C	-1.01611400	-0.32532400	3.16824500
H	-0.89131700	-0.05507400	4.22317900
H	-1.99274700	0.01535800	2.80829200
H	-0.96333200	-1.41031300	3.07022200
H	0.04197500	1.17214900	2.42875800
C	2.68304500	-4.18765800	-0.14275200
C	3.51736800	-4.51960500	0.93702800
C	2.62220300	-5.06842700	-1.23501800
C	4.26630600	-5.69697000	0.92643300
H	3.56958900	-3.84936600	1.78998300
C	3.37195300	-6.24528700	-1.24677600
H	1.98790700	-4.81921200	-2.08055300
C	4.19600100	-6.56399600	-0.16568300
H	4.90178300	-5.93835200	1.77400000
H	3.31537000	-6.91077600	-2.10373300
H	4.77928100	-7.48035800	-0.17464000
C	-4.16704000	-2.65132200	-0.20092500
C	-4.46090100	-3.48094200	-1.29557800
C	-5.09256300	-2.58708300	0.85356600
C	-5.64183400	-4.22324100	-1.33402300
H	-3.75878000	-3.53317100	-2.12234900
C	-6.27311500	-3.33006400	0.81672700
H	-4.87687700	-1.95332900	1.70879300
C	-6.55196000	-4.15085400	-0.27764800
H	-5.85275300	-4.85438100	-2.19283100
H	-6.97320900	-3.27011400	1.64544900
H	-7.47121300	-4.72881400	-0.30733200
C	-2.63144600	4.19493200	-0.16927200
C	-3.49216300	4.52680600	0.88972200
C	-2.54603500	5.07647200	-1.25948600
C	-4.24152600	5.70357600	0.86225300
H	-3.56696400	3.85605000	1.74074300
C	-3.29566800	6.25304000	-1.28841300
H	-1.89228900	4.82774500	-2.09013700
C	-4.14537600	6.57131300	-0.22721100
H	-4.89752000	5.94388100	1.69435800
H	-3.21909200	6.91864800	-2.14368600
H	-4.72860500	7.48742900	-0.24966900
C	4.22096400	2.65487900	-0.13582000
C	5.11737500	2.59958100	0.94385700
C	4.54340500	3.47402300	-1.23001200
C	6.29872700	3.34227300	0.93114100
H	4.87813200	1.97297900	1.79808000
C	5.72515100	4.21603500	-1.24389800
H	3.86338900	3.51863500	-2.07558300
C	6.60668100	4.15304600	-0.16297700
H	6.97685400	3.28954200	1.77840400
H	5.95910300	4.83938700	-2.10245200
H	7.52667700	4.73053800	-0.17354100

4.3: Methanol

MeOH

O	0.74906300	0.12200600	-0.00000200
H	1.13487800	-0.76229200	-0.00001700
C	-0.66143700	-0.01947300	-0.00000200
H	-1.08250100	0.98944400	0.00123700
H	-1.03819800	-0.54212300	-0.89251000
H	-1.03806300	-0.54423600	0.89131500

Design of oxophilic metalloporphyrins: An experimental and DFT study of methanol binding
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5: DFT Data

Table 32: Calculated energies for optimized systems.

B3LYP

Ligand	Porphyrin	State	mb energy	D3-disp	gibbs corrections	Sum of mb Gibbs25 with D3-disp	Comments
	Al(III)	*S*	-1691.192499	-0.10929949	0.232284	-1691.069515	
		T	-1691.126011	-0.10905382	0.225921	-1691.009144	
		Qui	-1691.057617	-0.10900384	0.223631	-1690.94299	
	Co(III)	*S*	-1594.506281	-0.11234396	0.231057	-1594.387568	
		T	-1594.501141	-0.11139802	0.228716	-1594.383823	
		Qui	-1594.505504	-0.1089732	0.225913	-1594.388564	
	Co(II)	*D*	-1134.318635	-0.10133585	0.232573	-1134.187398	
		Qua	-1134.311733	-0.10071191	0.228389	-1134.184055	
		Sex	-1134.247163	-0.10026658	0.222199	-1134.125231	
	Fe(III)	*D*	-1572.59177	-0.11454968	0.229045	-1572.477274	
		Qua	-1572.60893	-0.11379458	0.228398	-1572.494327	
		Sex	-1572.615011	-0.11203502	0.226608	-1572.500438	
	Fe(II)	*S*	-1112.379068	-0.1039149	0.231556	-1112.251427	
		T	-1112.396242	-0.10393117	0.230815	-1112.269358	
		Qui	-1112.393471	-0.10320455	0.22754	-1112.269136	
	Mg(II)	*S*	-1188.588176	-0.09946188	0.231104	-1188.456533	
		T	-1188.524054	-0.09913653	0.224106	-1188.399085	
		Qui	-1188.455454	-0.09911561	0.222844	-1188.331725	
	Mn(III)	*S*	-1553.025503	-0.11518717	0.230035	-1552.910655	
		T	-1553.038721	-0.11538688	0.229406	-1552.924702	
		Qui	-1553.066748	-0.11434228	0.22758	-1552.953511	
	Ni(II)	*S*	-1159.414359	-0.10334901	0.231547	-1159.286161	
		T	-1159.406382	-0.10272436	0.229538	-1159.279568	
		Qui	-1159.340009	-0.10226104	0.222611	-1159.219659	
	Ti(IV)	*S*	-1122.132277	-0.11049332	0.232873	-1122.009897	
		T	-1122.066573	-0.11013192	0.225421	-1121.951284	
		Qui	-1121.998003	-0.11007751	0.224306	-1121.883774	
	V(IV)	*D*	-1135.469398	-0.10928958	0.233089	-1135.345598	
		Qua	-1135.36192	-0.10907147	0.228627	-1135.242365	
		Sex	-1135.333838	-0.10889427	0.22513	-1135.217602	
	Zn(II)	*S*	-1215.585294	-0.10107322	0.229323	-1215.457045	
		T	-1215.519157	-0.10063123	0.221533	-1215.398255	
		Qui	-1215.449781	-0.10057642	0.220366	-1215.329991	
MeOH							
		S	-115.7218576	-0.0031035	0.028687	-115.6962741	

Table 33: Calculated energies for optimized systems.

B3LYP

Ligand	Porphyrin	State	mb energy	D3-disp	gibbs corrections	Sum of mb Gibbs25 with D3-disp	Comments
		S	-1806.926759	-0.12701775	0.280239	-1806.773538	
MeOH	**Al(III)P**	*T*	-1806.864515	-0.12692579	0.274756	-1806.716685	
		Qui	-1806.795354	-0.12679906	0.272421	-1806.649732	
		S	-1710.24834	-0.12834265	0.281048	-1710.095634	
MeOH	**Co(III)P**	*T*	-1710.232187	-0.12662781	0.27541	-1710.083405	H-bond!
		Qui	-1710.235206	-0.12055196	0.269996	-1710.085762	H-bond!
		D	-1250.054259	-0.11600815	0.278238	-1249.892029	
MeOH	**Co(II)P**	*Qua*	-1250.050003	-0.11491678	0.27525	-1249.889669	
		Sex	-1249.986822	-0.11437526	0.266809	-1249.834388	
		D	-1688.331608	-0.12648159	0.27973	-1688.17836	
MeOH	**Fe(III)P**	*Qua*	-1688.339926	-0.12907023	0.274944	-1688.194052	
		Sex	-1688.344843	-0.12396386	0.270521	-1688.198286	H-bond!
		S	-1228.117373	-0.11944393	0.279371	-1227.957446	
MeOH	**Fe(II)P**	*T*	-1228.130576	-0.11839457	0.276899	-1227.972071	
		Qui	-1228.129657	-0.11599846	0.272826	-1227.972829	
		S	-1304.335722	-0.113326	0.277951	-1304.171097	
MeOH	**Mg(II)P**	*T*	-1304.273654	-0.11316541	0.270761	-1304.116058	
		Qui	-1304.205101	-0.11301792	0.2696	-1304.048519	
		S	-1668.764453	-0.13346878	0.278662	-1668.61926	
MeOH	**Mn(III)P**	*T*	-1668.781045	-0.12930843	0.278682	-1668.631672	
		Qui	-1668.798243	-0.1292186	0.273646	-1668.653815	
		S	-1275.145822	-0.11494781	0.274558	-1274.986212	H-bond!
MeOH	**Ni(II)P**	*T*	-1275.151863	-0.1159836	0.277101	-1274.990746	
		Qui	-1275.087507	-0.11675995	0.270714	-1274.933553	
		S	-1237.862911	-0.12401041	0.277782	-1237.709139	H-bond!
MeOH	**Ti(IV)P**	*T*	-1237.765119	-0.12713616	0.275711	-1237.616544	
		Qui	-1237.730881	-0.1256671	0.270285	-1237.586263	
		D	-1251.200223	-0.12521054	0.27935	-1251.046084	
MeOH	**V(IV)P**	*Qua*	-1251.136726	-0.12540474	0.273923	-1250.988207	
		Sex	-1251.06784	-0.12521913	0.272311	-1250.920748	
		S	-1331.3224	-0.11483776	0.275813	-1331.161425	
MeOH	**Zn(II)P**	*T*	-1331.259535	-0.11453952	0.269077	-1331.104997	
		Qui	-1331.189881	-0.11447045	0.267238	-1331.037113	

Table 34: Calculated energies for optimized systems.

B3LYP

Ligand	Porphyrin	State	mb energy	D3-disp	gibbs corrections	Sum of mb Gibbs25 with D3-disp	Comments
	Mg(II)PF_8	*S*	-1982.376541	-0.10270087	0.157533	-1982.321709	
		T	-1982.309523	-0.10243642	0.151253	-1982.260706	
		Qui	-1982.240084	-0.1023725	0.148565	-1982.193892	
	Mg(II)PCl_8	*S*	-4865.292937	-0.13612837	0.139017	-4865.290048	
		T	-4865.229541	-0.1357406	0.131798	-4865.233483	
		Qui	-4865.16305	-0.13577896	0.130533	-4865.168296	
	Mg(II)PBr_8	*S*	-1290.711423	-0.14634886	0.124477	-1290.733295	
		T	-1290.647948	-0.14596877	0.117824	-1290.676092	
		Qui	-1290.58153	-0.14601916	0.117301	-1290.610248	
	Zn(II)PF_8	*S*	-2009.372309	-0.10438514	0.155726	-2009.320968	
		T	-2009.303562	-0.10405024	0.149322	-2009.25829	
		Qui	-2009.233241	-0.10391736	0.146173	-2009.190985	
	Zn(II)PCl_8	*S*	-4892.288584	-0.13802984	0.137238	-4892.289376	
		T	-4892.223288	-0.13759146	0.130608	-4892.230272	
		Qui	-4892.156021	-0.13753466	0.128154	-4892.165401	
	Zn(II)PBr_8	*S*	-1317.71917	-0.14819384	0.122351	-1317.745013	
		T	-1317.654386	-0.14768111	0.115202	-1317.686865	
		Qui	-1317.587249	-0.14770028	0.113287	-1317.621663	
	Co(III)PF_8Cl	*S*	-2388.290883	-0.11575542	0.157863	-2388.248775	
		T	-2388.285182	-0.11480299	0.155374	-2388.244611	
		Qui	-2388.289995	-0.11258145	0.152671	-2388.249905	
	Co(III)PCl_8Cl	*S*	-5271.203374	-0.1498265	0.13854	-5271.214661	
		T	-5271.197191	-0.14891899	0.138236	-5271.207874	
		Qui	-5271.204605	-0.1463846	0.133847	-5271.217142	
	Co(III)PBr_8Cl	*S*	-1696.632246	-0.1601244	0.12333	-1696.66904	
		T	-1696.625897	-0.15921889	0.123704	-1696.661411	
		Qui	-1696.634211	-0.15661378	0.118863	-1696.671962	
MeOH		S	-115.7218576	-0.0031035	0.028687	-115.6962741	

Table 35: Calculated energies for optimized systems.

B3LYP

Ligand	Porphyrin	State	mb energy	D3-disp	gibbs corrections	Sum of mb Gibbs25 with D3-disp	Comments
MeOH	**Mg(II)PF_8**	*S*	-2098.126836	-0.11610018	0.203899	-2098.039037	

		T	-2098.061292	-0.1158852	0.196512	-2097.980666	
		Qui	-2097.992138	-0.1157739	0.196717	-2097.911195	
MeOH	**$Mg(II)PCl_8$**	*S*	-4981.044472	-0.14967889	0.185276	-4981.008875	
		T	-4980.98388	-0.14909742	0.179038	-4980.95394	
		Qui	-4980.916697	-0.14927897	0.178837	-4980.887139	
MeOH	**$Mg(II)PBr_8$**	*S*	-1406.465584	-0.15968115	0.171836	-1406.453429	
		T	-1406.405488	-0.15943584	0.164577	-1406.400347	
		Qui	-1406.338187	-0.15940438	0.163142	-1406.334449	
MeOH	**$Zn(II)PF_8$**	*S*	-2125.111804	-0.11789084	0.202443	-2125.027252	
		T	-2125.04506	-0.11770253	0.194588	-2124.968175	
		Qui	-2124.975383	-0.11749944	0.193387	-2124.899496	
MeOH	**$Zn(II)PCl_8$**	*S*	-5008.029317	-0.15174601	0.183718	-5007.997345	
		T	-5007.967564	-0.15125156	0.176738	-5007.942078	
		Qui	-5007.89988	-0.1513206	0.175291	-5007.87591	
MeOH	**$Zn(II)PBr_8$**	*S*	-1433.46003	-0.16093284	0.170544	-1433.450418	
		T	-1433.399065	-0.16055997	0.164097	-1433.395528	
		Qui	-1433.332051	-0.16152738	0.16037	-1433.333208	
MeOH	**$Co(III)PF_8Cl$**	*S*	-2504.034657	-0.13150551	0.207574	-2503.958588	
		T	-	-	-	-	Fail
		Qui	-2504.019071	-0.12395013	0.196707	-2503.946314	
MeOH	**$Co(III)PCl_8Cl$**	*S*	-5386.948608	-0.16580937	0.188401	-5386.926016	
		T	-5386.930576	-0.16478498	0.183138	-5386.912223	
		Qui	-5386.933362	-0.15785746	0.177009	-5386.914211	
MeOH	**$Co(III)PBr_8Cl$**	*S*	-1812.378206	-0.17620541	0.173868	-1812.380543	
		T	-1812.359985	-0.17522745	0.167641	-1812.367572	
		Qui	-1812.363069	-0.16807798	0.162115	-1812.369032	

Table 36: Calculated energies for optimized systems.

B3LYP

Symetry	Ligand	porphyrin	State	mb energy	D3-disp	gibbs corrections	Sum of mb Gibbs25 with D3-disp	Comments
/		**Mg(II)TPP**	*S*	-2112.793537	-0.21997169	0.526863	-2112.486646	
			T	-2112.734799	-0.22022079	0.521714	-2112.433306	
			Qui	-2112.666408	-0.22003165	0.518781	-2112.367658	
X		**Mg(II)TPP**	*S*	-2112.793093	-0.21983428	0.526285	-2112.486642	
			T	-	-	-	-	
			Qui	-	-	-	-	
/		**Mg(II)TPFPP**	*S*	-4097.27002	-0.23442741	0.338041	-4097.166406	

		T	-4097.207581	-0.2344421	0.317307	-4097.124716	
		Qui	-4097.143153	-0.2345162	0.316819	-4097.060851	
X	**Mg(II)TPFPP**	*S*	-4097.269994	-0.22884848	0.337384	-4097.161458	
		T	-	-	-	-	
		Qui	-	-	-	-	
Saddle	**Mg(II)TPPBr$_8$**	*S*	-2214.829271	-0.29330208	0.421345	-2214.701228	
		T	-2214.786062	-0.29087843	0.418078	-2214.658862	
		Qui	-2214.718192	-0.29082125	0.414249	-2214.594764	
/	**Co(III)TPPCl**	*S*	-	-	-	-	Fail
		T	-	-	-	-	Fail
		Qui	-2518.71393	-0.23032911	0.520994	-2518.423265	
X	**Co(III)TPPCl**	*S*	-2518.635567	-0.22922686	0.515355	-2518.349439	
		T	-	-	-	-	
		Qui	-2518.713646	-0.23021909	0.520744	-2518.423121	
/	**Co(III)TPFPPCl**	*S*	-	-	-	-	
		T	-	-	-	-	
		Qui	-4503.183252	-0.24001515	0.333972	-4503.089295	
X	**Co(III)TPFPPCl**	*S*	-	-	-	-	Fail
		T	-	-	-	-	Fail
		Qui	-4503.183023	-0.23990758	0.331686	-4503.091245	
Saddle	**Co(III)TPPBr$_8$Cl**	*S*	-2620.697742	-0.30362623	0.412929	-2620.588439	
		T	-2620.769396	-0.30363329	0.416605	-2620.049158	
		Qui	-2620.764163	-0.30483838	0.415072	-2620.653929	
/	**Zn(II)TPP**	*S*	-2139.790759	-0.22190301	0.52488	-2139.487782	
		T	-2139.730099	-0.22205638	0.519433	-2139.432722	
		Qui	-2139.661018	-0.22183177	0.516133	-2139.366717	
X	**Zn(II)TPP**	*S*	-2139.7907	-0.22198369	0.525032	-2139.487651	
		T	-	-	-	-	
		Qui	-	-	-	-	
/	**Zn(II)TPFPP**	*S*	-4124.266305	-0.23097884	0.33665	-4124.160633	
		T	-	-	-	-	
		Qui	-	-	-	-	
X	**Zn(II)TPFPP**	*S*	-4124.266202	-0.23099861	0.33588	-4124.161321	
		T	-4124.202582	-0.23103623	0.331725	-4124.101893	
		Qui	-4124.137874	-0.231218	0.330036	-4124.039056	

Saddle	**Zn(II)TPPBr$_8$**	*S*	-2241.837526	-0.2960306	0.419628	-2241.713928	
		T	-2241.796357	-0.29341368	0.41591	-2241.67386	
		Qui				0	Fail
MeOH		S	-115.7218576	-0.0031035	0.028687	-115.6962741	

Table 37: Calculated energies for optimized systems.

B3LYP								
Symetry	**Ligand**	**porphyrin**	**State**	**mb energy**	**D3-disp**	**gibbs corrections**	**Sum of mb Gibbs25 with D3-disp**	**Comments**
/	**MeOH**	**Mg(II)TPP**	*S*	-2228.540518	-0.23500657	0.574053	-2228.201471	
			T	-	-	-	-	
			Qui	-	-	-	-	
X	**MeOH**	**Mg(II)TPP**	*S*	-2228.540024	-0.23462023	0.571838	-2228.202806	
			T	-2228.483168	-0.23486199	0.567902	-2228.150128	
			Qui	-2228.414648	-0.23463089	0.564311	-2228.084968	
/	**MeOH**	**Mg(II)TPFPP**	*S*	-4213.021109	-0.24319515	0.385721	-4212.878583	
			T	-	-	-	-	
			Qui	-	-	-	-	
X	**MeOH**	**Mg(II)TPFPP**	*S*	-4213.021255	-0.24347062	0.385	-4212.879726	
			T	-4212.961739	-0.24352327	0.38011	-4212.825153	
			Qui	-4212.897146	-0.24372716	0.378786	-4212.762087	
Saddle	**MeOH**	**Mg(II)TPPBr$_8$**	*S*	-2330.584603	-0.30846203	0.46827	-2330.424795	
			T	-2330.546053	-0.30723087	0.465203	-2330.388081	
			Qui	2330.477724	-0.30661899	0.461095	2330.6322	
/	**MeOH**	**Co(III)TPPCl**	*S*	-2634.45467	-0.2506575	0.575634	-2634.129693	
			T				0	Fail
			Qui				0	Fail
X	**MeOH**	**Co(III)TPPCl**	*S*	-2634.455412	-0.25092964	0.576957	-2634.129384	
			T	-	-	-	-	
			Qui	-	-	-	-	
/X	**MeOH**	**Co(III)TPFPPCl**	*S*	-4618.931008	-0.25990091	0.386711	-4618.804198	
			T	-4618.868275	0.26066322	0.383839	-4618.223773	

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			Qui	-4618.913306	-0.25294026	0.378439	-4618.787807
X	**MeOH**	**Co(III)TPFPPCl**	*S*	-4618.930941	-0.25994417	0.387691	-4618.803194
			T	-	-	-	-
			Qui	-	-	-	-
Saddle	**MeOH**	**Co(III)TPPBr$_8$Cl**	*S*	-2736.5043	-0.3274984	0.471628	-2736.36017
			T	-2734.490342	-0.32604699	0.464394	-2734.351994
			Qui	-2736.495474	-0.31875349	0.459354	-2736.354873
/	**MeOH**	**Zn(II)TPP**	*S*	-2255.527222	-0.23668272	0.571207	-2255.192697
			T	-	-	-	-
			Qui	-	-	-	-
X	**MeOH**	**Zn(II)TPP**	*S*	-2255.52763	-0.23672425	0.571411	-2255.192943
			T	-2255.471484	-0.23759057	0.567828	-2255.141246
			Qui	-2255.402148	-0.23721223	0.564786	-2255.074574
/	**MeOH**	**Zn(II)TPFPP**	*S*	-4240.006579	-0.24593721	0.382828	-4239.869688
			T	-4239.945267	-0.24586982	0.373949	-4239.817188
			Qui	-4239.880092	-0.24593971	0.376144	-4239.749888
X	**MeOH**	**Zn(II)TPFPP**	*S*	-4239.934306	-0.24713413	0.389128	-4239.792312
			T	-	-	-	-
			Qui	-	-	-	-
Saddle	**MeOH**	**Zn(II)TPPBr$_8$**	*S*	-2357.579474	-0.31144195	0.465306	-2357.42561
			T	-2357.543345	-0.30940481	0.463337	-2357.389413
			Qui	-2357.47528	-0.3096032	0.459285	-2357.325598

Table 38: Calculated theoretican binding constants and M-MeOH bond lengths.

Porphyrin	au	kcal/mol	kJ/mol	K	Bond length
Al(III)PCl	-0.00775	-4.9	-20.4	3.70E+03	2.2827
Co(III)PCl	-0.0108	-6.8	-28.4	9.37E+04	2.10608
Co(II)P	-0.00836	-5.2	-22.0	7.06E+03	2.32675
Fe(III)PCl	0.00266	1.7	7.0	-	3.56094
Fe(II)P	-0.0072	-4.5	-18.9	2.06E+03	2.23481
Mg(II)P	-0.01829	-11.5	-48.1	2.65E+08	2.15116
Mn(III)PCl	-0.00403	-2.5	-10.6	7.18E+01	2.63986
Ni(II)P	-0.00831	-5.2	-21.8	6.72E+03	2.15364
O=Ti(IV)P	0.089627	56.2	235.5	-	3.11836

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O=V(IV)P	-0.00421	-2.6	-11.1	8.70E+01	2.65046
Zn(II)P	-0.00811	-5.1	-21.3	5.41E+03	2.29161
Co(III)PF_8Cl	-0.01354	-8.5	-35.6	1.72E+06	2.10555
Co(III)PCl_8Cl	-0.01508	-9.5	-39.6	8.81E+06	2.10003
Co(III)PBr_8Cl	-0.01523	-9.6	-40.0	1.03E+07	2.09873
MgPF_8	-0.02105	-13.2	-55.3	4.96E+09	2.13421
MgPCl_8	-0.02255	-14.2	-59.3	2.43E+10	2.12815
MgPBr_8	-0.02386	-15.0	-62.7	9.72E+10	2.07883
Zn(II)PF_8	-0.01001	-6.3	-26.3	4.07E+04	2.26006
Zn(II)PCl_8	-0.01169	-7.3	-30.7	2.43E+05	2.24746
Zn(II)PBr_8	-0.00913	-5.7	-24.0	1.60E+04	2.23730

Table 39: Calculated theoretican binding constants and M-MeOH bond lengths.

Porphyrin	au	kcal/mol	kJ/mol	K	Bond length
Mg(II)TPP	-0.01989	-12.5	-52.2	1.44E+09	2.15602
Mg(II)TPFPP	-0.01705	-10.7	-44.8	7.07E+07	2.13171
Mg(II)TPPBr8	-0.02729	-17.1	-71.7	3.70E+12	2.06569
Co(III)TPPCl	-0.01015	-6.4	-26.7	4.74E+04	2.10823
Co(III)TPFPPCl	-0.01668	-10.5	-43.8	4.80E+07	2.09931
Co(III)TPPBr8Cl	-0.00997	-6.3	-26.2	3.89E+04	2.11001
Zn(II)TPP	-0.00889	-5.6	-23.3	1.24E+04	2.30294
Zn(II)TPFPP	-0.01209	-7.6	-31.8	3.71E+05	2.26497
Zn(II)TPPBr8	-0.01541	-9.7	-40.5	1.25E+07	2.21946

Table 40: Natural charges for methanol in MP-MeOH complex.

Porphyrin	Natural charges for Methanol in porphyrin complex. change from free in brackets								
	H		O		C		CH_3		Total change
MeOH	0.24		-0.37		-0.16		0.10		
Al(III)P	0.51	(0.28)	-0.75	(-0.38)	-0.31	(-0.16)	0.22	(0.12)	-0.14
Co(III)P	0.52	(0.28)	-0.66	(-0.29)	-0.31	(-0.15)	0.22	(0.12)	-0.04
Co(II)P	0.26	(0.02)	-0.35	(0.03)	-0.16	(0.001)	0.11	(0.01)	0.06
Fe(II)P	0.24	(0.01)	-0.35	(0.03)	-0.15	(0.003)	0.11	(0.01)	0.05
Mg(II)P	0.52	(0.28)	-0.78	(-0.41)	-0.31	(-0.16)	0.22	(0.12)	-0.16
Mn(III)P	0.25	(0.01)	-0.34	(0.03)	-0.15	(0.01)	0.10	(0.01)	0.05
Ni(II)P	0.26	(0.02)	-0.34	(0.03)	-0.16	(0.001)	0.11	(0.01)	0.07
V(IV)P	0.25	(0.01)	-0.36	(0.03)	-0.15	(0.002)	0.10	(0.01)	0.04
Zn(II)P	0.51	(0.27)	-0.75	(-0.38)	-0.31	(-0.15)	0.21	(0.11)	-0.14

*Non-bonding porphyrins omitted.

Table 41: Natural charges for methanol in MTPP-MeOH complex.

Porphyrin	Natural charges for Methanol in porphyrin complex. change from free in brackets										
	Metall		H		O		C		CH_3		
Non	-		0.24		-0.37		-0.16		0.10		
Co(III)P	0.43	(-1.36)	0.52	(0.28)	-0.66	(-0.29)	-0.31	(-0.15)	0.22	(0.12)	
Co(III)TPPCl	0.43	(-1.37)	0.52	(0.28)	-0.66	(-0.29)	-0.31	(-0.15)	0.22	(0.12)	
Co(III)TPFPPCl	0.41	(-1.38)	0.52	(0.28)	-0.66	(-0.30)	-0.31	(-0.15)	0.22	(0.12)	
Co(III)TPPBr$_8$Cl	0.41	(-1.36)	0.52	(0.28)	-0.67	(-0.29)	-0.31	(-0.15)	0.22	(0.12)	
Mg(II)P	1.40	(-0.03)	0.52	(0.28)	-0.78	(-0.41)	-0.31	(-0.15)	0.22	(0.12)	
Mg(II)TPP	1.40	(-0.06)	0.52	(0.28)	-0.78	(-0.41)	-0.31	(-0.15)	0.22	(0.12)	
Mg(II)TPFPP	1.40	(-0.08)	0.52	(0.28)	-0.79	(-0.42)	-0.31	(-0.15)	0.22	(0.12)	
Mg(II)TPPBr$_8$	1.42	(-0.03)	0.52	(0.28)	-0.80	(-0.43)	-0.31	(-0.15)	0.22	(0.12)	LanL2DZ
Zn(II)P	1.22	(-0.01)	0.51	(0.27)	-0.75	(-0.38)	-0.31	(-0.15)	0.21	(0.11)	
Zn(II)TPP	1.22	(-0.01)	0.51	(0.27)	-0.75	(-0.38)	-0.31	(-0.15)	0.21	(0.11)	
Zn(II)TPFPP	1.23	(0.57)	0.51	(0.27)	-0.76	(-0.39)	-0.31	(-0.15)	0.22	(0.12)	

Table 42:Natural charges for the metal and nitrogens in MTPP.

Porphyrin	Charge metall	N1	N2	N3	N4	
Co(III)P	1.790	-0.160	-0.160	-0.160	-0.160	
Co(III)PF$_8$Cl	1.782	-0.162	-0.162	-0.162	-0.162	
Co(III)PCl$_8$Cl	1.781	-0.155	-0.155	-0.155	-0.155	
Co(III)PBr$_8$Cl	1.780	-0.154	-0.154	-0.154	-0.154	
Mg(II)P	1.429	-0.682	-0.682	-0.682	-0.682	
MgPF$_8$	1.436	-0.680	-0.680	-0.680	-0.680	
MgPCl$_8$	1.446	-0.669	-0.669	-0.669	-0.669	
MgPBr$_8$	1.451	-0.663	-0.663	-0.663	-0.663	LanL2DZ
Zn(II)P	1.236	-0.649	-0.649	-0.649	-0.649	
Zn(II)PF$_8$	1.244	-0.648	-0.648	-0.648	-0.648	
Zn(II)PCl$_8$	1.254	-0.637	-0.637	-0.637	-0.637	
Zn(II)PBr$_8$	1.258	-0.634	-0.634	-0.634	-0.634	

6: UV spectra

UV-vis spectra of all synthesized metalloporphyrins.

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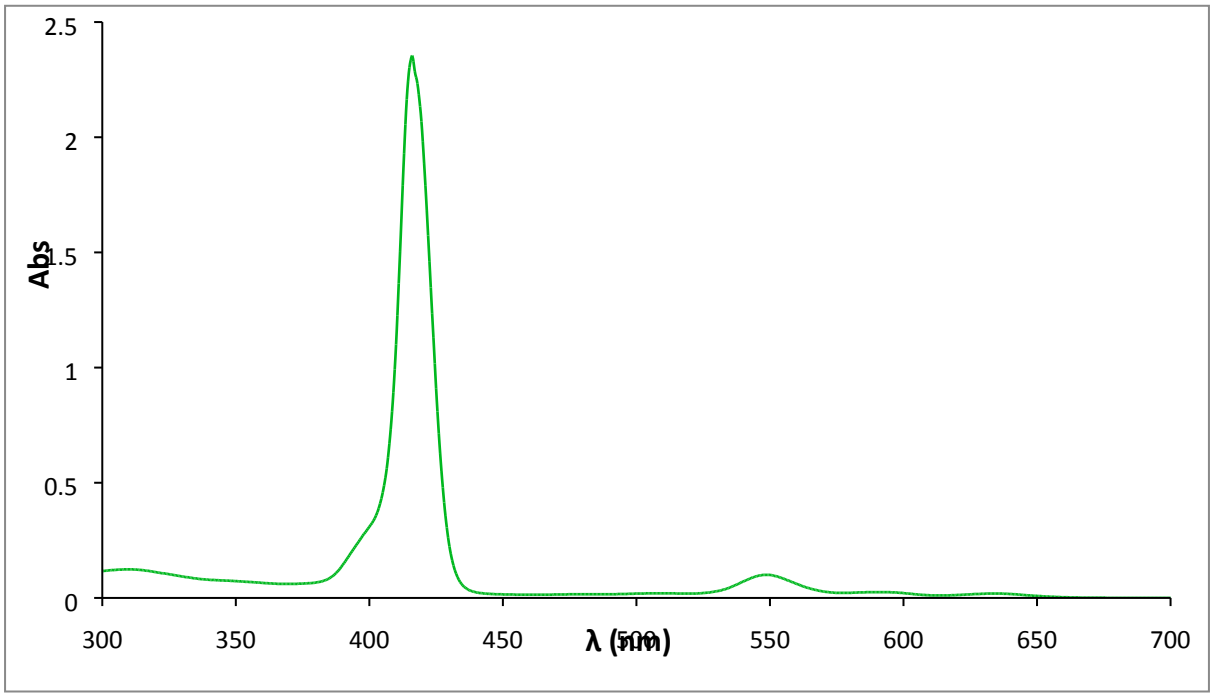

Figure 1: UV-vis spectrum of AlTPPCl.

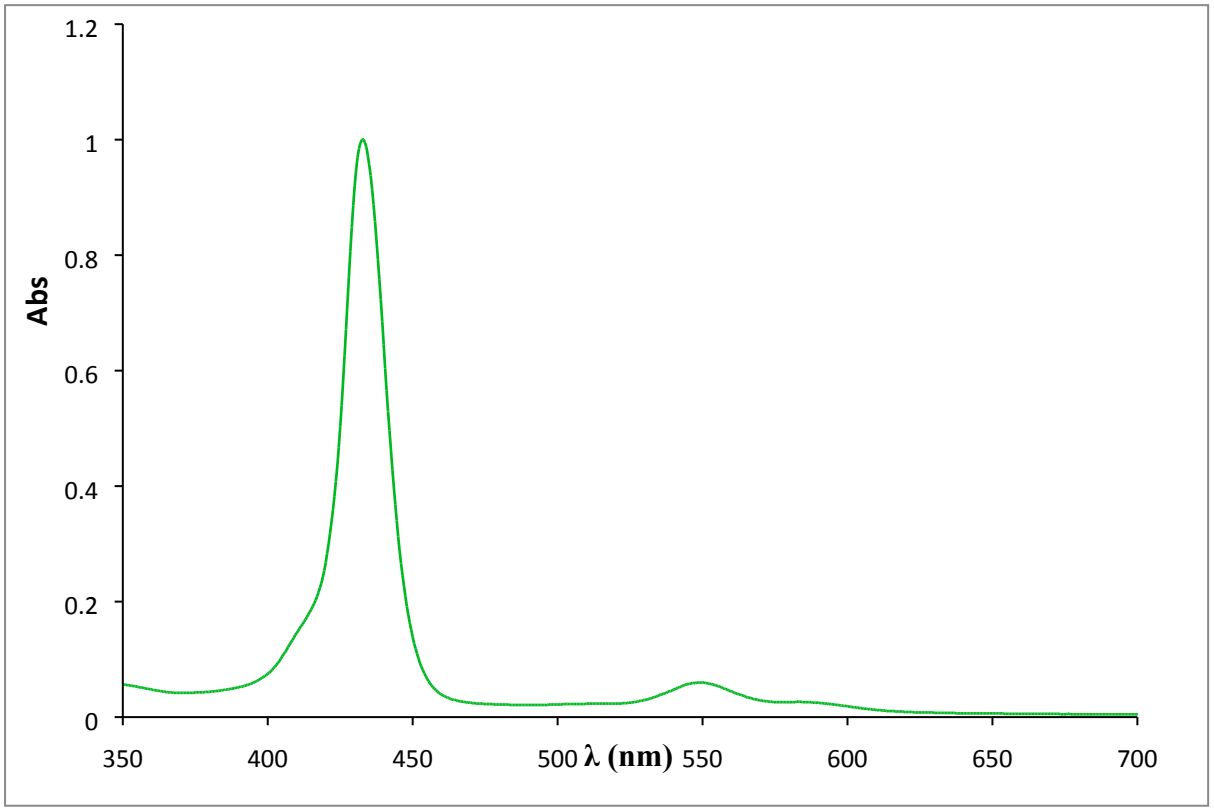

Figure 2: UV-vis spectrum of CoTPPCl.

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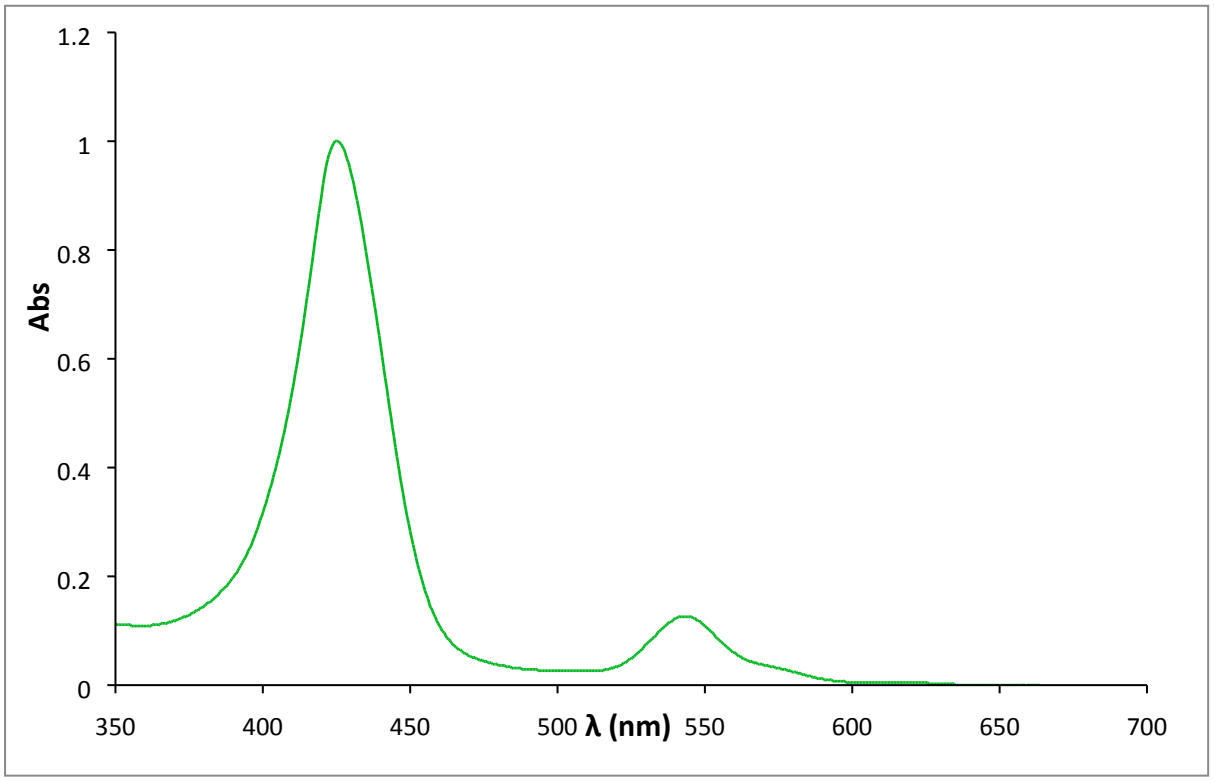

Figure 3: UV-vis spectrum of CoTPFPPCl.

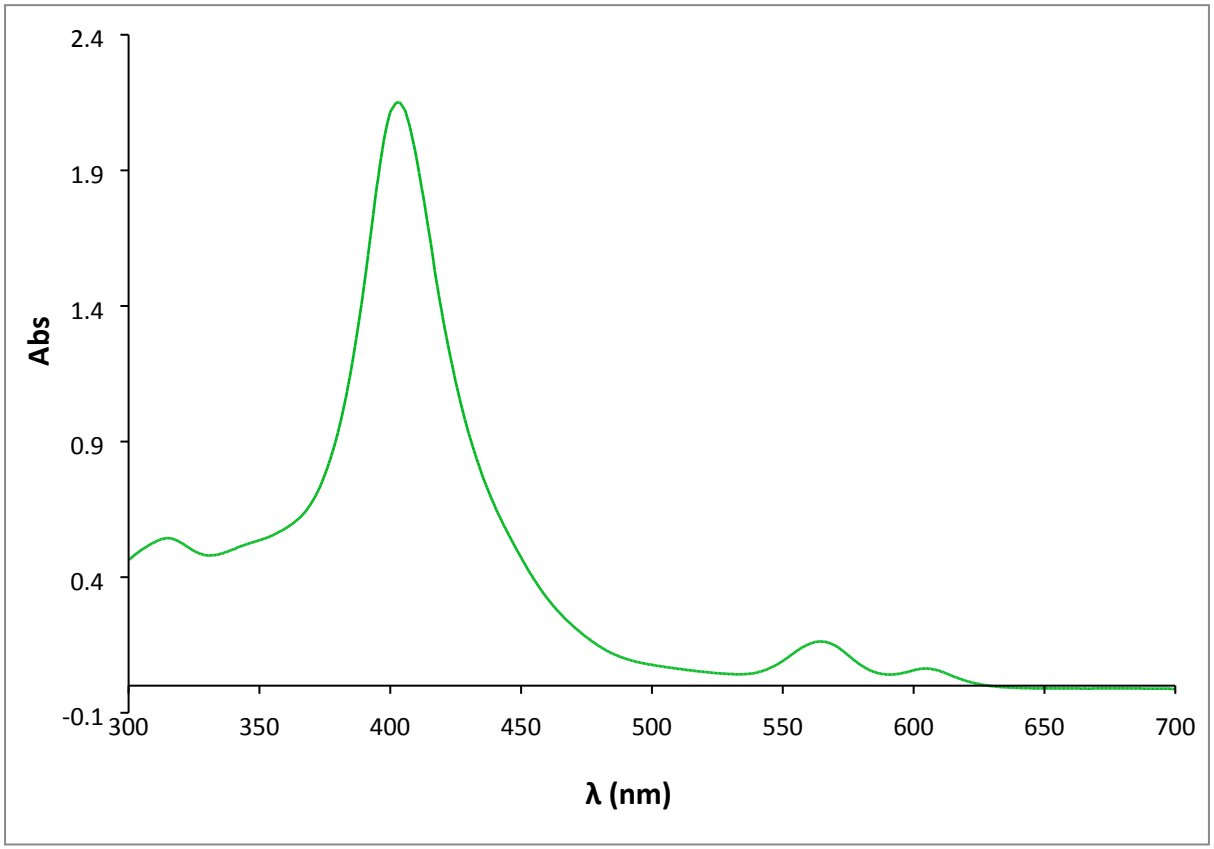

Figure 4: UV-vis spectrum of FeTPP.

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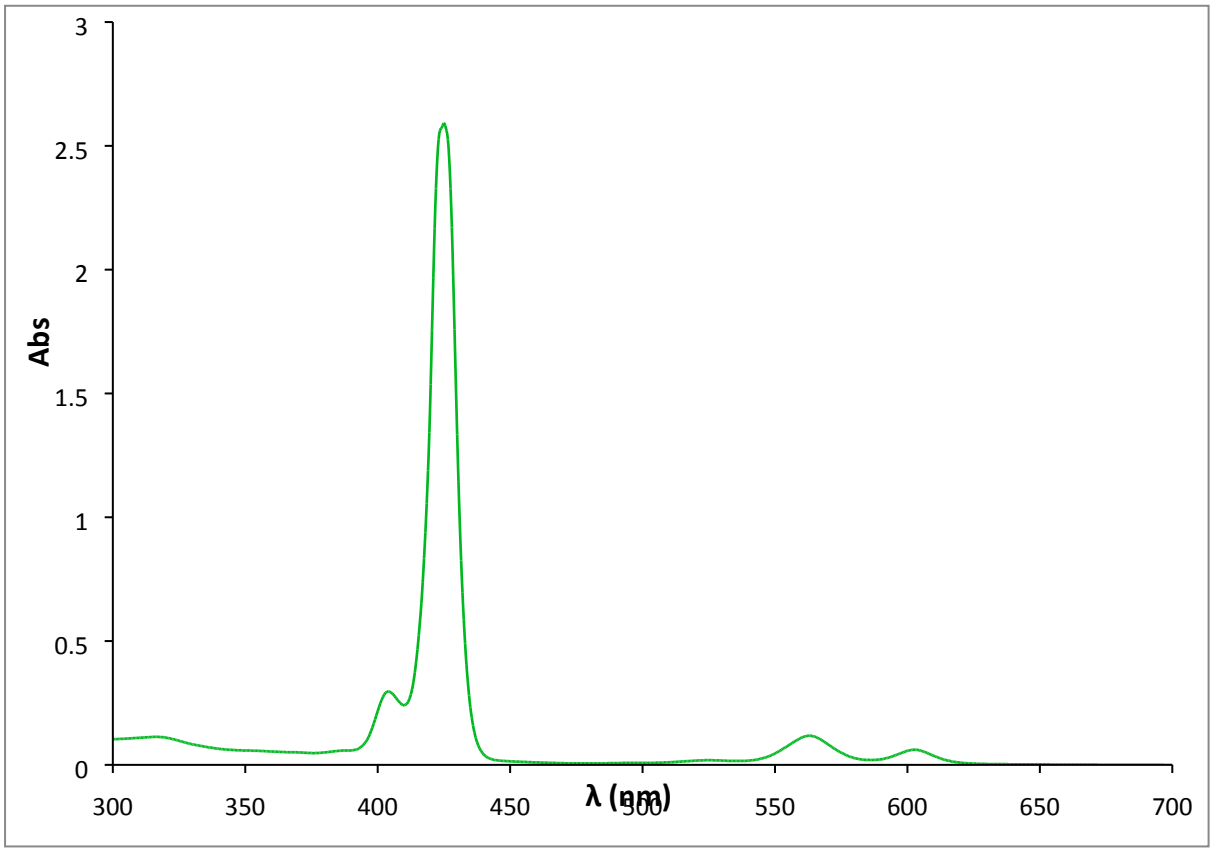

Figure 5: UV-vis spectrum of MgTPP.

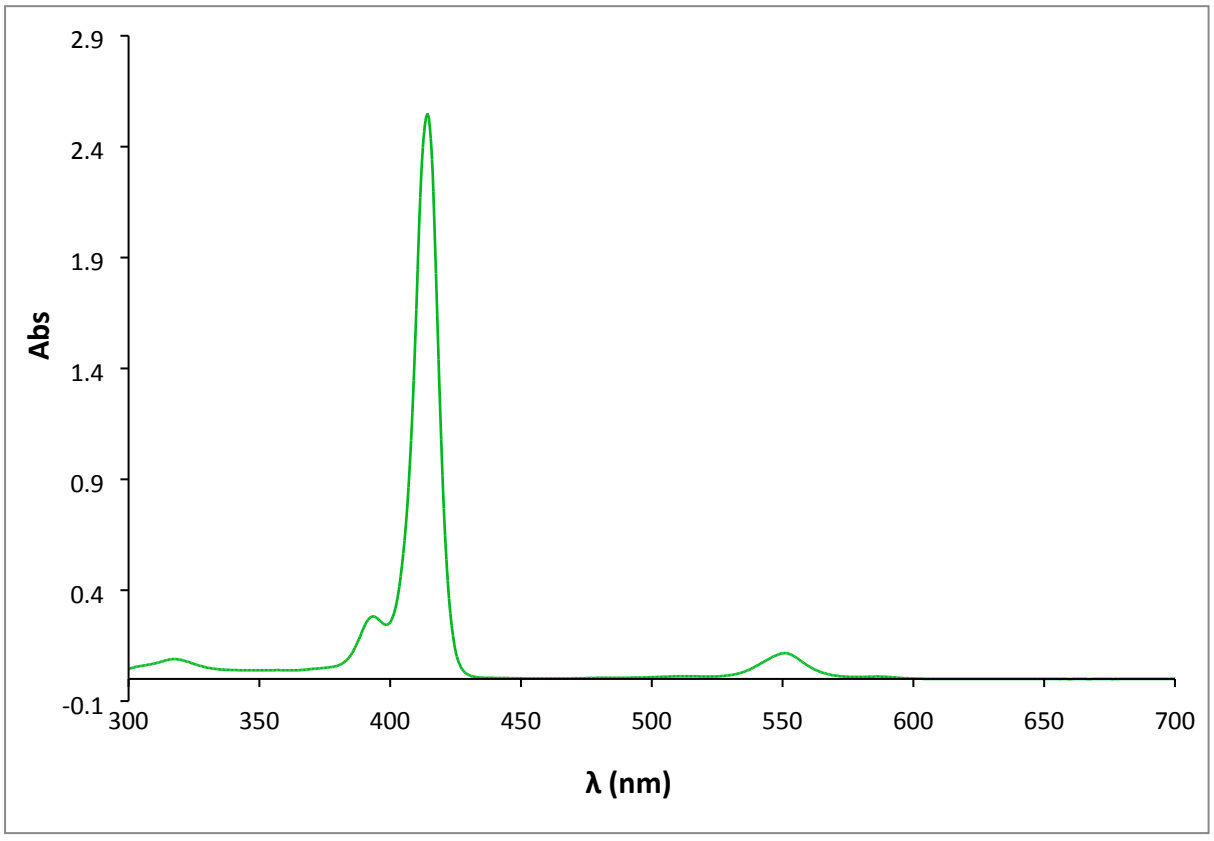

Figure 6: UV-vis spectrum of MgTPFPP.

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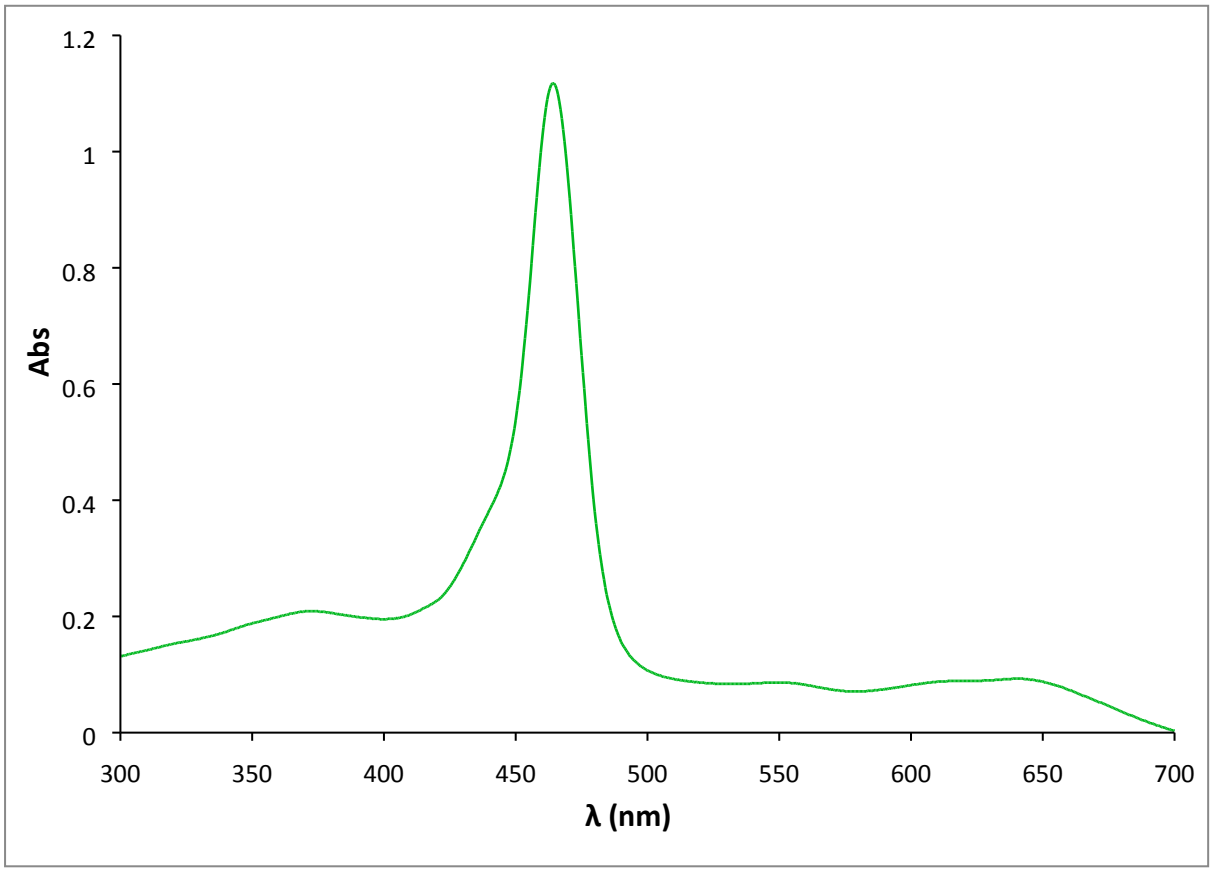

Figure 7: UV-vis spectrum of $MgTPPBr_8$.

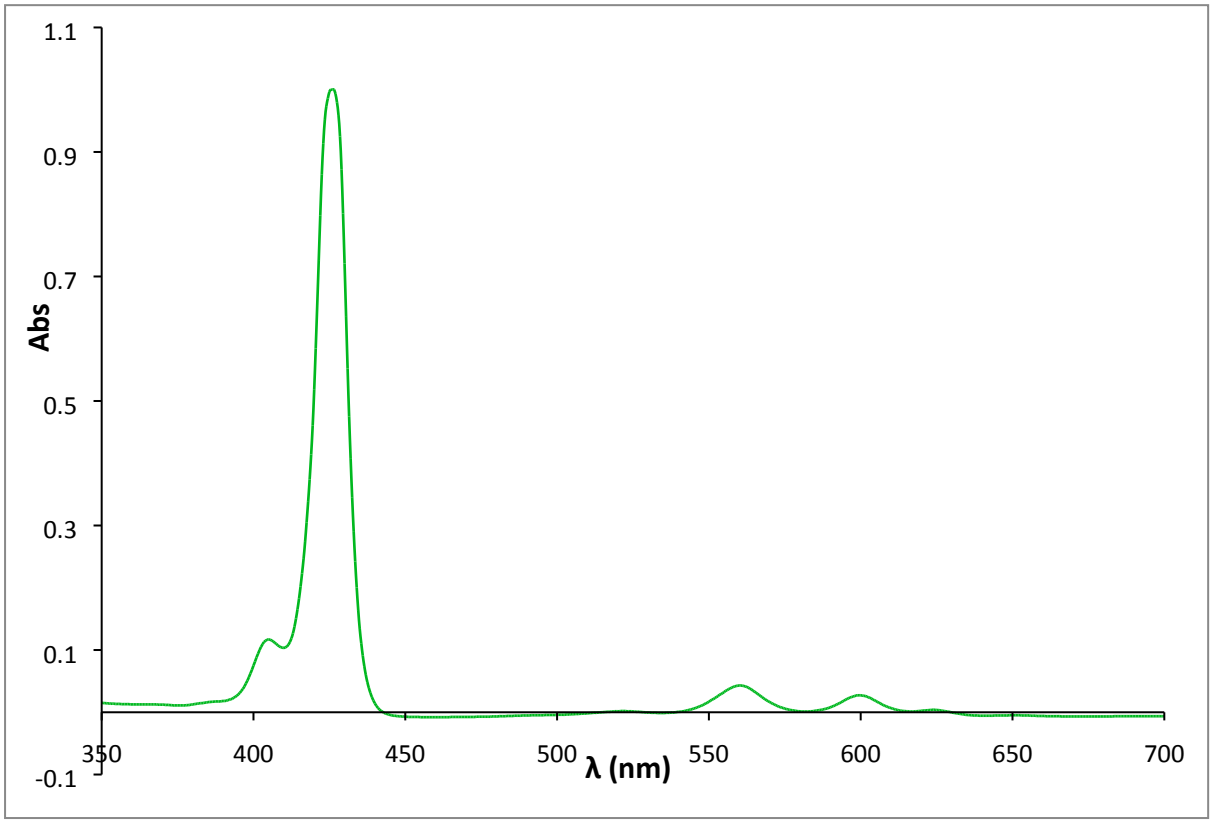

Figure 8: UV-vis spectrum of $SnTPP(OH)_2$.

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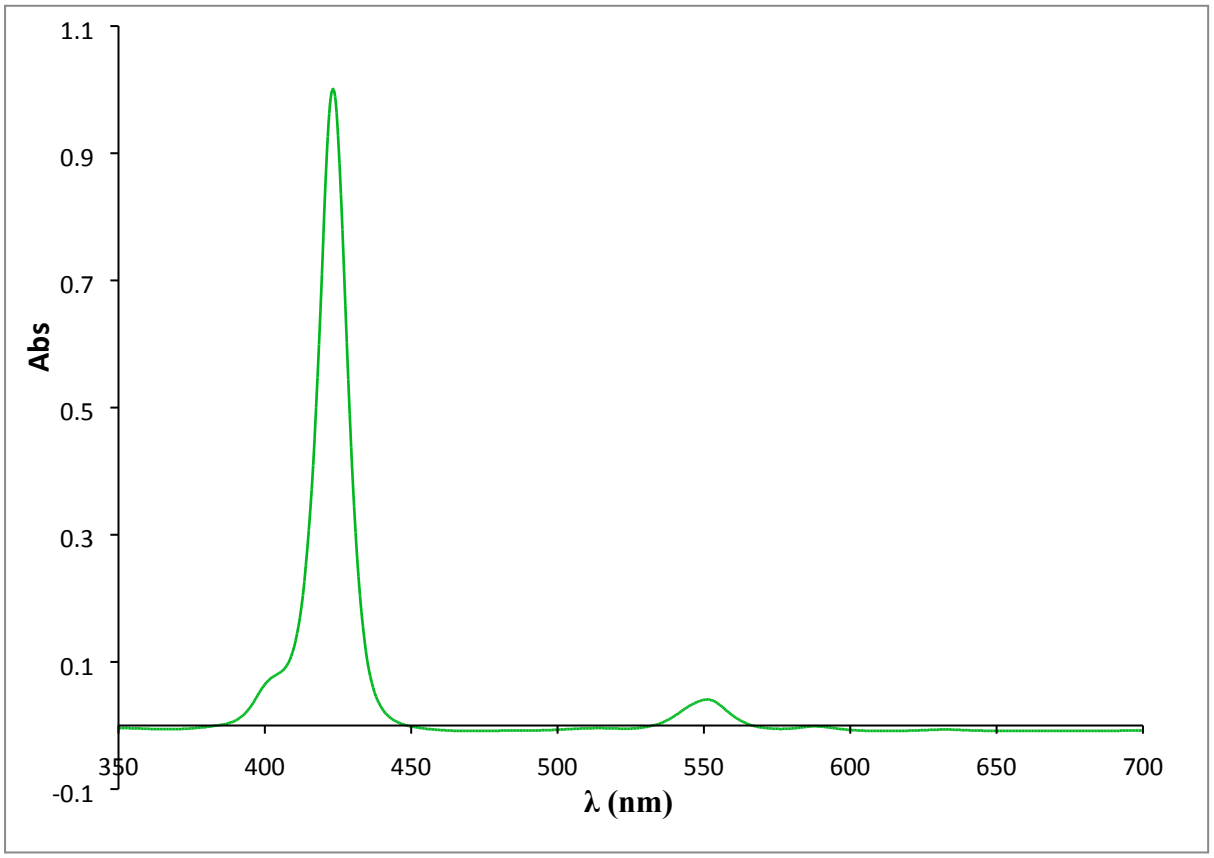

Figure 9: UV-vis spectrum of O=TiTPP.

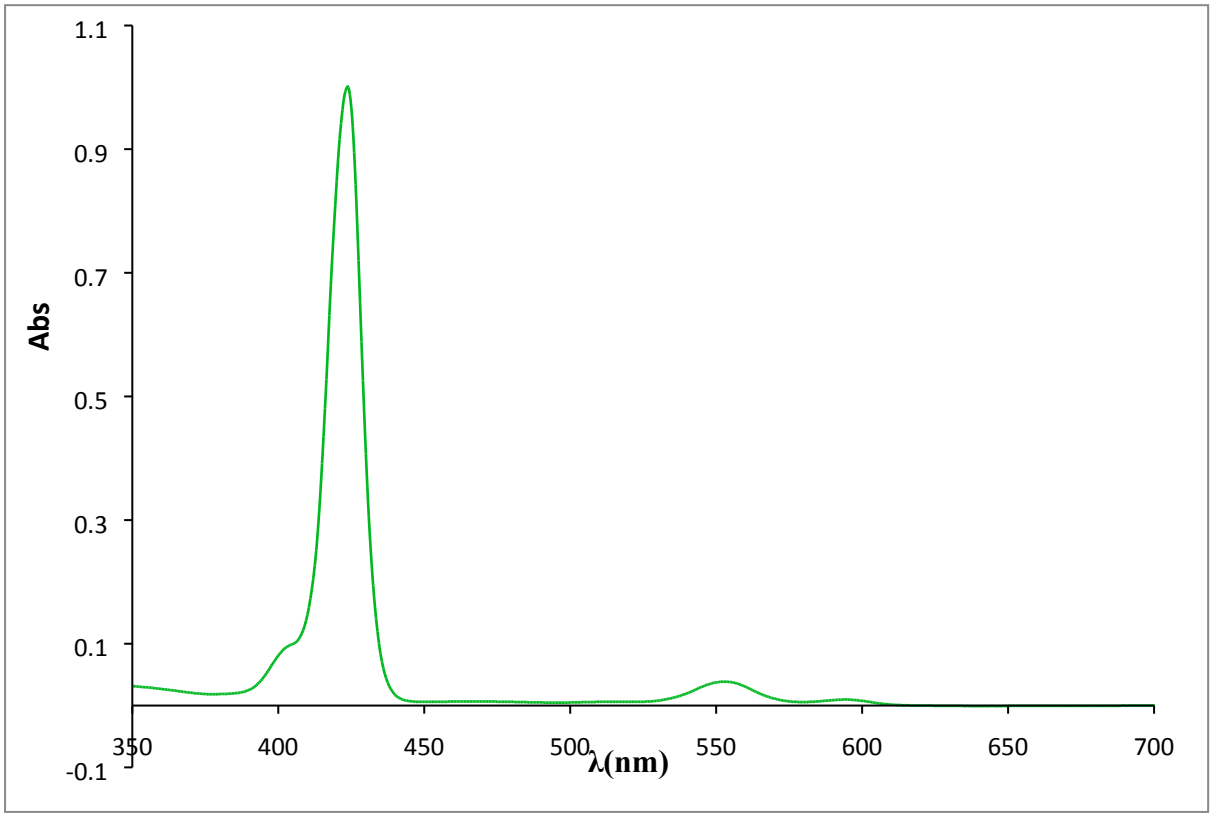

Figure 10: UV-vis spectrum of ZnTPP.

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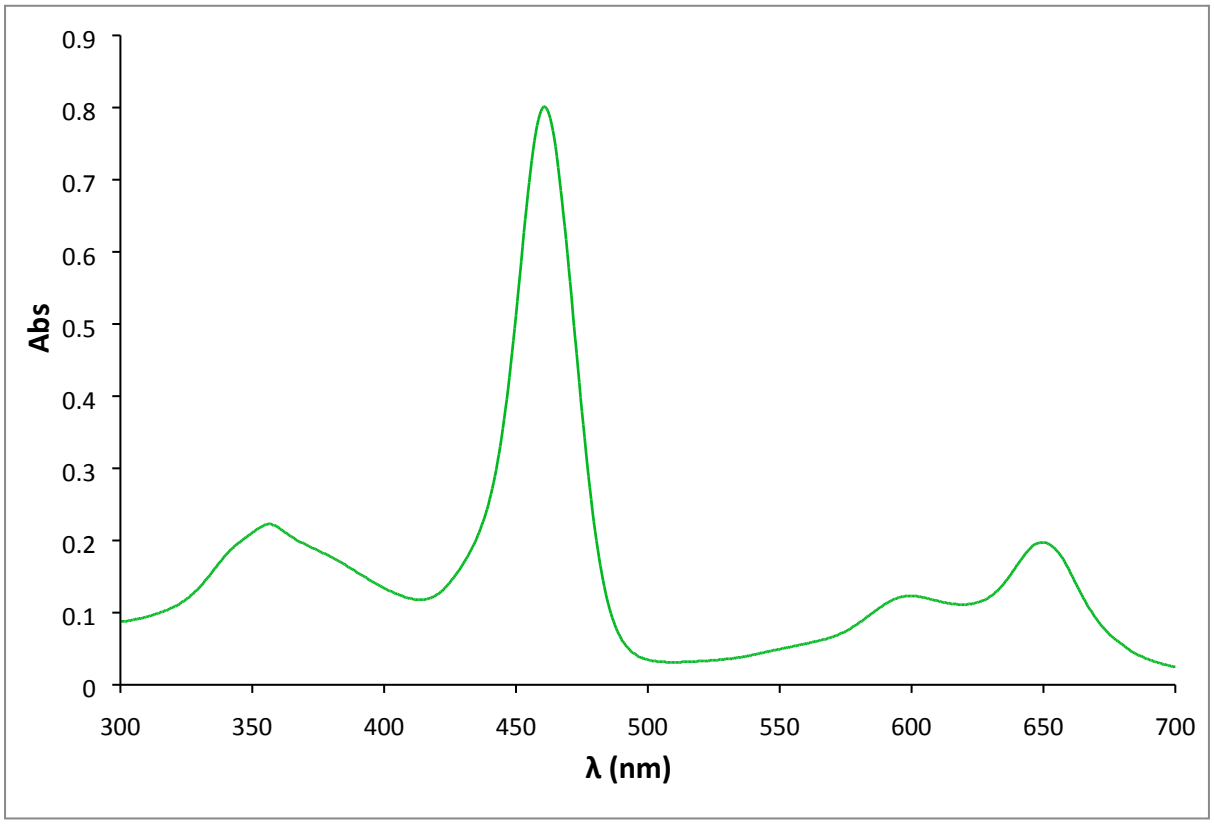

Figure 11: UV-vis spectrum of $ZnTPPBr_8$.

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7: NMR spectra

NMR spectra of all metalloporphyrins in the titrations, both syntezised and comercial.

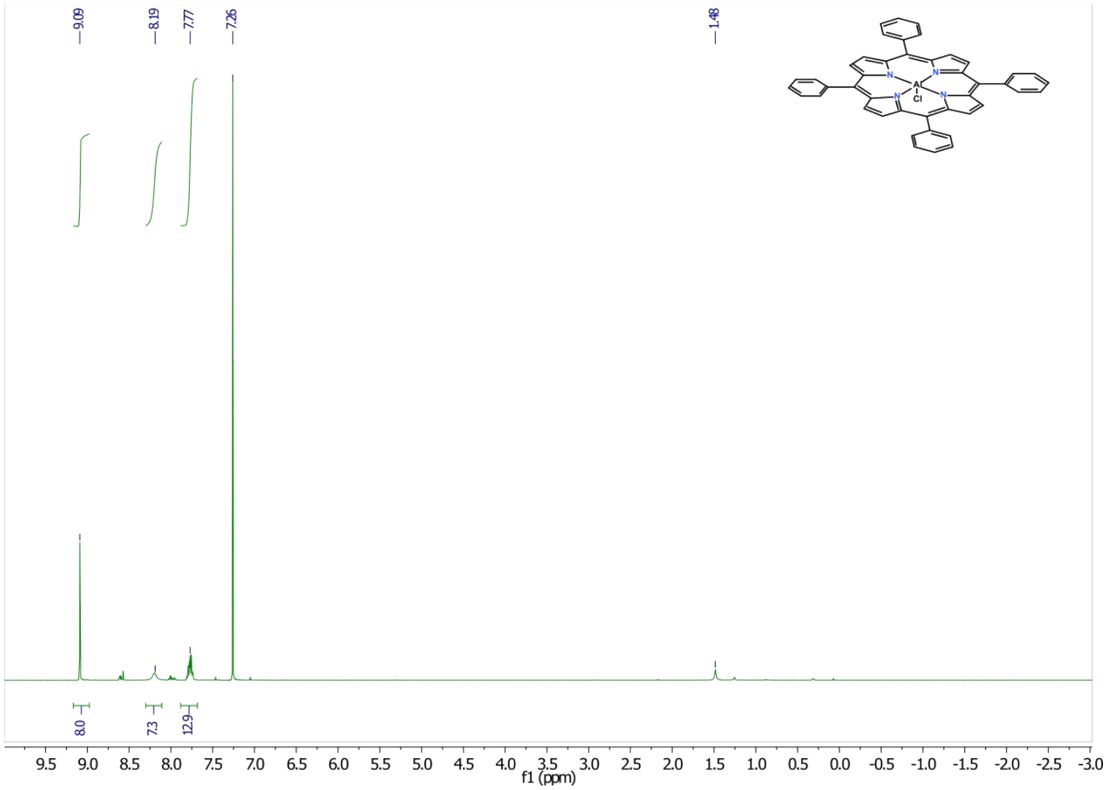

Figure 12: ^{1}H NMR spectrum of AlTPPCl.

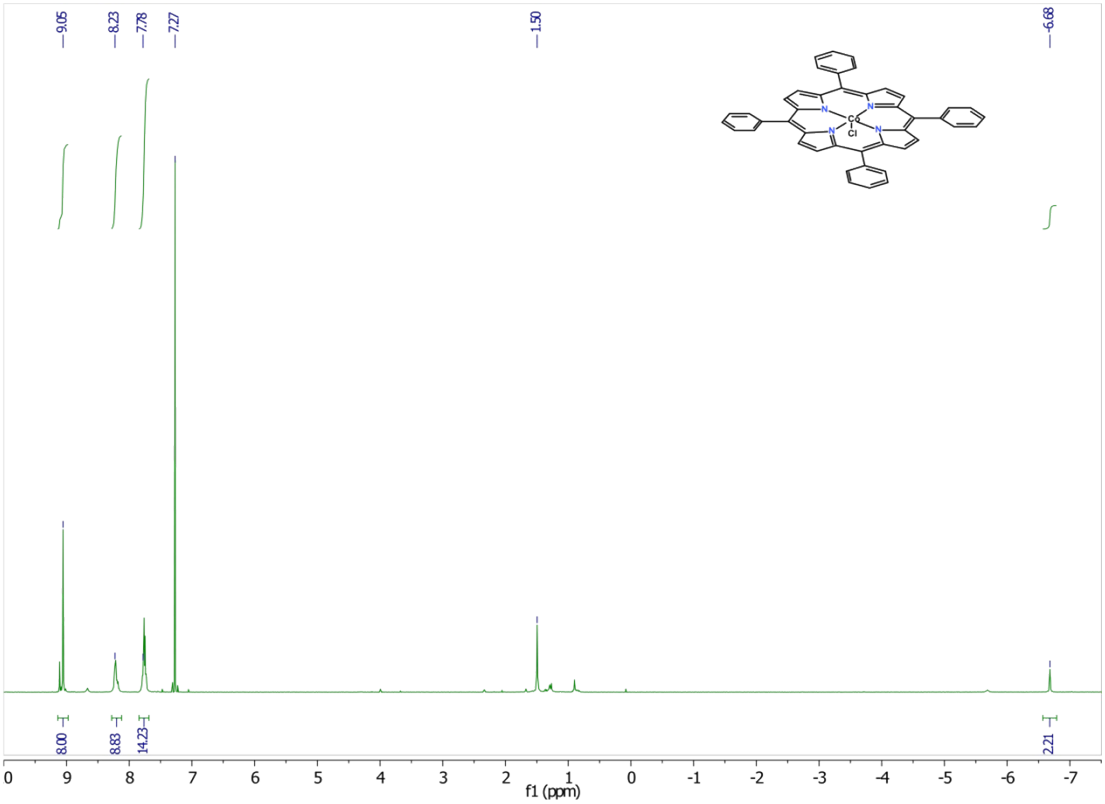

Figure 13: ^{1}H NMR spectrum of CoTPPCl, complexing water.

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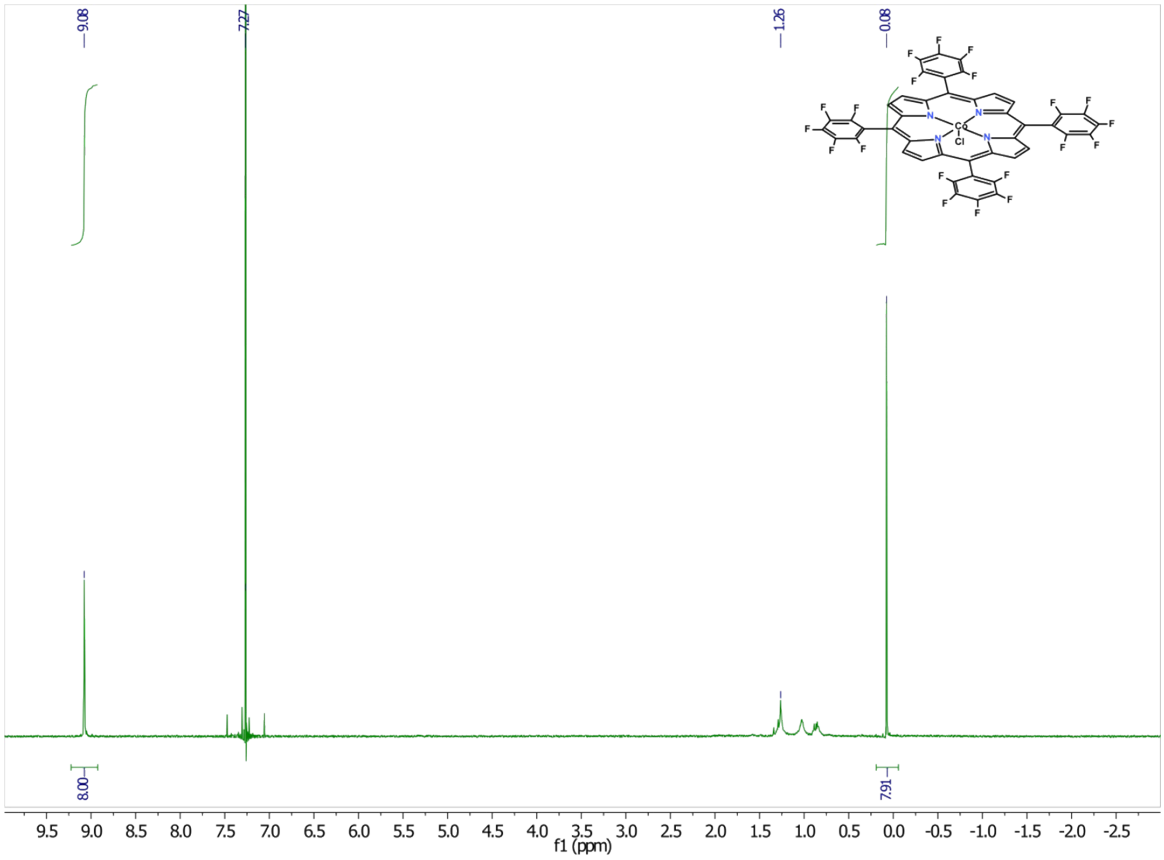

Figure 14: ^{1}H NMR spectrum of CoTPFPPCl, contains silicon grease.

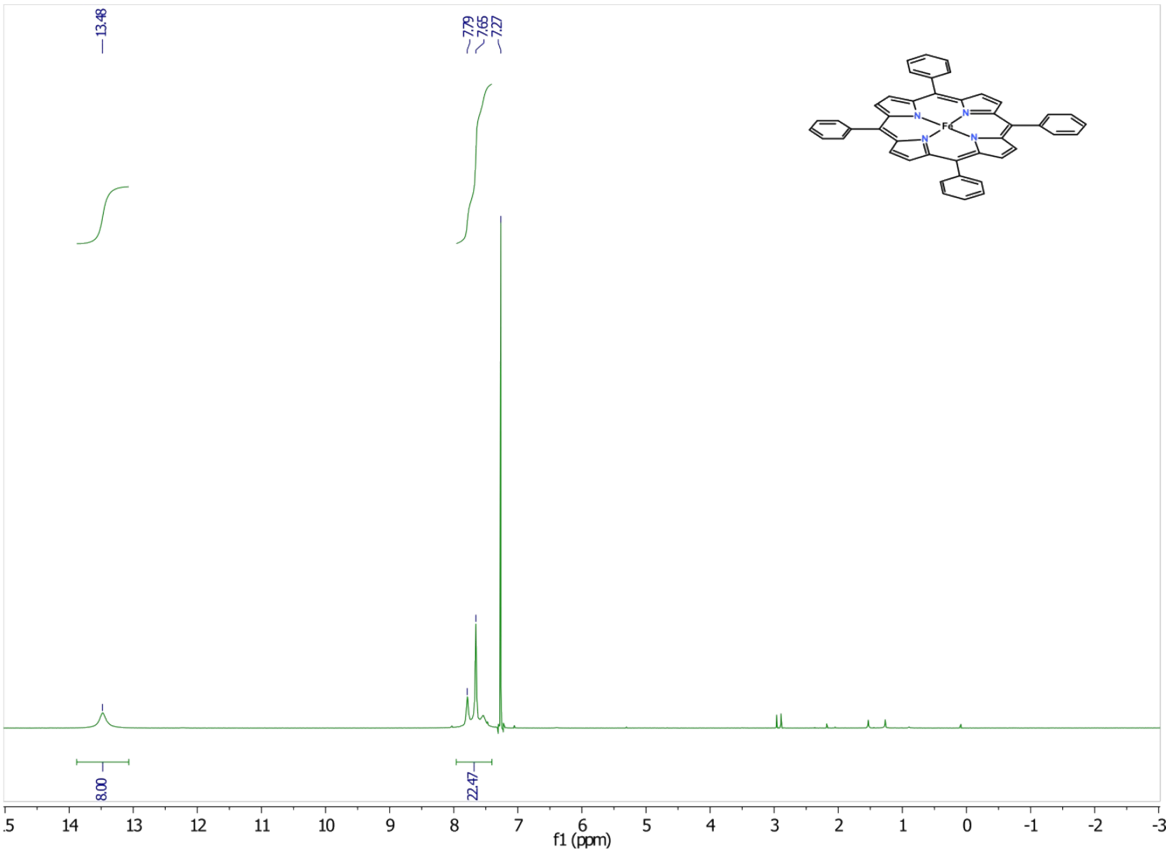

Figure 15: ^{1}H NMR spectrum of FeTPP.

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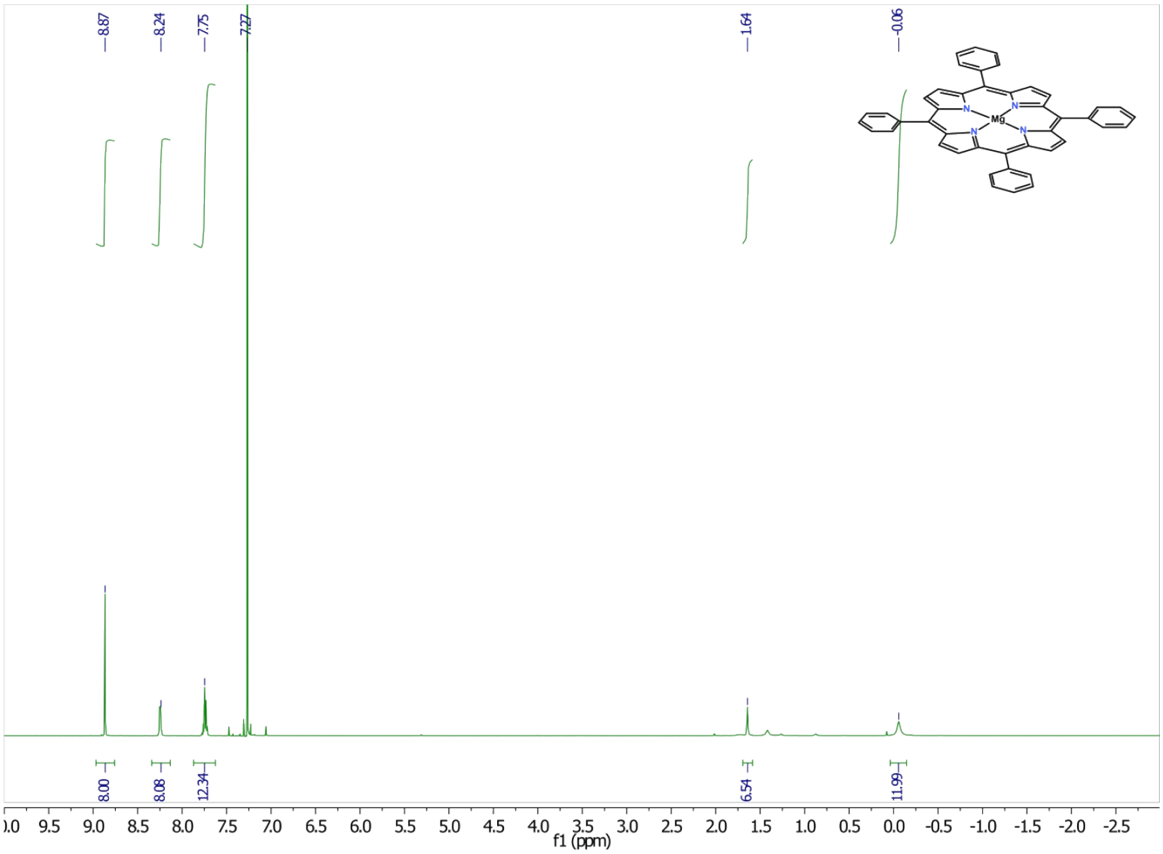

Figure 16: ^{1}H NMR spectrum of MgTPP.

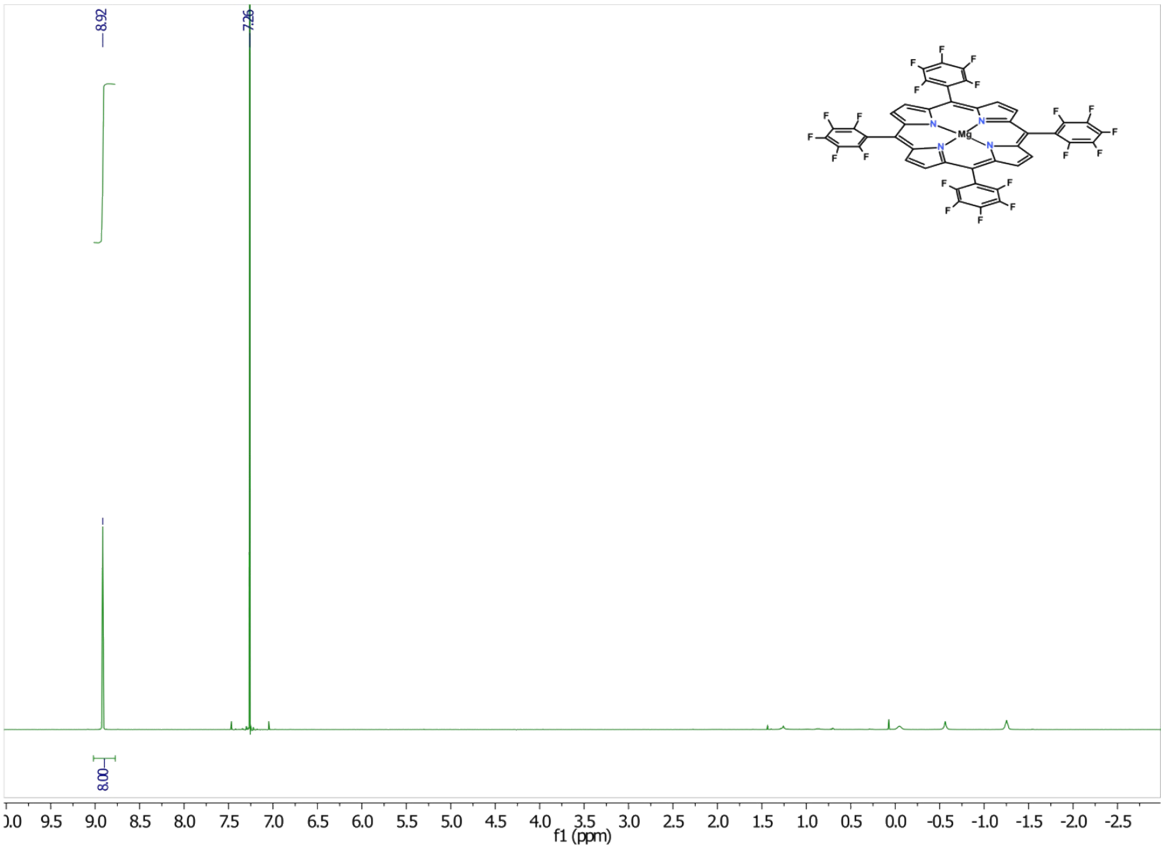

Figure 17: ^{1}H NMR spectrum of MgTPFPP.

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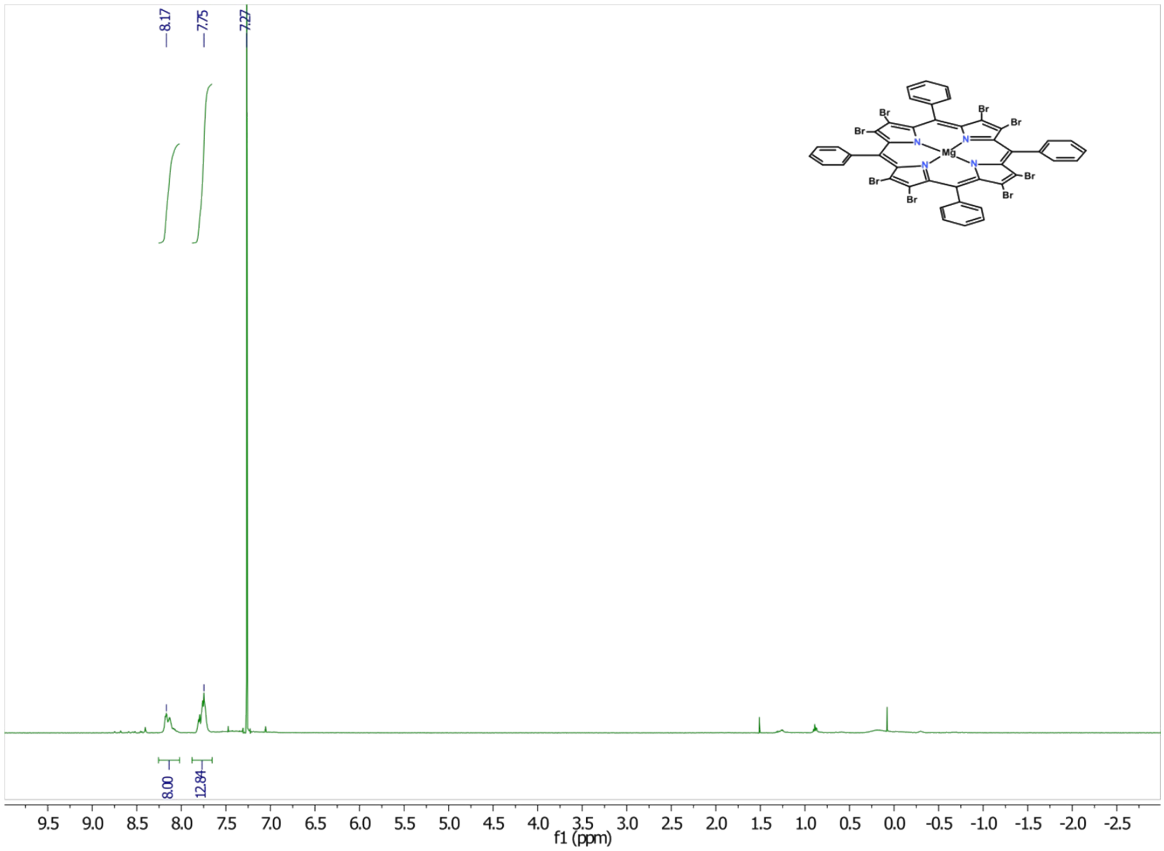

Figure 18: ^{1}H NMR spectrum of $MgTPPBr_8$.

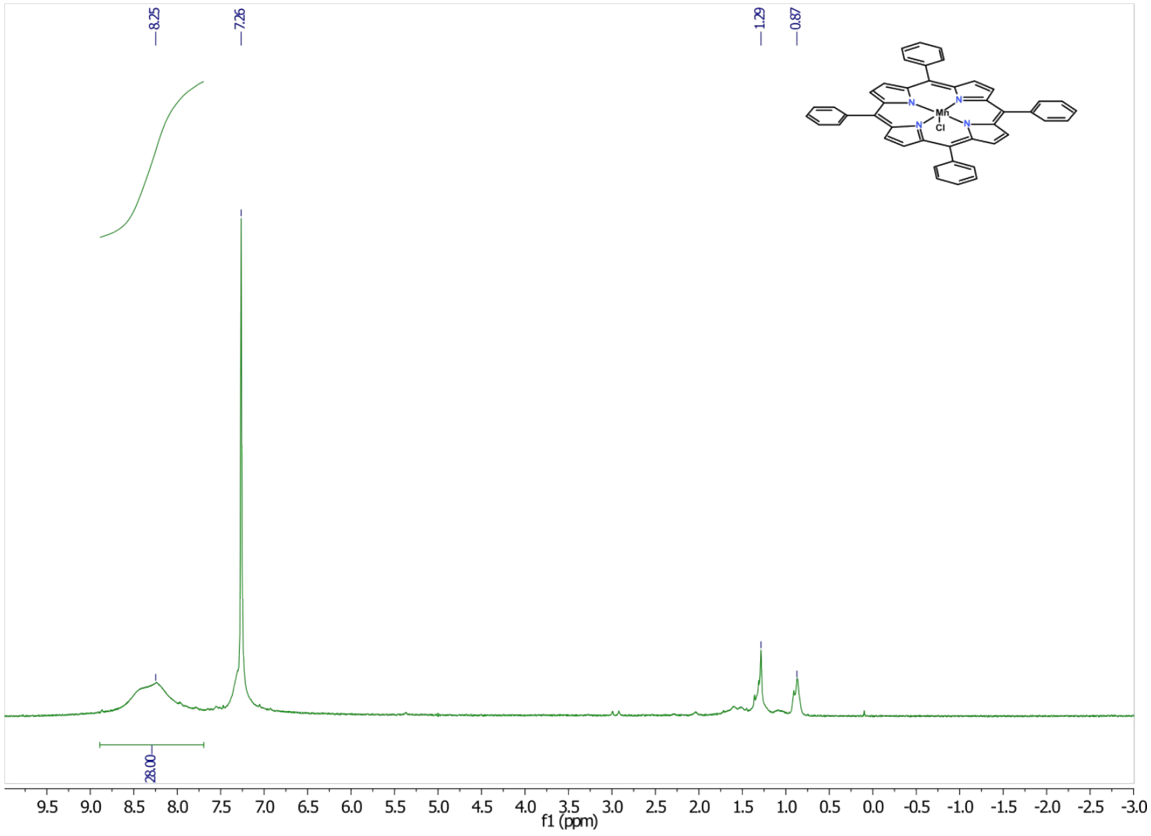

Figure 19: ^{1}H NMR spectrum of MnTPPCl.

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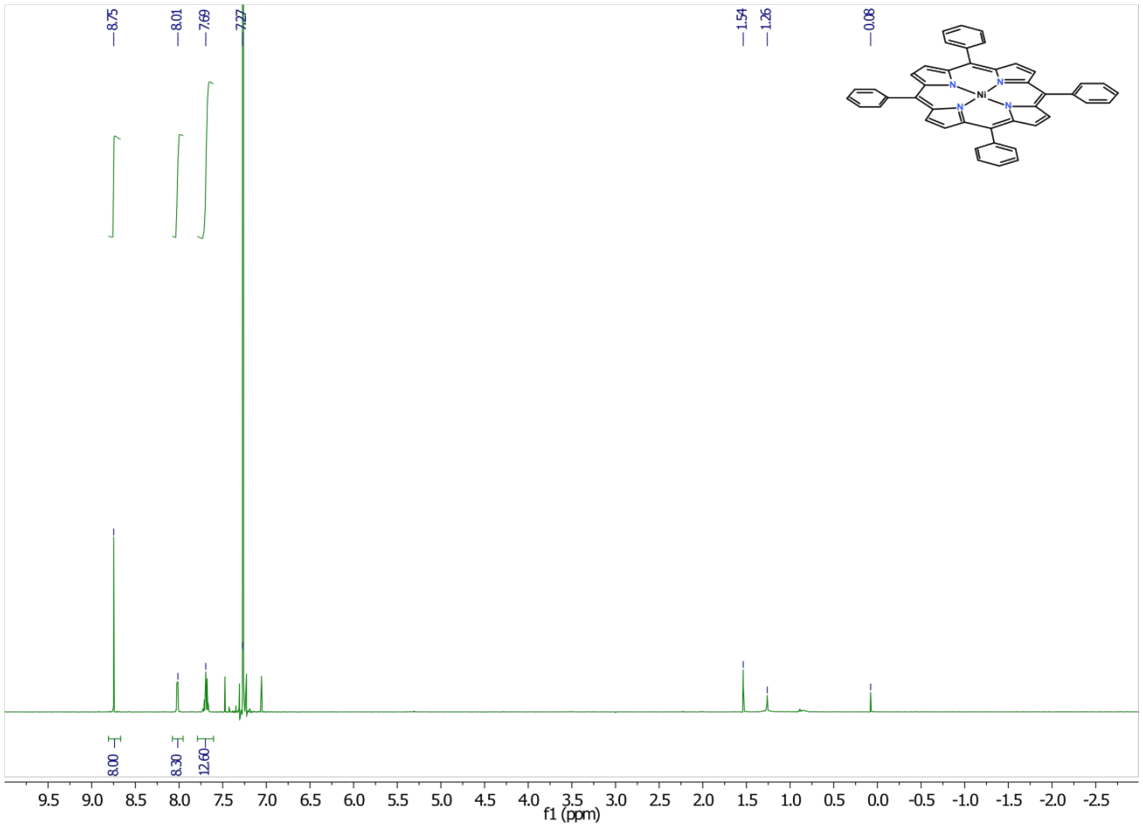

Figure 20: ^{1}H NMR spectrum of NiTPP.

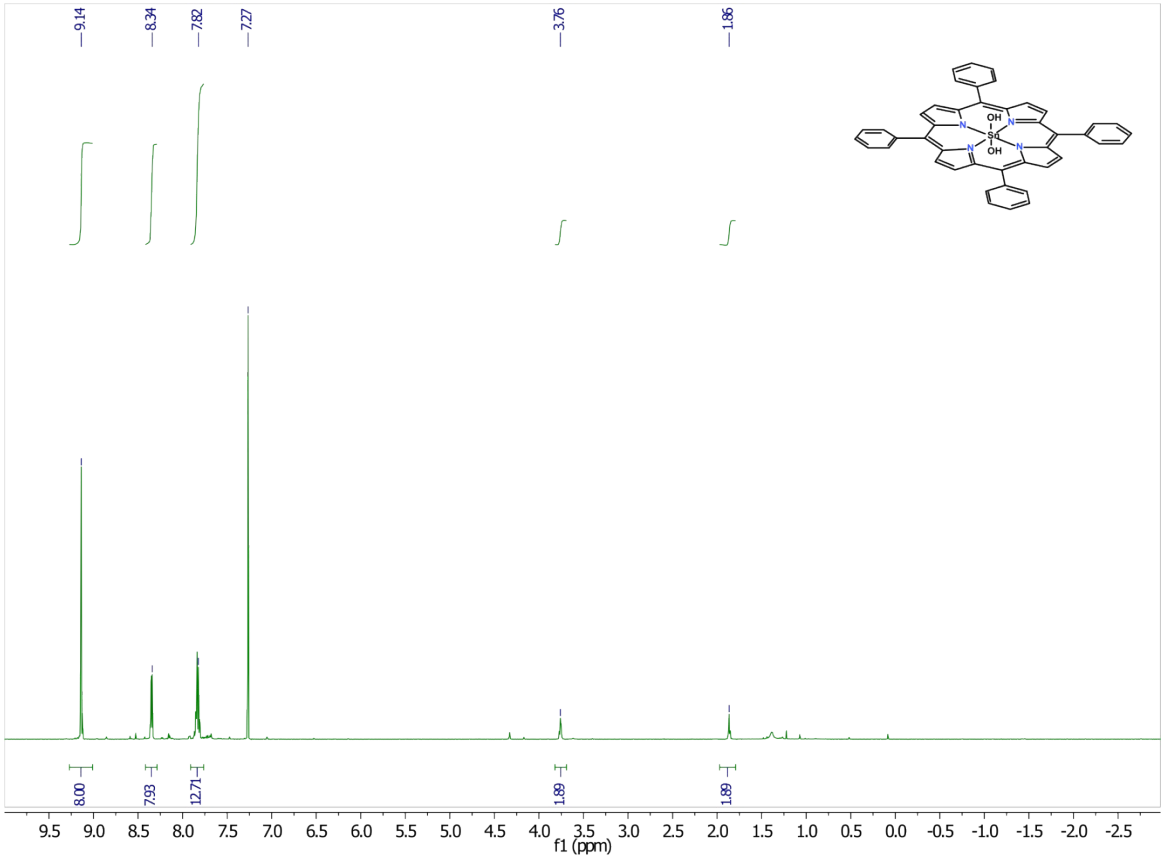

Figure 21: ^{1}H NMR spectrum of SnTPP(OH)$_2$.

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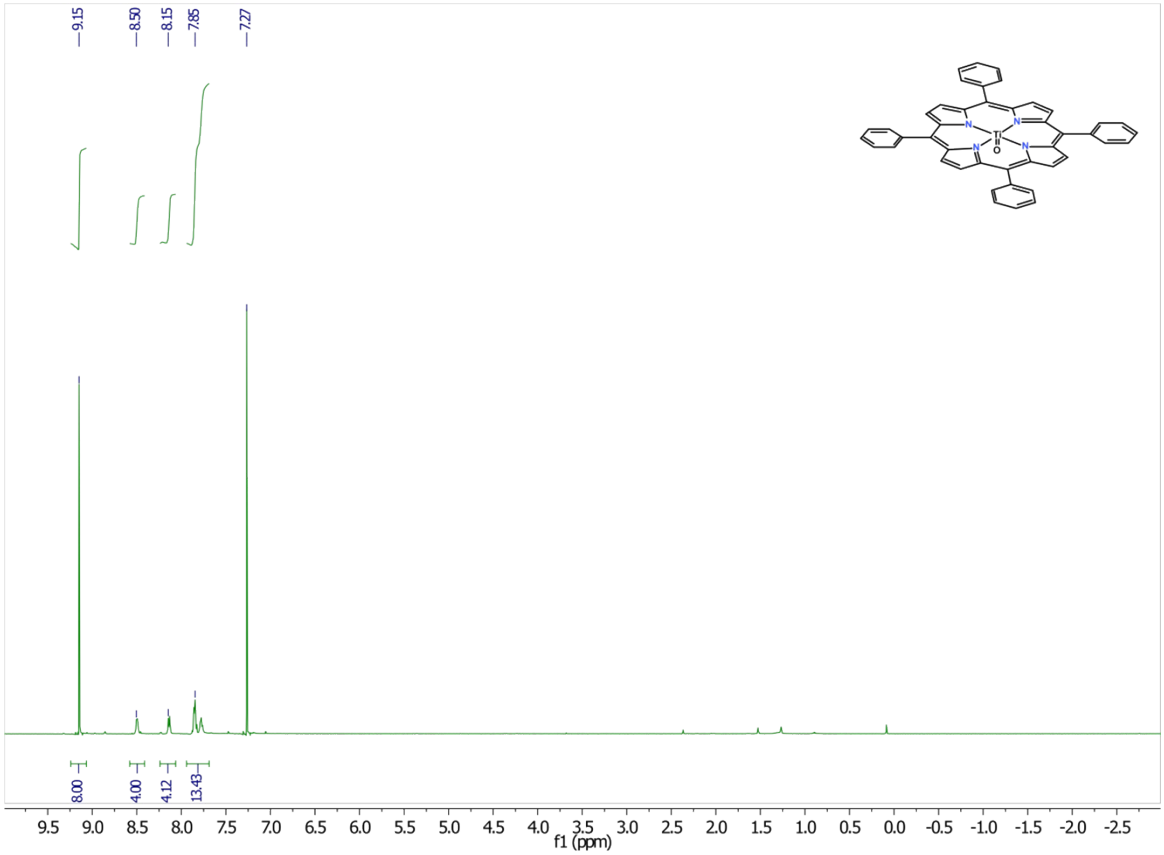

Figure 22: ^{1}H NMR spectrum of O=TiTPP.

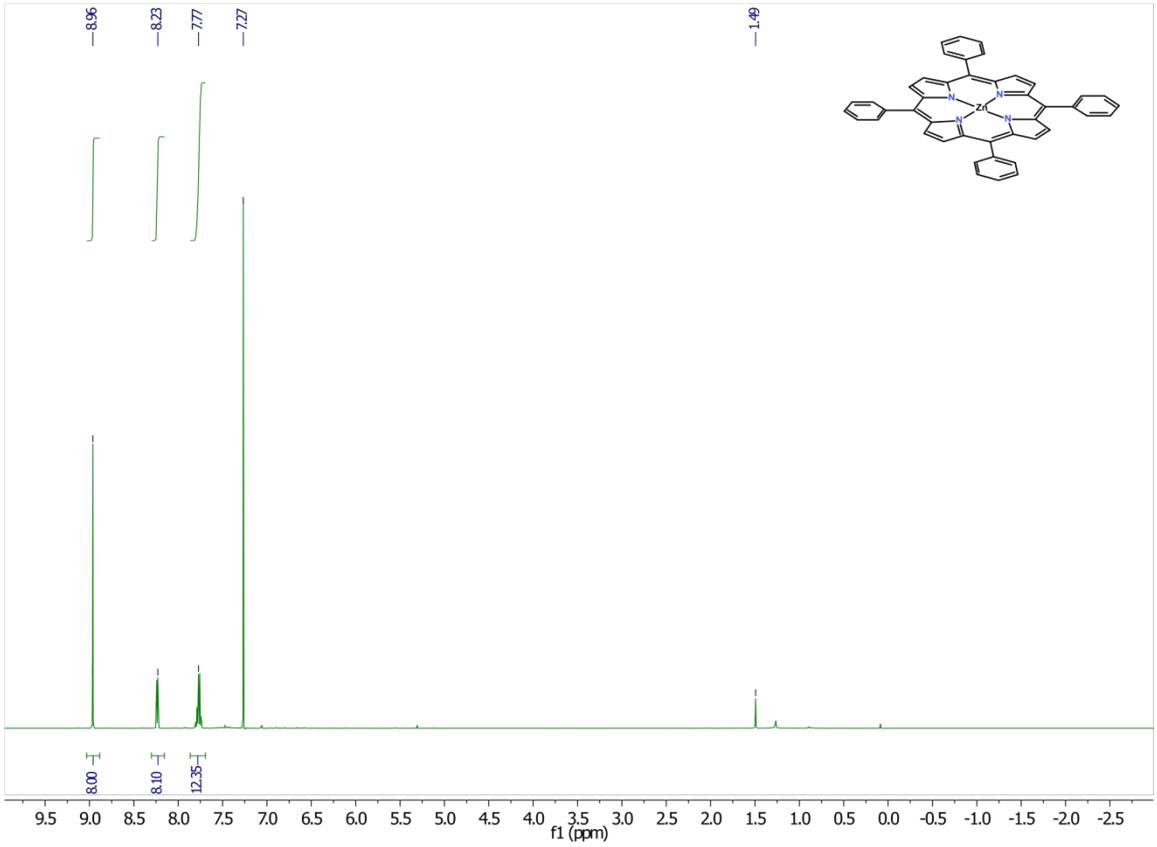

Figure 23: ^{1}H NMR spectrum of ZnTPP.

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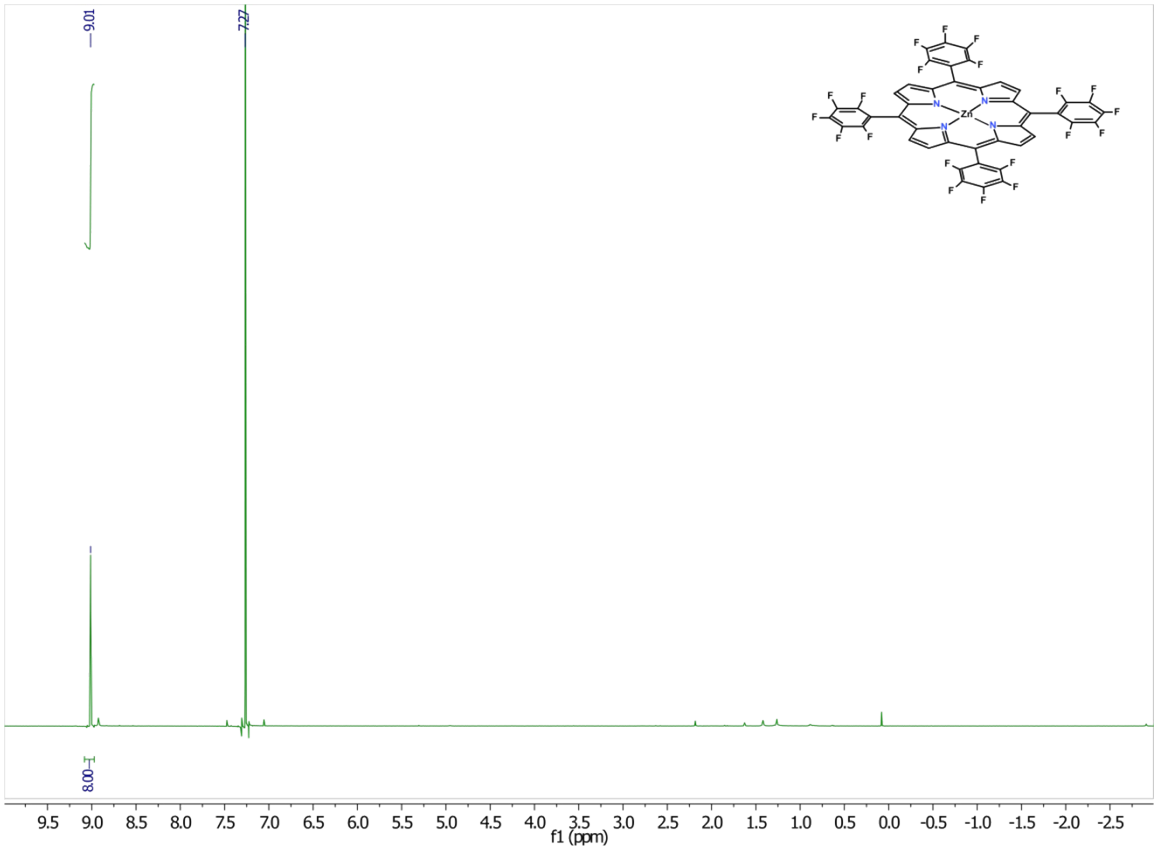

Figure 24: ^{1}H NMR spectrum of ZnTPFPP.

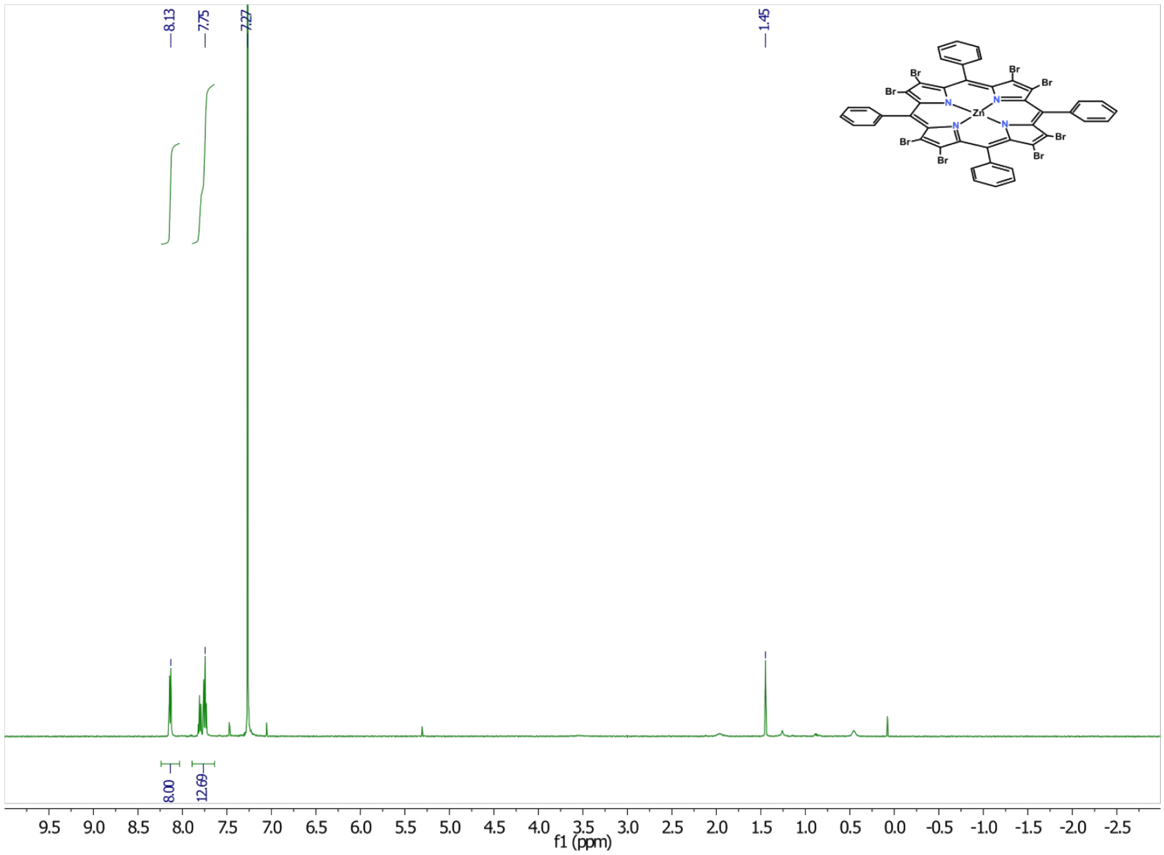

Figure 25: ^{1}H NMR spectrum of ZnTPPBr$_8$.

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8: MALDI spectra

MALDI-MS spectra of all synthesized metalloporphyrins. The spectra show a consistant systematic error of $\Delta_{m/z}$ = -2. However, correct fragmentation patterns are obtained.

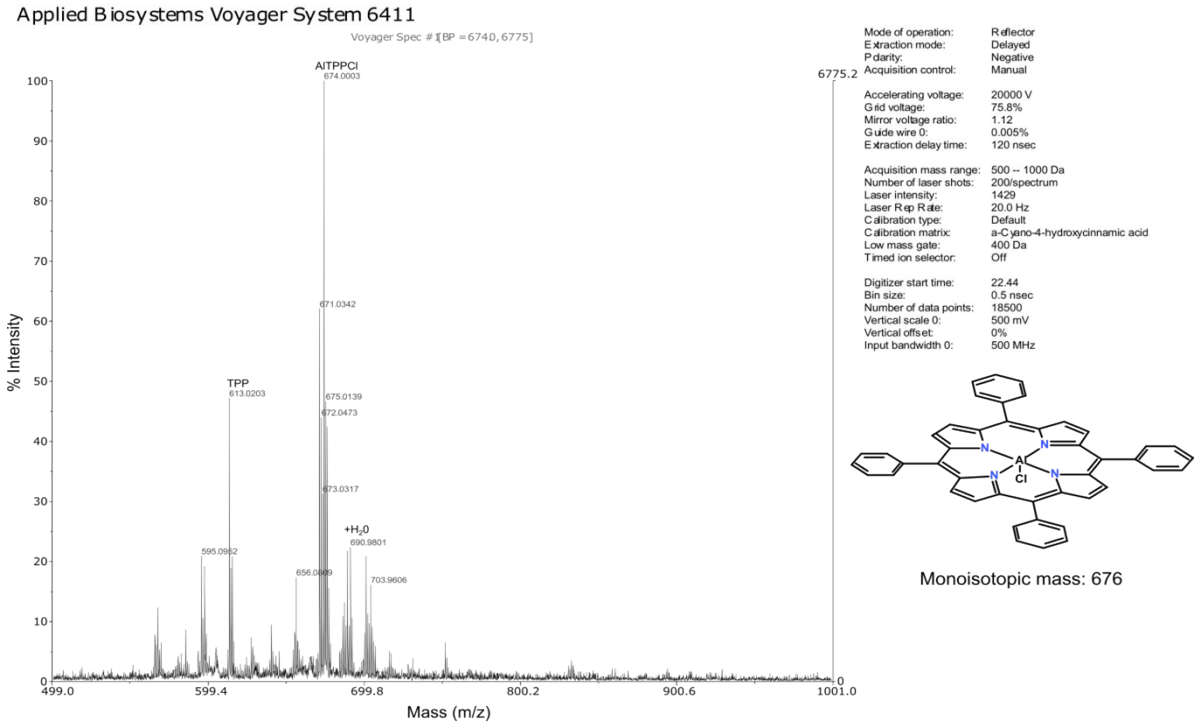

Figure 26: MALDI-MS spectrum of AlTPPCl, showing both full system and the metalloporphyrin with the chloride displaced.

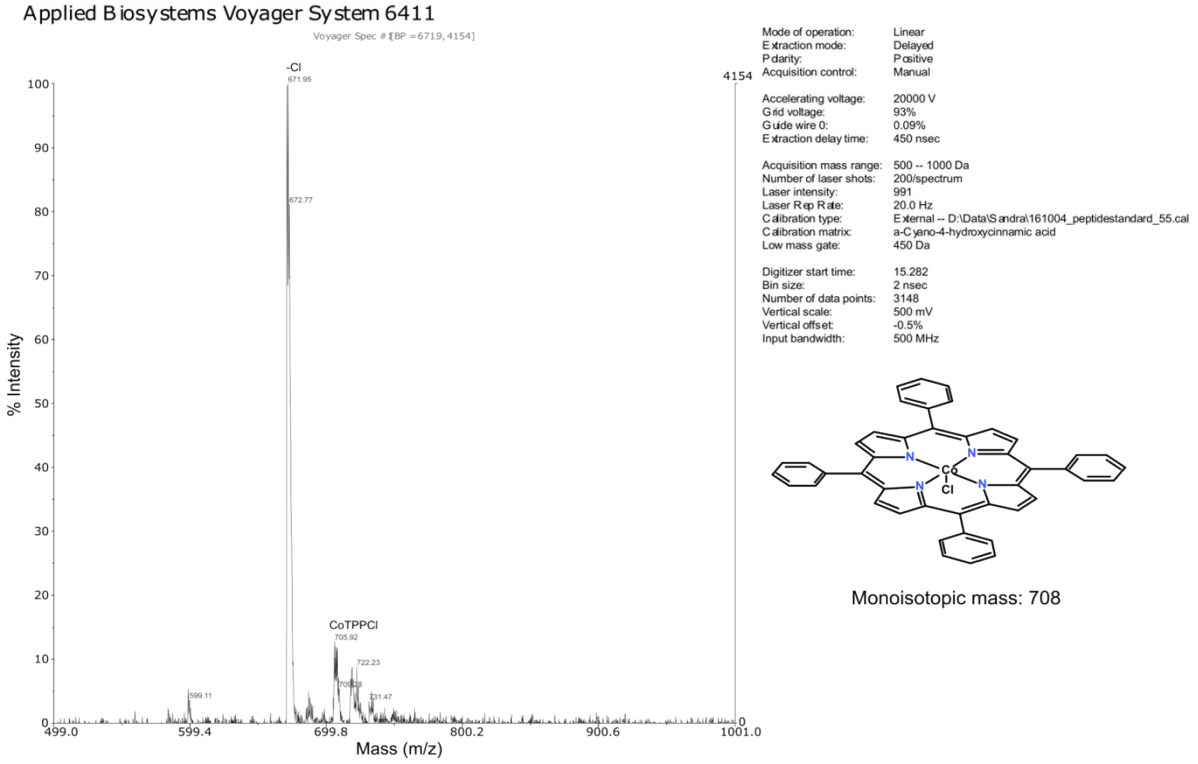

Figure 27: MALDI-MS spectrum of CoTPPCl, showing both full system and the metalloporphyrin with the chloride displaced.

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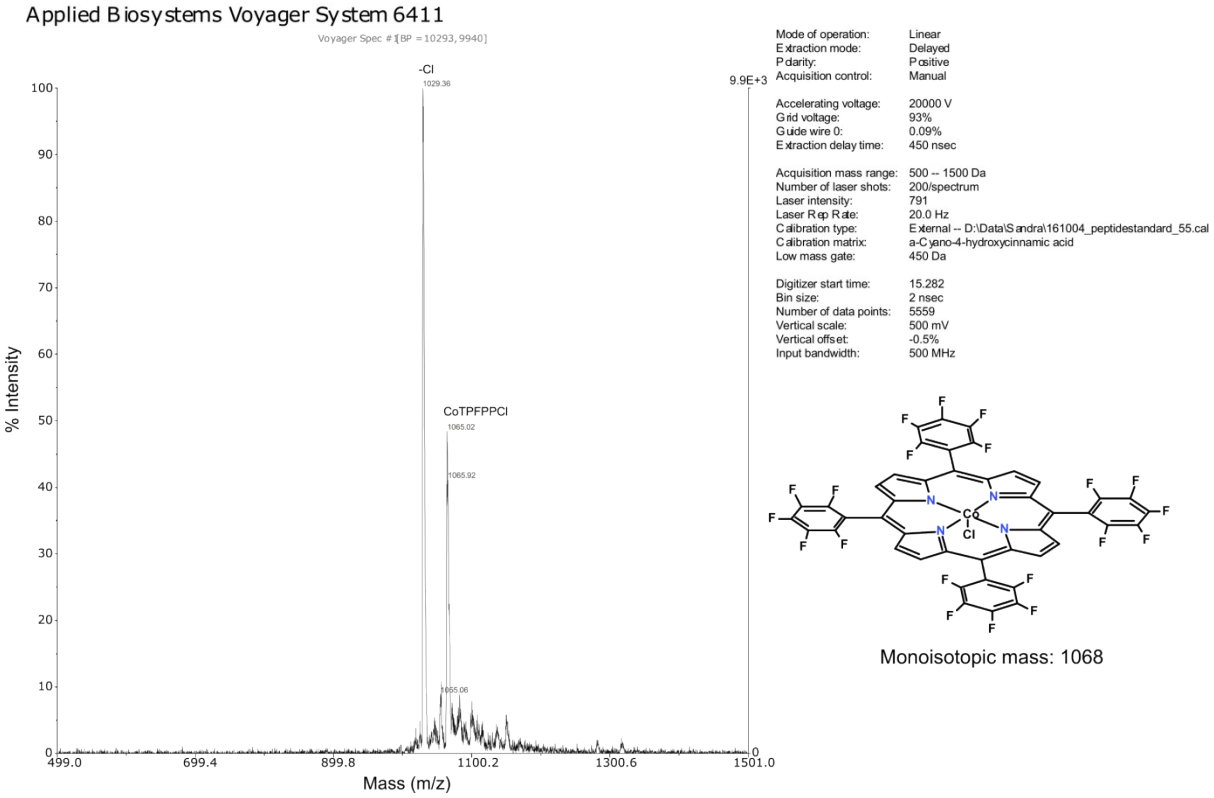

Figure 28: MALDI-MS spectrum of CoTPFPPCl, showing both full system and the metalloporphyrin with the chloride displaced.

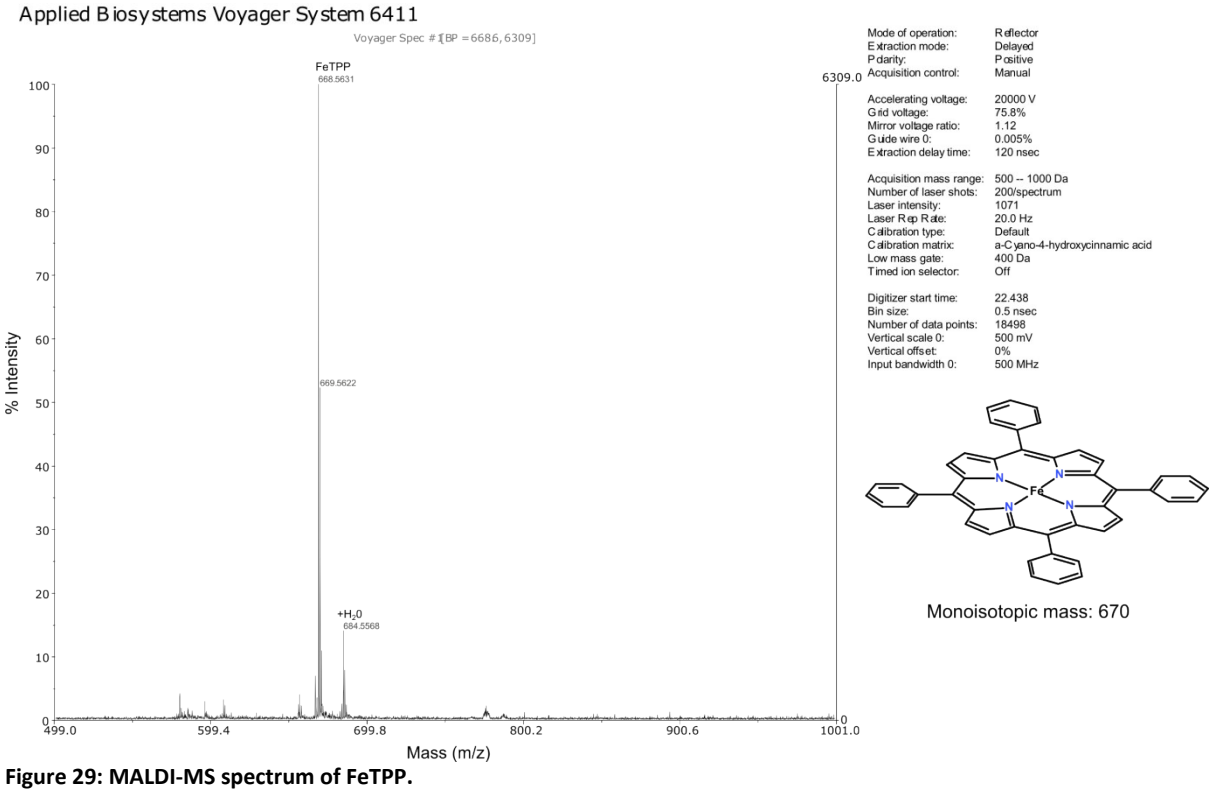

Figure 29: MALDI-MS spectrum of FeTPP.

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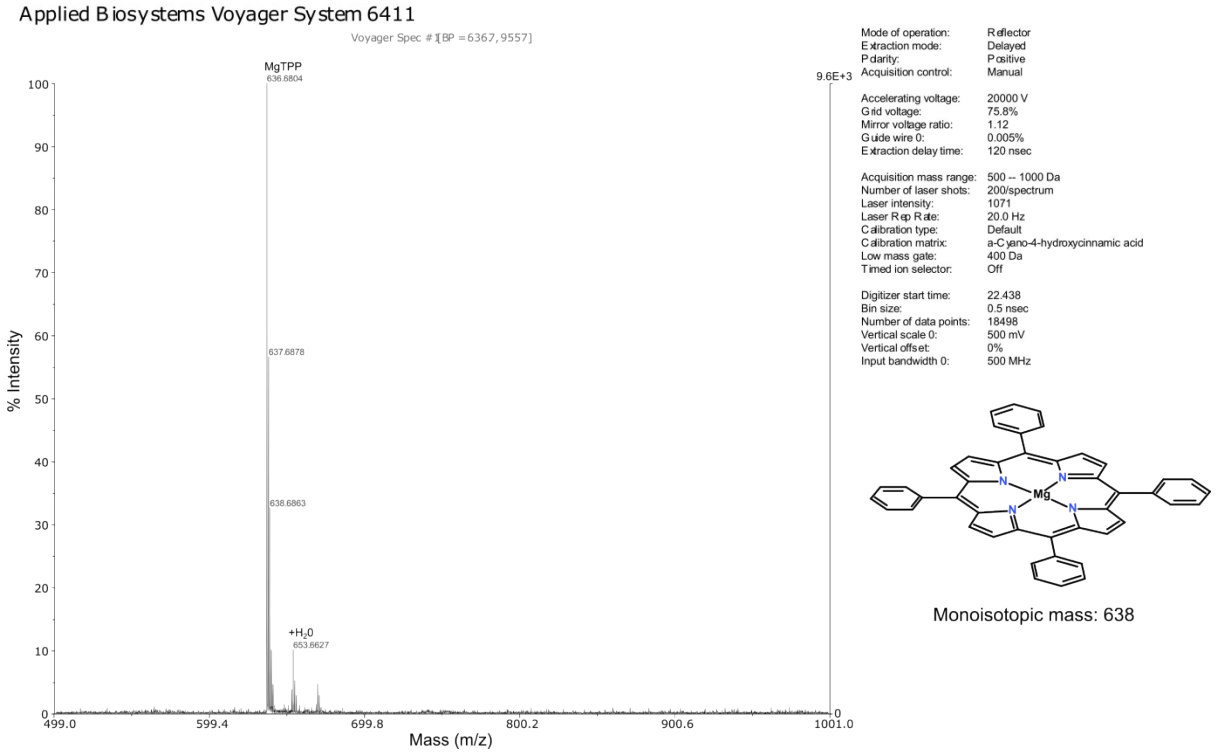

Figure 30: MALDI-MS spectrum of MgTPP.

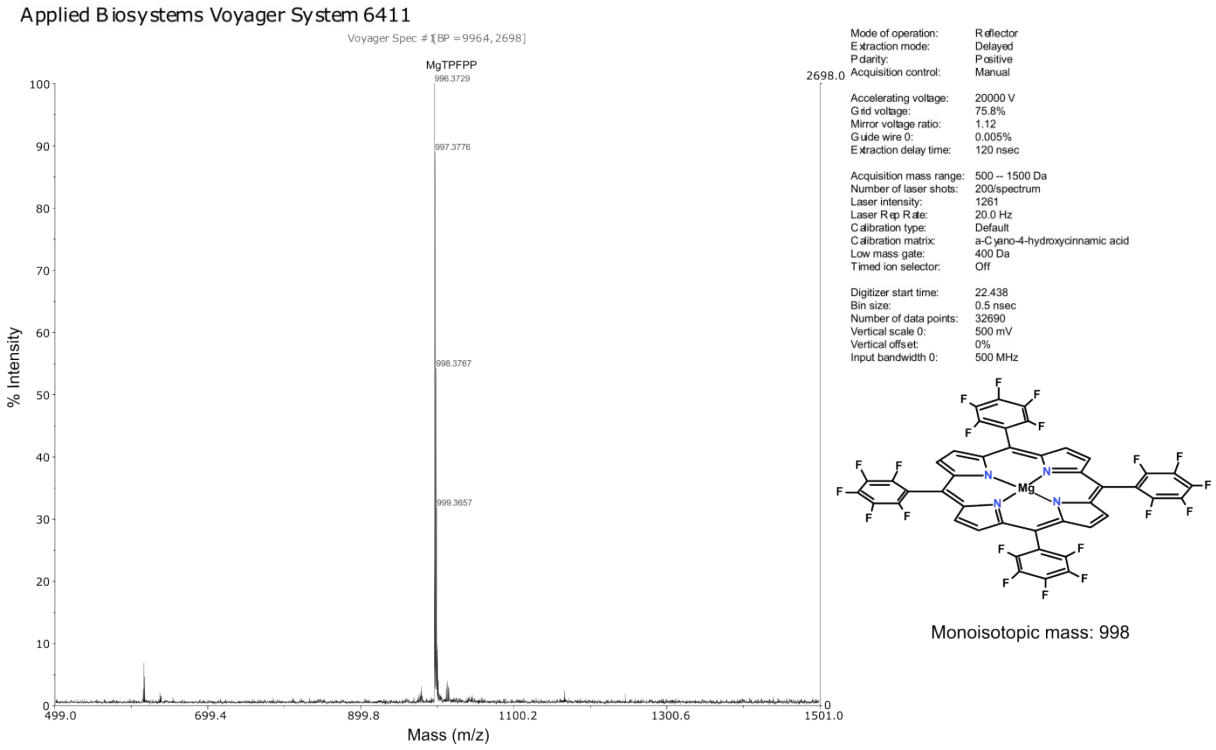

Figure 31: MALDI-MS spectrum of MgTPFPP.

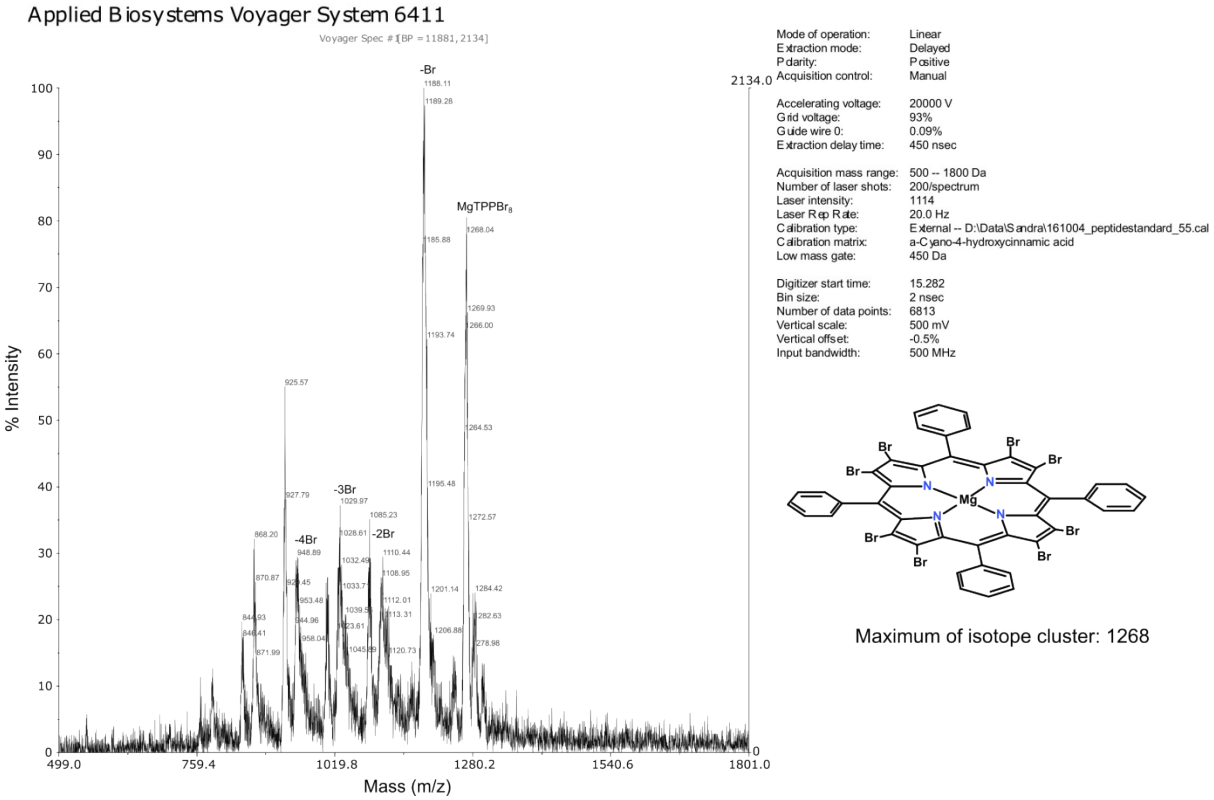

Figure 32: MALDI-MS spectrum of $MgTPPBr_8$.

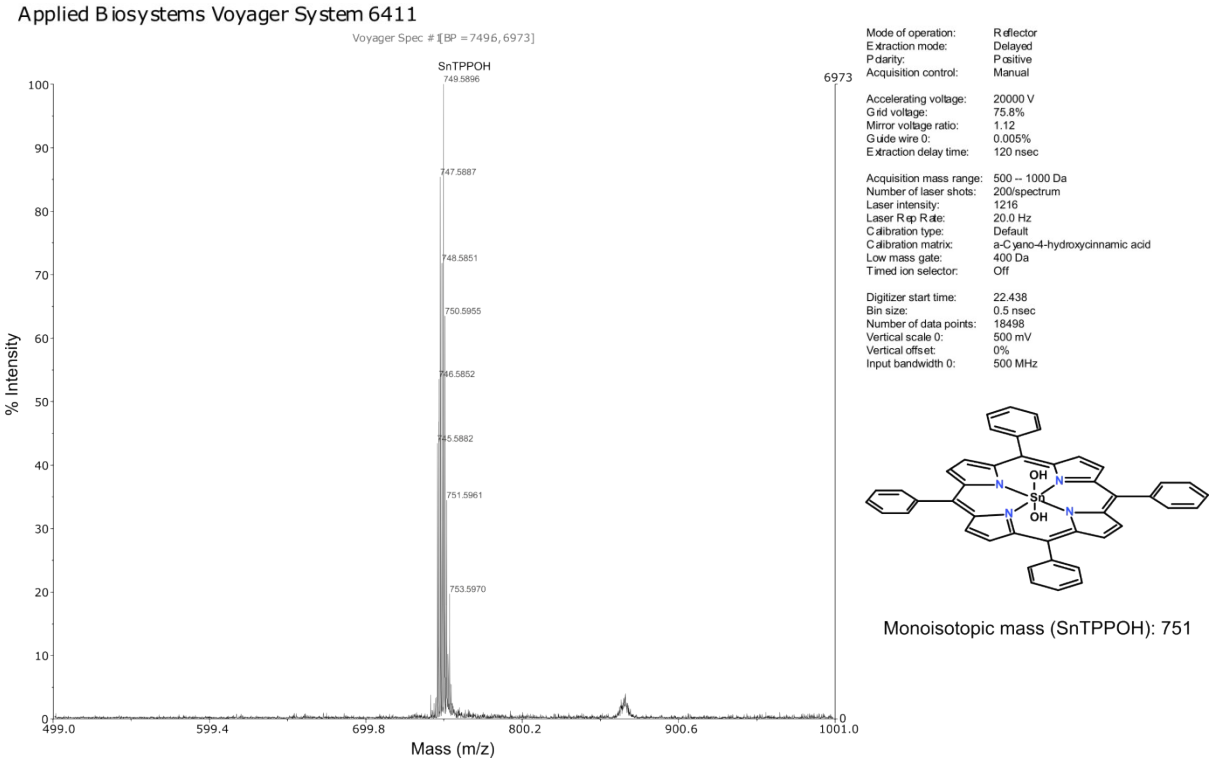

Figure 33: MALDI-MS spectrum of $SnTPP(OH)_2$, showing up with one OH-ligand displaced.

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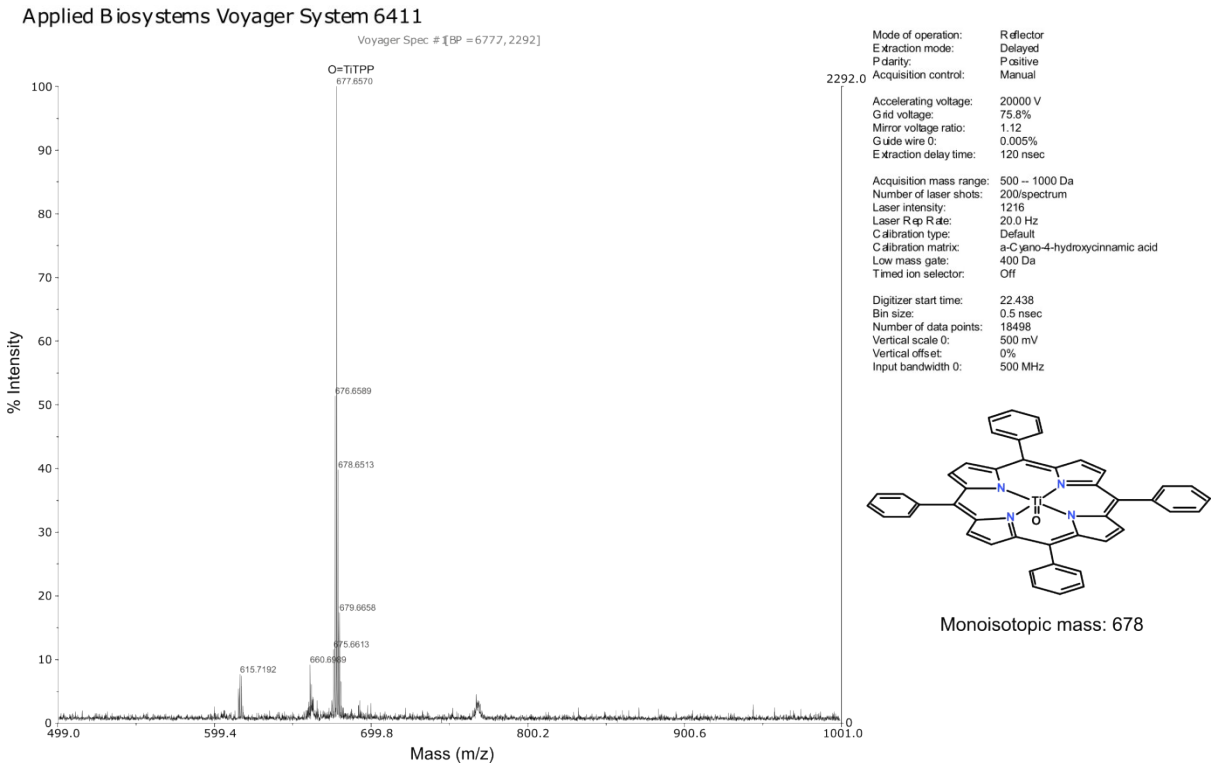

Figure 34: MALDI-MS spectrum of O=TiTPP.

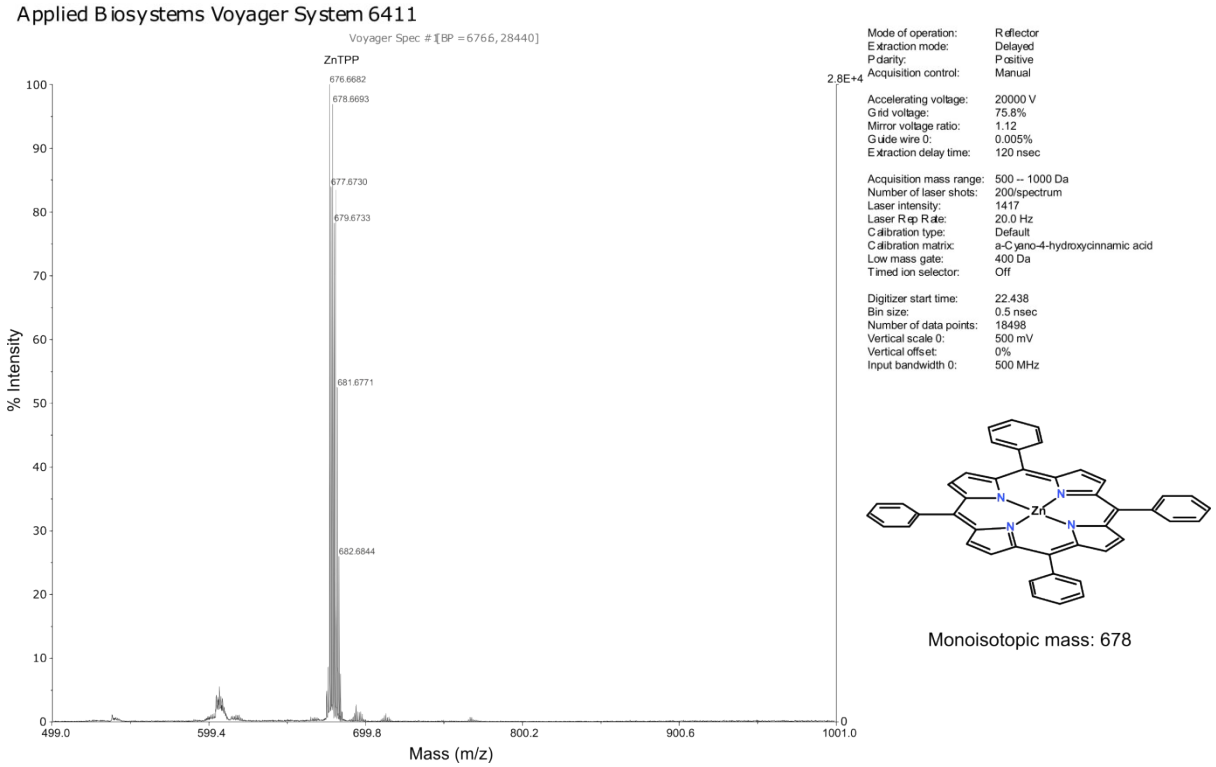

Figure 35: MALDI-MS spectrum of ZnTPP.

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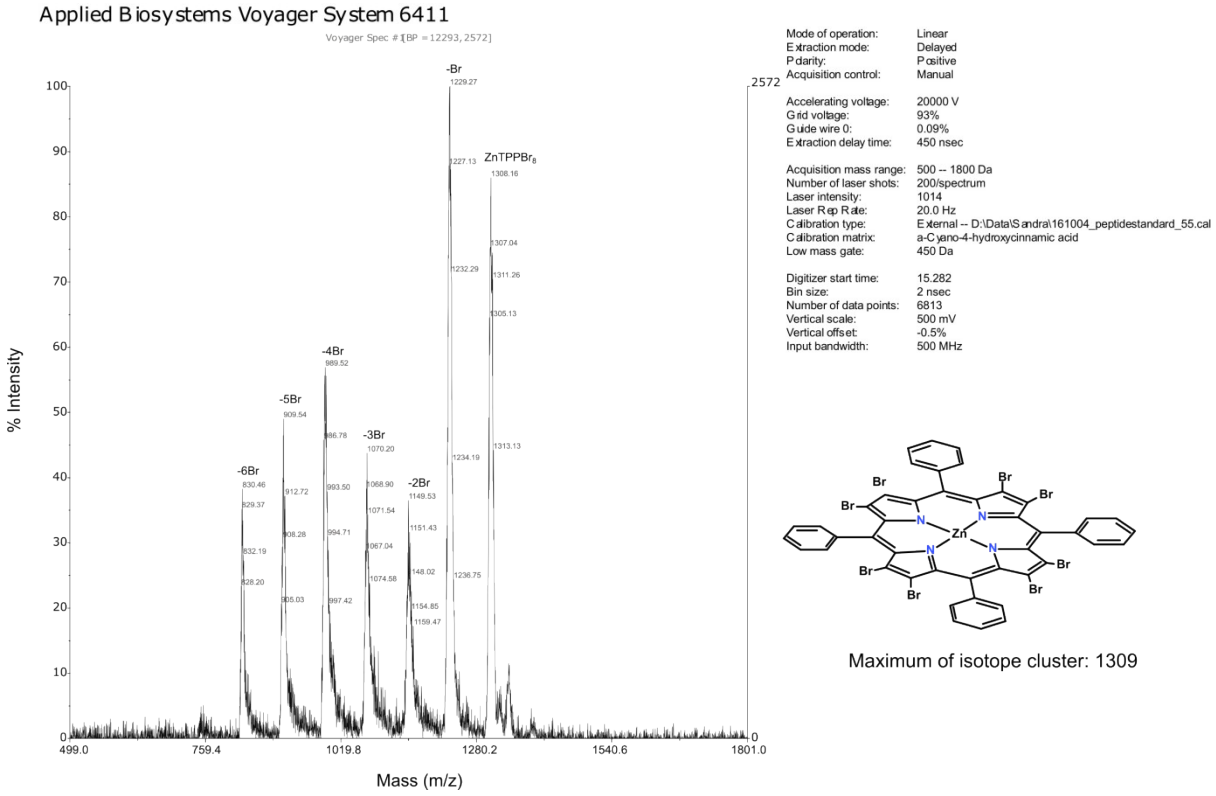

Figure 36: MALDI-MS spectrum of $ZnTPPBr_8$.

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