# Electronic effects on polypyridyl Co complex-based water reduction catalysts.

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# 1. Synthesis

**L2, 6-MeOTPA, ((6-methoxyl-2-pyridyl)methyl)bis(2-pyridylmethyl)amine**

Similar to the method in literature,[1-3] the ligand **L2** was synthesized in an argon saturated flask. 6-Methoxypyridine-2-carbaldehyde (549 mg, 4 mmol), *N,N*-bis(2-pyridinylmethyl)amine (797 mg, 4 mmol) and sodium triacetoxyborohydride (1.3 g, 5.86 mmol) were dissolved in 1,2-dichloroethane and stired for 2 days at room temperature. Afterwards, the solvent was removed and the crude product was dissolved in dichloromethane, then the solution was washed by saturated $NaCO_3$ aqueous solution for three times. After drying by anhydrous $MgSO_4$, the crude product was purified by column chromatography, and pure product was obtained as yellow oil (1.1 g, 85.9%). $^1$H NMR (400 MHz, Chloroform-*d*) δ 8.53 (dd, *J* = 4.8, 1.4 Hz, 2H), 7.66 (d, *J* = 4.3 Hz, 4H), 7.53 (t, *J* = 7.8 Hz, 1H), 7.15 (q, *J* = 4.5 Hz, 2H), 7.06 (d, *J* = 7.2 Hz, 1H), 6.60 (d, *J* = 8.2 Hz, 1H), 4.02 (s, 3H), 3.94 (d, *J* = 1.1 Hz, 4H), 3.87 (s, 2H). $^{13}$C NMR (101 MHz, Chloroform-d) δ ppm =163.61, 159.81, 156.86, 149.03, 138.75, 136.37, 122.73, 121.89, 115.43, 108.71, 60.23, 60.00, 53.26. ESI-MS: m/z = 321.1699 (calcd m/z = 321.17 for [M+H$^+$] )

**L3, 5-MeOTPA, ((5-methoxyl-2-pyridyl)methyl)bis(2-pyridylmethyl)amine**

Following the above mentioned procedures and using 5-methoxypyridine-2-carbaldehyde (250 mg, 1.8 mmol) instead of 6-methoxypyridine-2-carbaldehyde, we got **L3** as yellow oily product (289.8 mg, 49.6%). $^1$H NMR (400 MHz, Chloroform-*d*) δ 8.55 (d, *J* = 4.9 Hz, 2H), 8.25 (d, *J* = 2.9 Hz, 1H), 7.67 (t, *J* = 7.7 Hz, 2H), 7.59 (d, *J* = 7.8 Hz, 2H), 7.49 (d, *J* = 8.5 Hz, 1H), 7.22 – 7.12 (m, 3H), 3.93 (d, *J* = 26.3 Hz, 5H), 3.84 (s, 3H). $^{13}$C NMR (101 MHz, Chloroform-d) δ ppm =159.52, 154.58, 151.21, 149.05, 136.34, 136.29, 123.44, 122.97, 121.91, 121.27, 60.03, 59.43, 55.60. ESI-MS: m/z = 321.1703 (calcd m/z = 321.17 for [M+H$^+$])

**L4, 4-MeOTPA, ((4-methoxyl-2-pyridyl)methyl)bis(2-pyridylmethyl)amine**

Following the above mentioned procedures and using 4-methoxypyridine-2-carbaldehyde (440 mg, 3 mmol) instead of 6-methoxypyridine-2-carbaldehyde, we obtained **L4** as yellow oily product (706.6 mg, 73.5%). $^1$H NMR (400 MHz, DMSO-d6) δ 8.50 (d, *J* = 4.8 Hz, 2H), 8.30 (d, *J* = 5.7 Hz, 1H), 7.77 (d, *J* = 7.6 Hz, 2H), 7.58 (d, *J* = 7.8 Hz, 2H), 7.23-7.27 (m, 2H), 7.18 (s, 1H), 6.84 (d, *J* = 3.7 Hz, 1H), 3.82 (s, 3H), 3.80 (s, 4H), 3.74 (s, 2H). $^{13}$C NMR (101 MHz, Chloroform-d) δ ppm =166.25, 161.26, 159.35, 150.27, 149.11, 136.37, 122.93, 121.97, 108.67, 108.29, 60.21, 60.18, 55.07. ESI-MS: m/z = 321.1700 (calcd m/z = 321.17 for [M+H$^+$])

**L5, 4-MeTPA, ((4-methyl-2-pyridyl)methyl)bis(2-pyridylmethyl)amine**

Following the above mentioned procedures and using 4-methylpyridine-2-carbaldehyde (363 mg, 3 mmol) instead of 6-methoxypyridine-2-carbaldehyde, **L5** was achieved as yellow oily product (590.7 mg, 64.7%). $^1$H NMR (400 MHz, Chloroform-*d*) δ 8.57–8.48 (m, 2H), 8.38 (d, *J* = 5.1 Hz, 1H), 7.65 (tt, *J* = 7.6, 1.5 Hz, 2H), 7.57 (d, *J* = 7.8 Hz, 2H), 7.35 (s, 1H), 7.14 (dd, *J* = 7.3, 5.1 Hz, 2H), 6.96 (d, *J* = 5.1 Hz, 1H), 3.87 (d, *J* = 14.7 Hz, 6H), 2.34 (s, 3H). $^{13}$C NMR (101 MHz,

Chloroform-d) δ ppm =159.39, 158.99, 149.05, 148.81, 147.44, 136.37, 123.84, 123.05, 122.99, 121.94, 60.23, 60.15, 21.14. ESI-MS: m/z = 305.1752 (calcd m/z = 321.17 for $[M+H^+]$)

**C2, $[Co^{II}$(6-MeOTPA)Cl]Cl**

**L2** (320 mg, 1 mmol) and $CoCl_2 \cdot 6H_2O$ (238 mg, 1 mmol) were dissolved in dry acetonitrile and mixed under an argon atmosphere, then stirred for 4 h at room temperature. After removal of the solvent, the solid was washed by diethyl ether and hexane. After drying under vacuum overnight, the final product was obtained as green powders (290.8 mg, 64.6%). IR (KBr, $cm^{-1}$): 3414, 1604, 1469, 1436, 1307, 1268, 1153, 1032, 788, 754, 639. UV/Vis ($CH_3CN$) λ= 499, 627(nm). ESI-MS: m/z = 414.06543 (calcd m/z =414.07 for $[Co(6\text{-}MeOTPA)Cl]^+$), 424.09390 (calcd m/z = 424.09 for [Co(6-MeOTPA)COOH]). Elemental analysis: anal. calcd for C19H20Cl2CoN4O: C, 50.69; H ,4.48; N, 12.44. Found: C, 50.74; H, 4.55; N, 12.39.

**C3, $[Co^{II}$(5-MeOTPA)Cl]Cl**

Similar to **C2**, **C3** was obtained (182.6 mg, 81.2%). IR (KBr, $cm^{-1}$): 3429, 1609, 1573, 1492, 1438, 1293, 1265, 1026, 839, 774, 651. UV/Vis ($CH_3CN$) λ= 487, 633(nm). ESI-MS: m/z = 414.06534 (calcd m/z = 414.07 for $[Co(5\text{-}MeOTPA)Cl]^+$). Elemental analysis: anal. calcd for C19H20Cl2CoN4O: C, 50.69; H ,4.48; N, 12.44. Found: C, 50.61; H, 4.39; N, 12.42.

**C4, $[Co^{II}$(4-MeOTPA)Cl]Cl**

Similar to **C2**, **C4** was obtained (350.9 mg, 77.9%). IR (KBr, $cm^{-1}$): 3424, 1612, 1489, 1437, 1312, 1263, 1038, 847, 775, 649. UV/Vis ($CH_3CN$) λ= 490, 636(nm). ESI-MS: m/z = 414.06488 (calcd m/z = 414.07 for $[Co(4\text{-}MeOTPA)Cl]^+$ ). Elemental analysis: anal. calcd for C19H20Cl2CoN4O: C, 50.69; H ,4.48; N, 12.44. Found: C, 50.67; H, 4.63; N, 12.56.

**C5, $[Co^{II}$(4-MeTPA)Cl] Cl**

Similar to **C2**, **C5** was obtained (392.8 mg, 90.5%). IR (KBr, $cm^{-1}$): 3446, 1607, 1482, 1438, 1310, 1266, 1025, 839, 775, 649. UV/Vis ($CH_3CN$) λ= 486, 634(nm). ESI-MS: m/z = 398.07074 (calcd m/z = 398.07 for $[Co(4\text{-}MeTPA)Cl]^+$). Elemental analysis: anal. calcd for C19H20Cl2CoN4: C, 52.55; H ,4.64; N, 12.90. Found: C, 52.73; H, 4.68; N, 12.77.

## 2. $^{1}$H NMR spectra

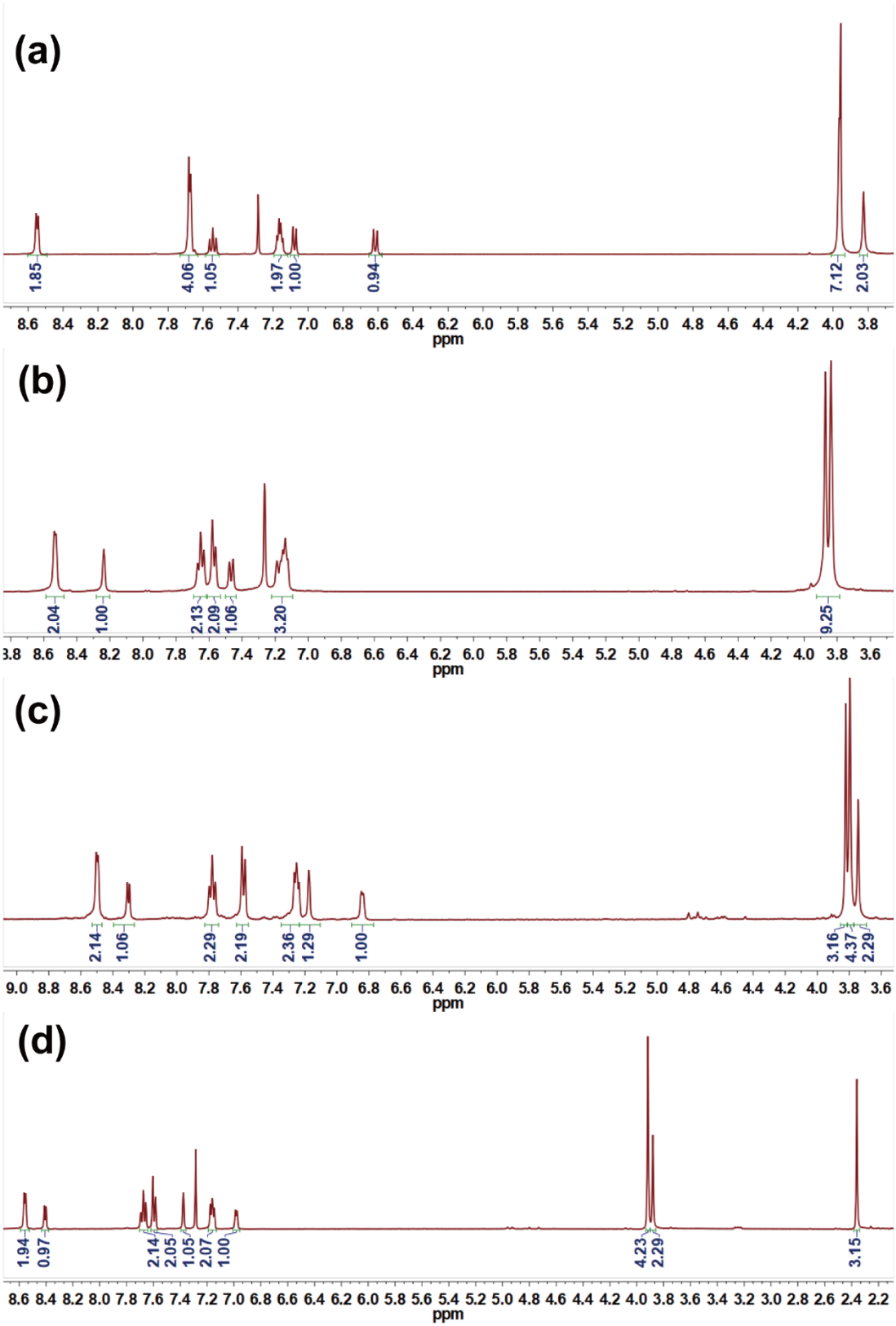


**Figure S1.** $^{1}$H NMR spectra of **L2** (**a**), **L3** (**b**), **L5** (**d**) in $CDCl_3$ and **L4** (**c**) in DMSO-$d_6$.

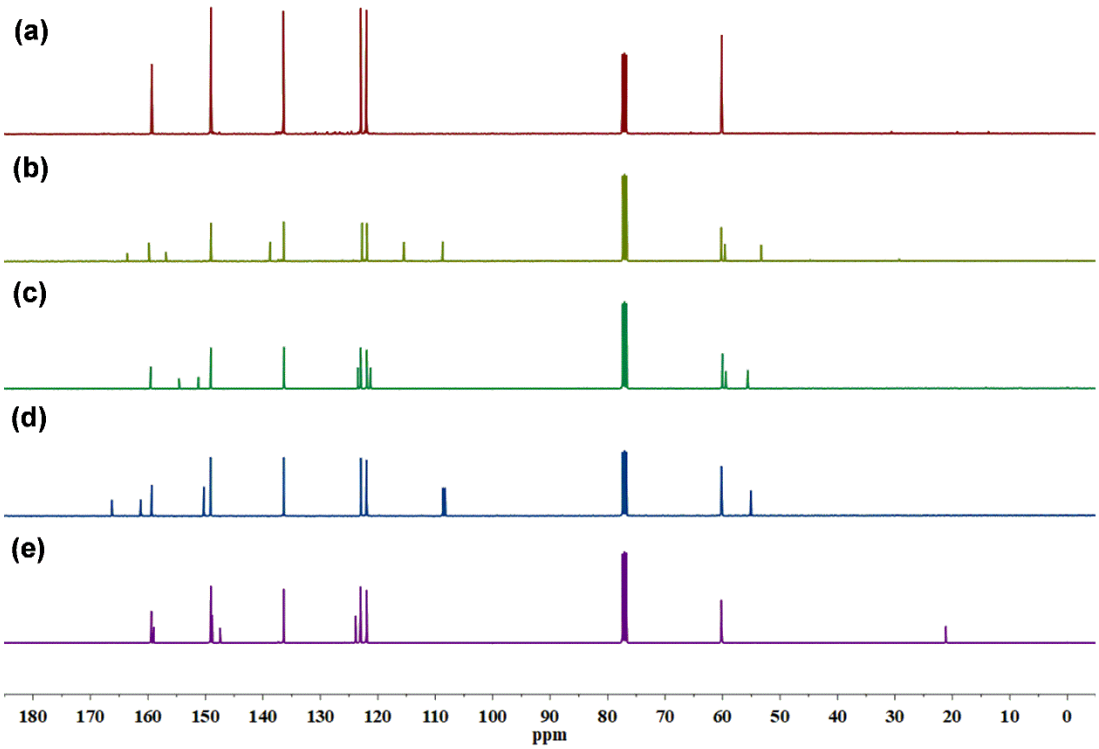


**Figure S2.** $^{13}C$ NMR spectra of **L1-L5** (**a-e**) in $CDCl_3$.

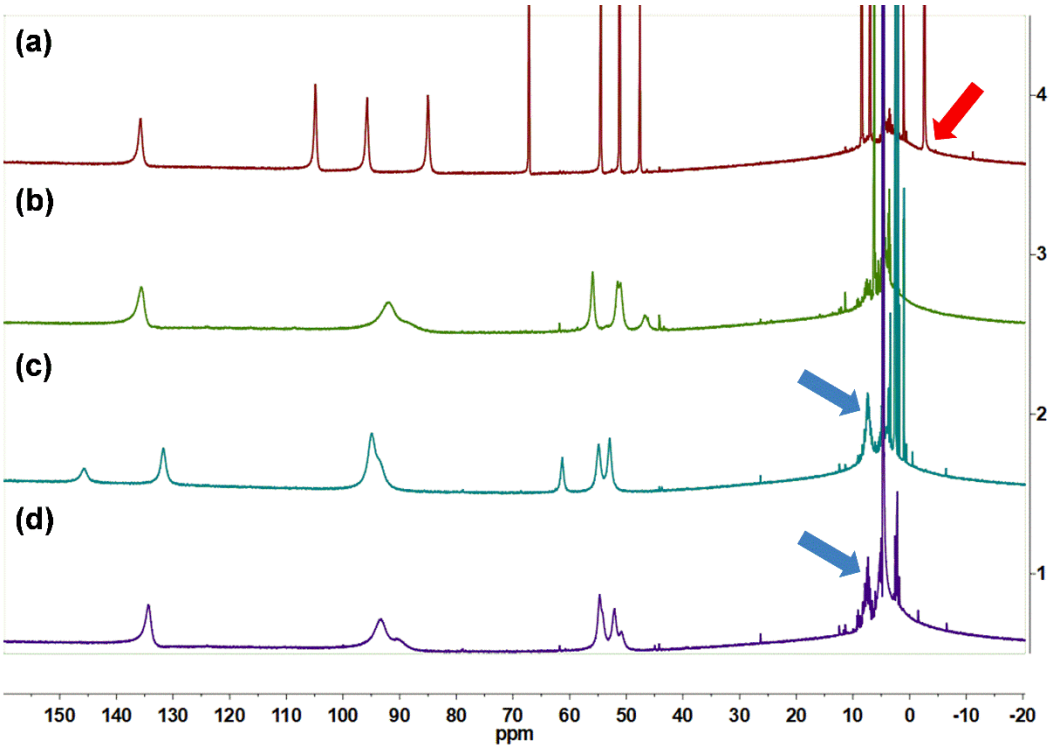


**Figure S3.** $^{1}H$ NMR spectra of **C2-C5** (**a-d**) in $D_2O$, the red arrow points to the signal of the methoxy group near the Co center and the blue arrows point to the signals of the methoxy and methyl groups far away from the Co center.

# 3. ESI-MS spectra

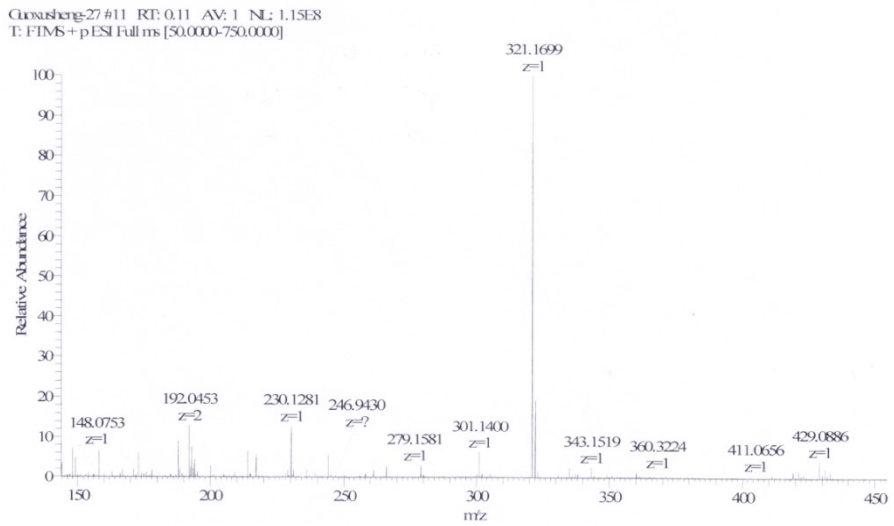


**Figure S4.** ESI-MS spectrum of **L2**.

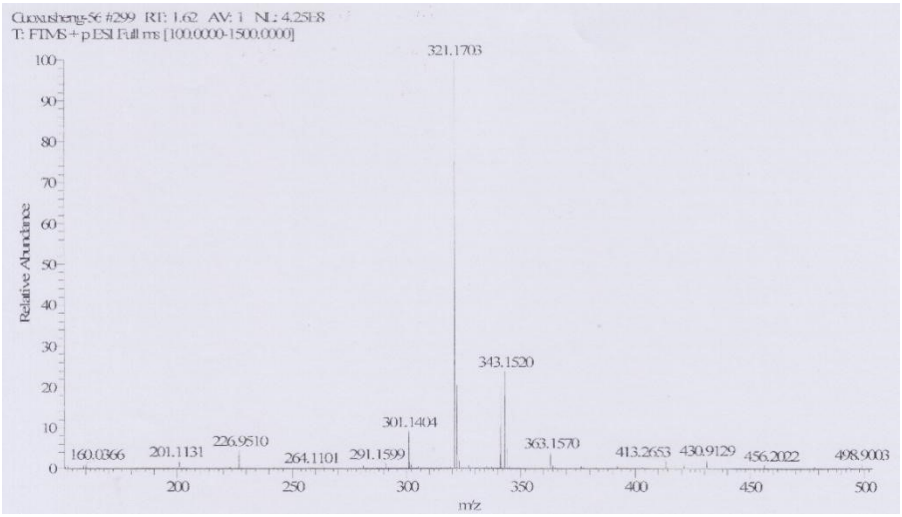


**Figure S5.** ESI-MS spectrum of **L3**.

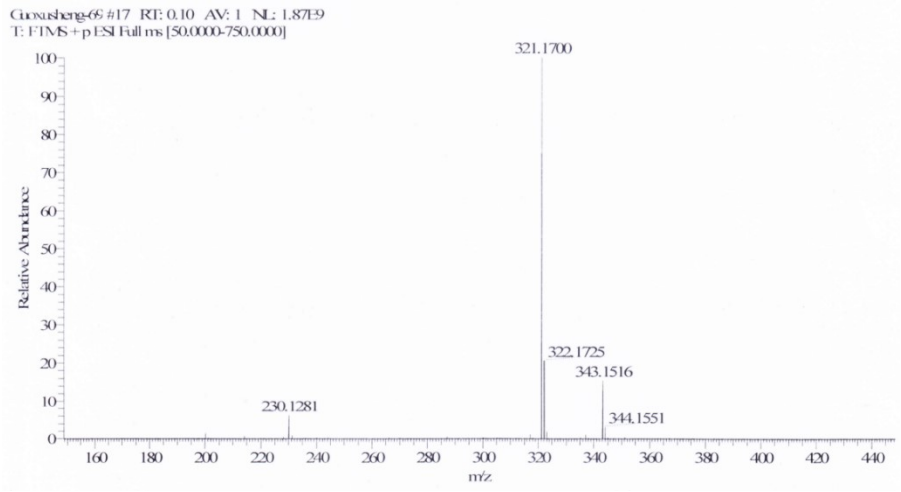


**Figure S6.** ESI-MS spectrum of **L4**.

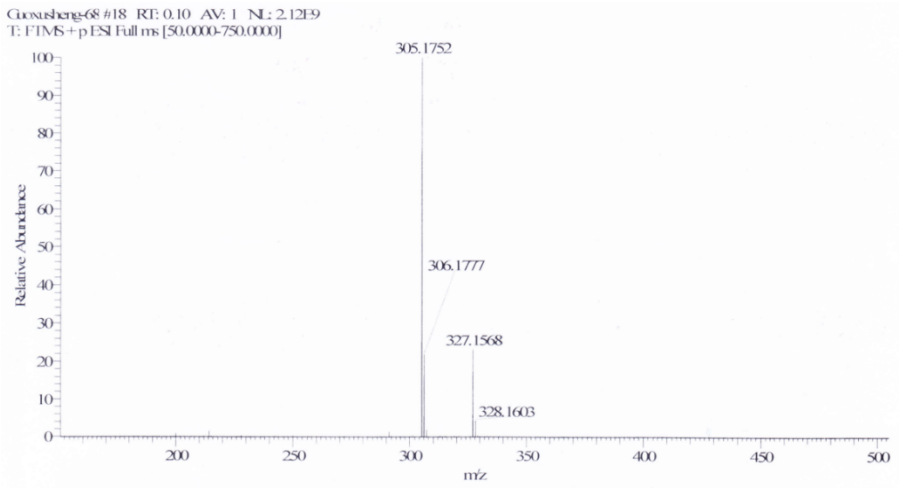


**Figure S7.** ESI-MS spectrum of **L5**.

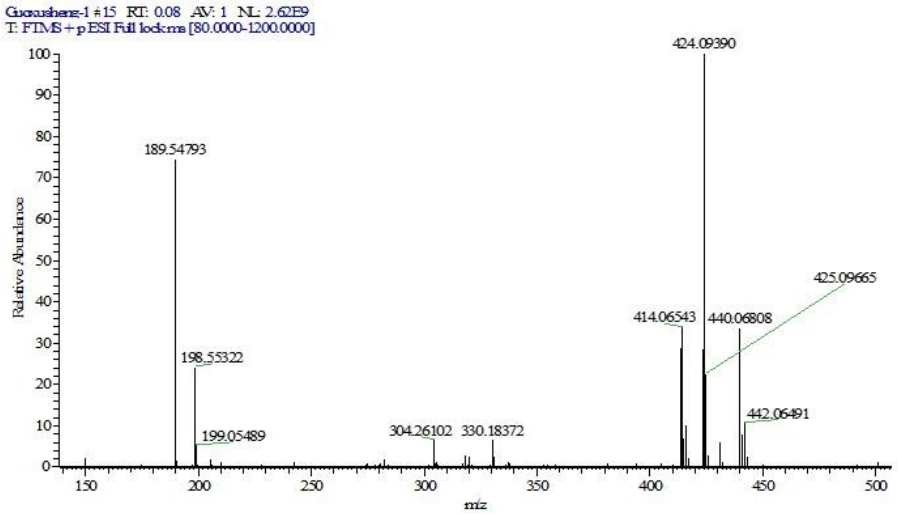


**Figure S8.** ESI-MS spectrum of **C2**.

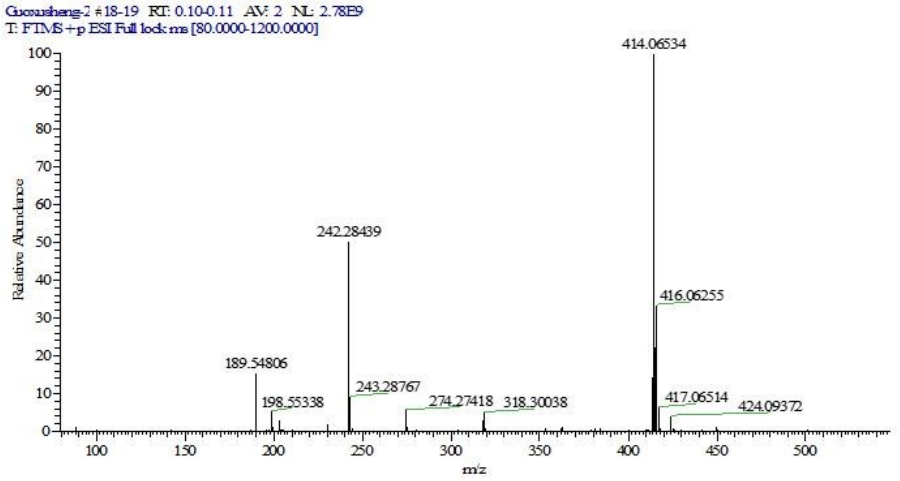


**Figure S9.** ESI-MS spectrum of **C3**.

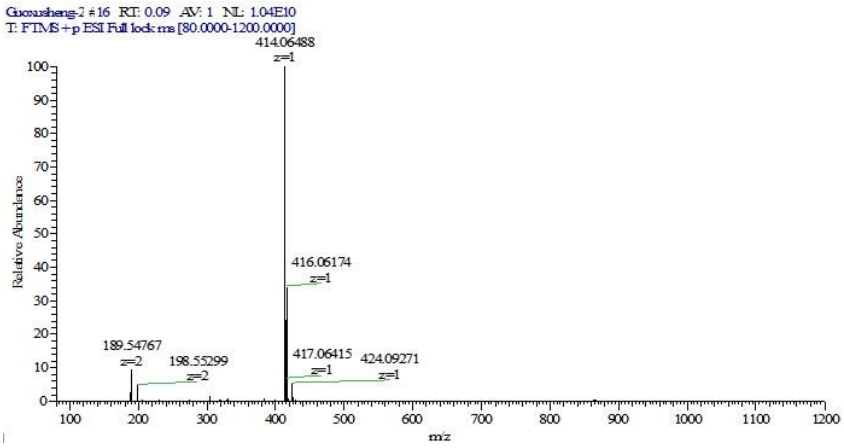


**Figure S10.** ESI-MS spectrum of **C4**.

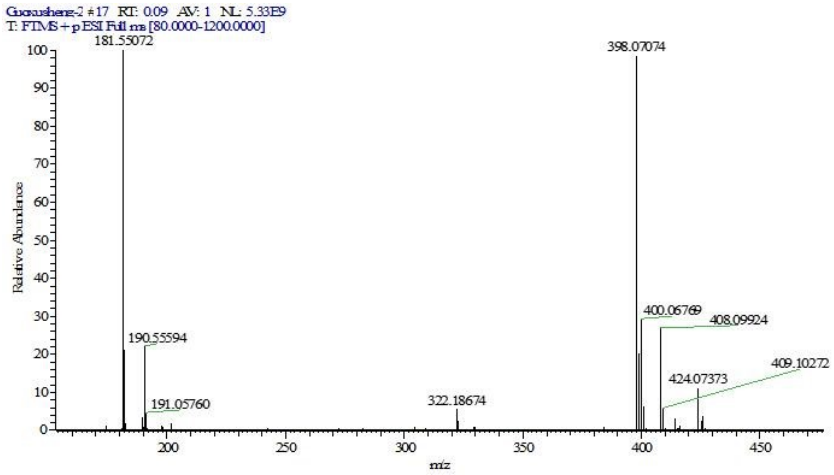


**Figure S11.** ESI-MS spectrum of **C5**.

# 4. IR spectra

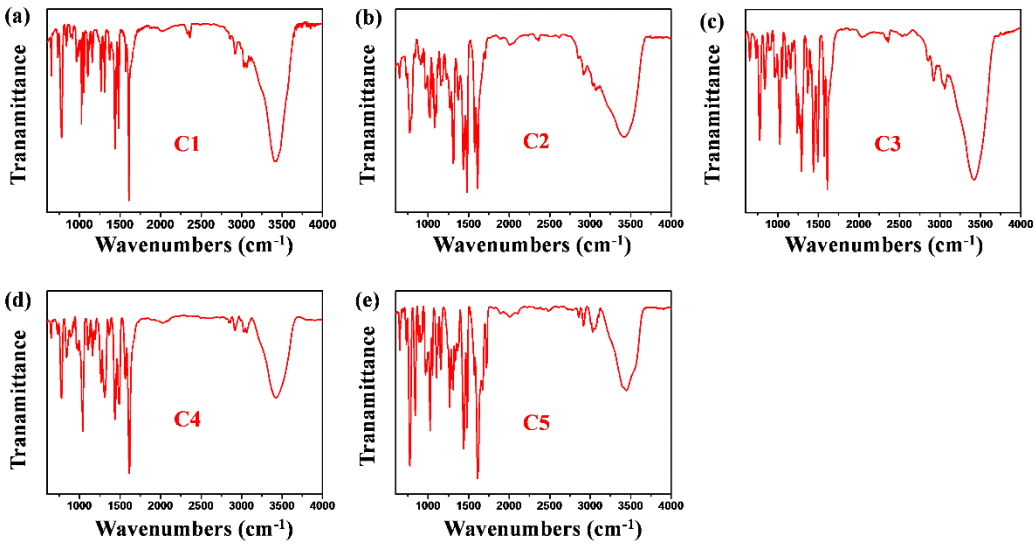


**Figure S12.** IR spectra of **C1-C5** (**a-e**).

## 5. UV-vis absorption spectra

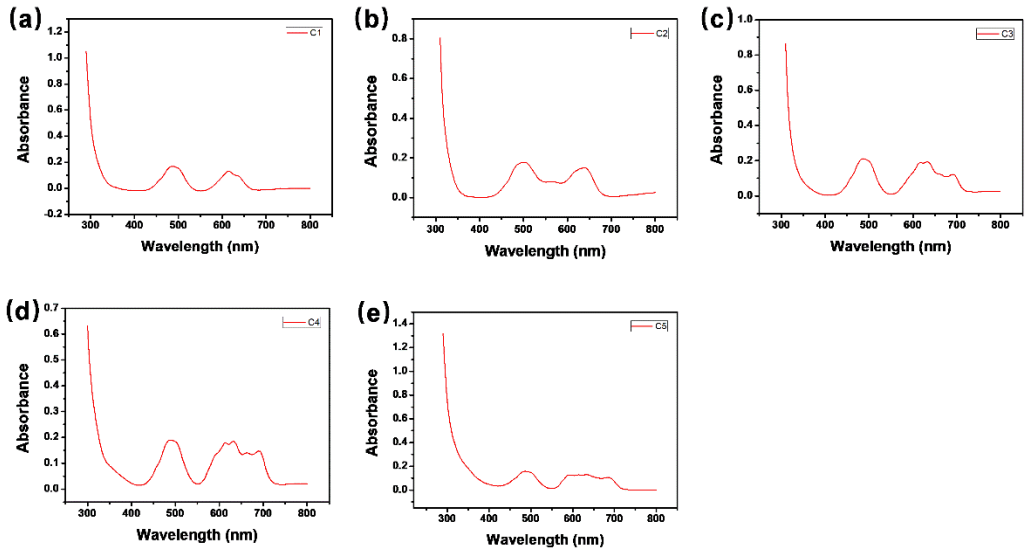


**Figure S13.** UV-vis absorption spectra of **C1-C5** (**a-e**).

**Table S1.** Absorption maxima and molar absorptivity (ε) of **C1-C5** in the region of 400-800 nm

| Complex | C1 | C2 | C3 | C4 | C5 |
|---|---|---|---|---|---|
| $\lambda_{max}$/nm | 489 | 499 | 487 | 490 | 486 |
| ε/mol$^{-1}$·cm$^{-1}$ | 168 | 179 | 214 | 192 | 159 |

## 6. Cyclic voltammetry

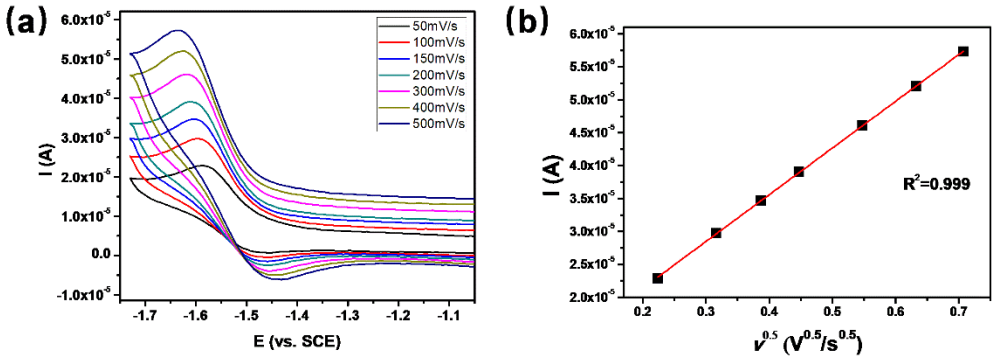


**Figure S14.** (a) CVs of 1.0 mM **C1** under various scan rates in anhydrous $CH_3CN$ with 0.1 M $TBAPF_6$ as supporting electrolyte under an argon atmosphere. (b) Plot of the reduction peak currents versus the square root of the scan rates.

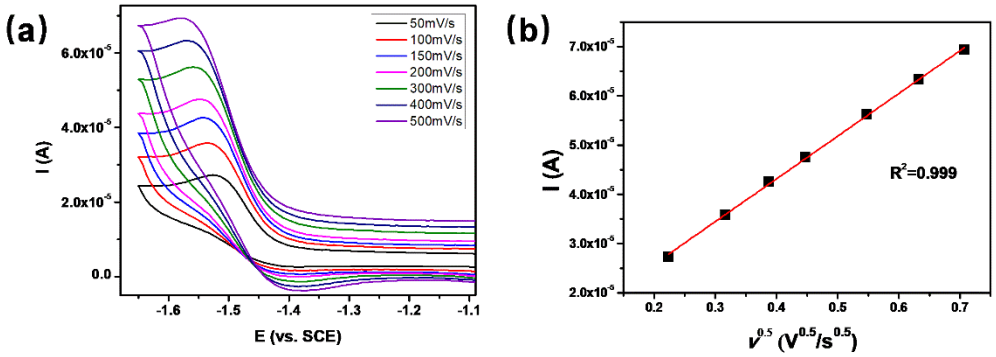


**Figure S15.** (a) CVs of 1.0 mM **C2** under various scan rates in anhydrous $CH_3CN$ with 0.1 M $TBAPF_6$ as supporting electrolyte under an argon atmosphere. (b) Plot of the reduction peak currents versus the square root of the scan rates.

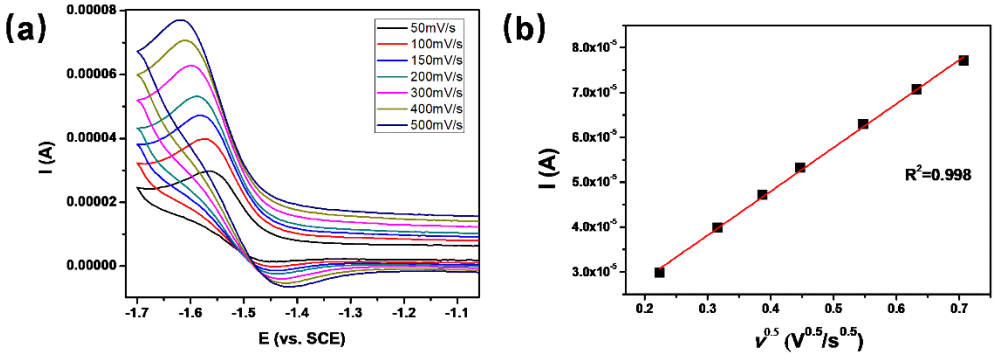


**Figure S16.** (a) CVs of 1.0 mM **C3** under various scan rates in anhydrous $CH_3CN$ with 0.1 M $TBAPF_6$ as supporting electrolyte under an argon atmosphere. (b) Plots of the reduction peak currents versus the square root of the scan rates.

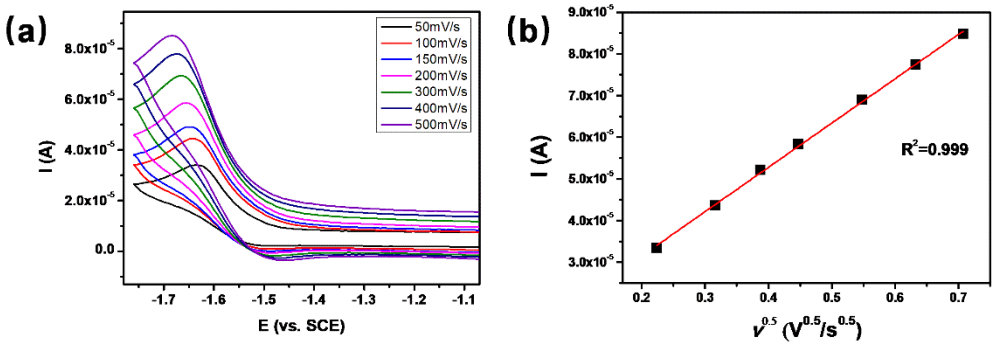


**Figure S17.** (a) CVs of 1.0 mM **C4** under various scan rates in anhydrous $CH_3CN$ with 0.1 M $TBAPF_6$ as supporting electrolyte under an argon atmosphere. (b) Plots of the reduction peak currents versus the square root of the scan rates.

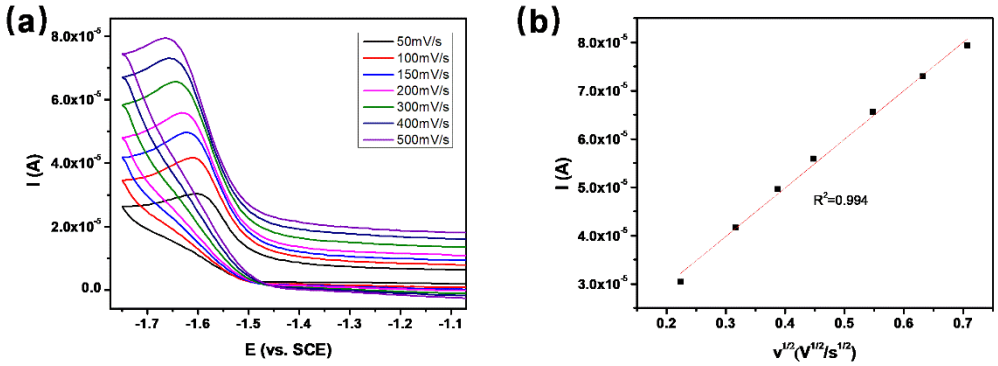


**Figure S18.** (a) CVs of 1.0 mM **C5** under various scan rates in anhydrous $CH_3CN$ with 0.1 M $TBAPF_6$ as supporting electrolyte under an argon atmosphere. (b) Plots of the reduction peak currents versus the square root of the scan rates.

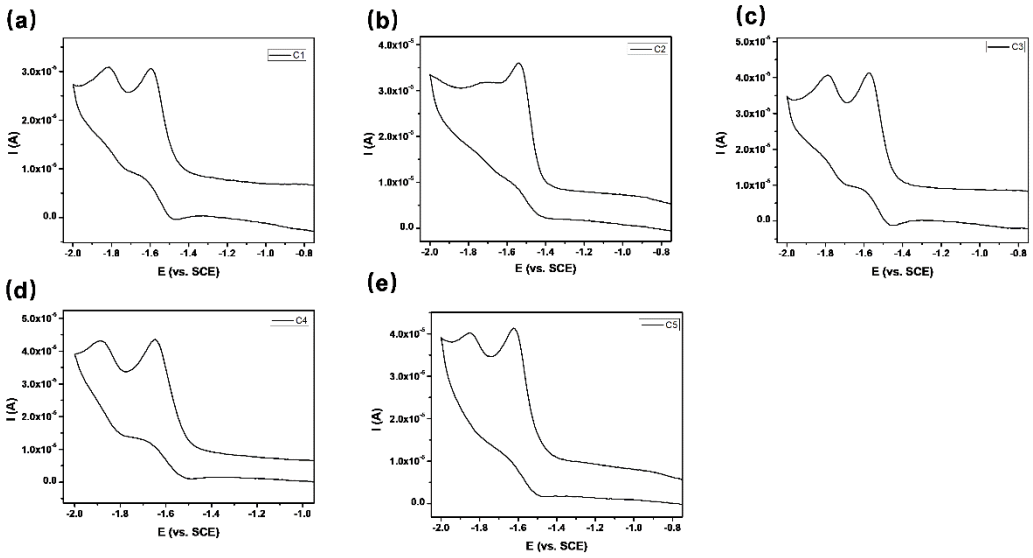


**Figure S19.** Wider range CVs of 1.0 mM **C1**-**C5** (**a**-**e**) in anhydrous $CH_3CN$ with 0.1 M $TBAPF_6$ as supporting electrolyte under an argon atmosphere with scan rate of 100 mV/s.

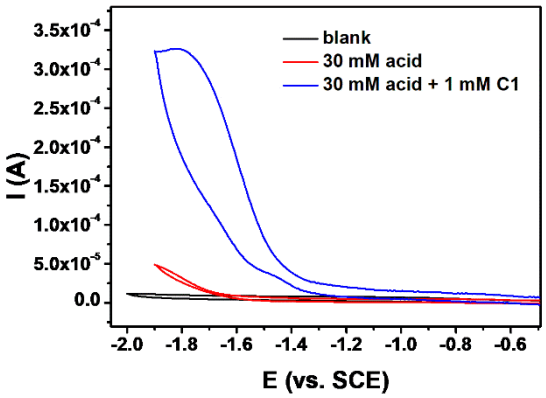


**Figure S20.** CVs of blank, 30 mM acetic acid and 30 mM acetic acid with 1 mM **C1** in Ar-saturated 0.1 M $TBAPF_6$ anhydrous $CH_3CN$ at a scan rate of 100 mV/s.

**Table S2.** Faradaic efficiencies of 1 mM **C1-C5** in controlled-potential electrolysis.

| | Charge / C | $n(H_2)_{tested}$ / mmol | $n(H_2)_{calcd}$ / mmol | Faradaic Efficiency/ % |
|---|---|---|---|---|
| **C1** | 1.44 | 0.00668 | 0.00749 | 89.2 |
| **C2** | 1.26 | 0.00587 | 0.00655 | 89.7 |
| **C3** | 1.35 | 0.00621 | 0.00700 | 88.7 |
| **C4** | 1.59 | 0.00745 | 0.00824 | 90.4 |
| **C5** | 1.46 | 0.00667 | 0.00759 | 87.9 |

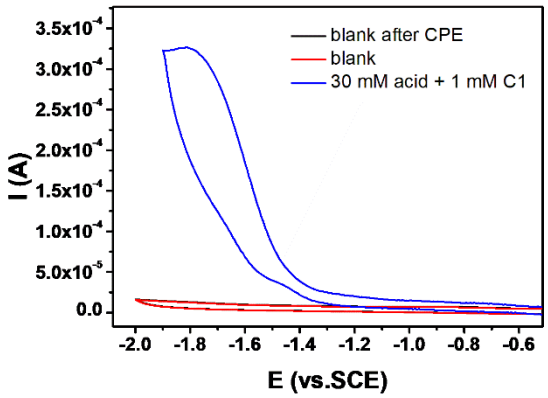


**Figure S21.** CVs of electrolyte solution using a same glassy carbon working electrode before and after use for electrolysis compared with CV of 1.0 mM **C1** with 30 mM acetic acid, The GC electrode after CPE experiment was rinsed by ethonal, water and used without further polishing.

## 7. Photocatalytic experiments

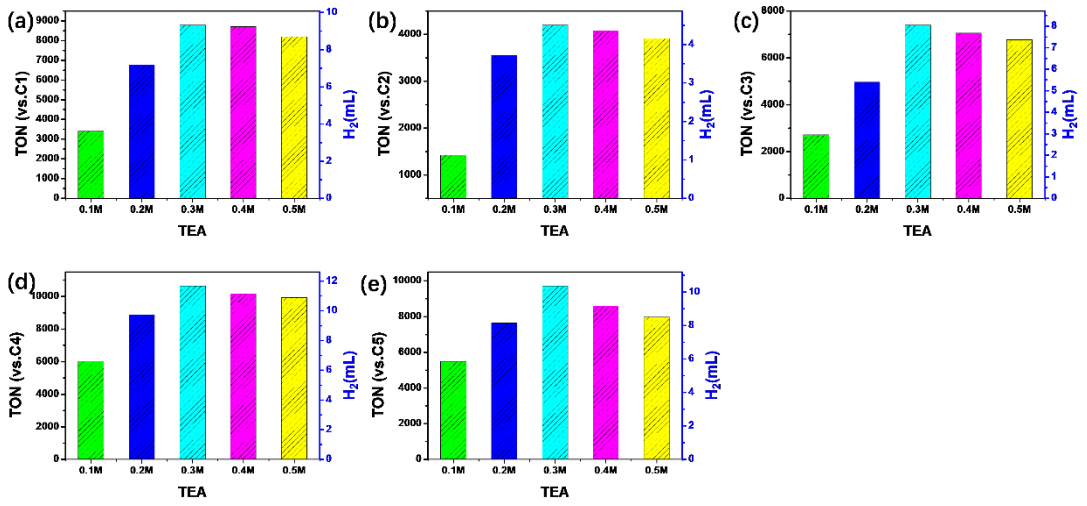


**Figure S22.** Photocatalytic $H_2$ evolution of **C1-C5** (**a-d**) after 6 h irradiation at various concentrations of TEA. Conditions: 0.2 mM $[Ir(ppy)_2(dtbpy)]Cl$, $CH_3CN/H_2O$ (8:2,v/v), 10 μM

Co complex.

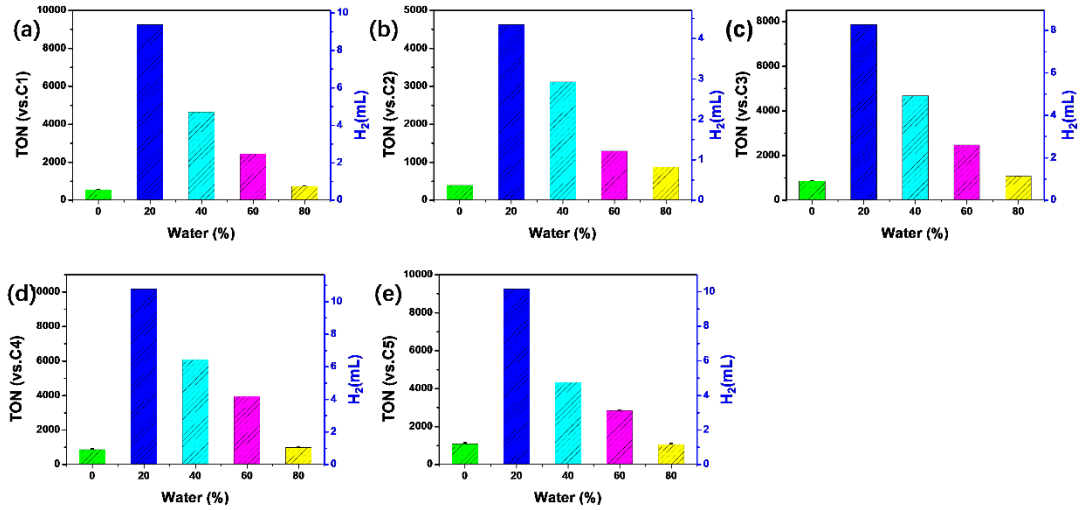


**Figure S23.** Photocatalytic $H_2$ evolution of **C1-C5** (**a-d**) after 6 h irradiation in $CH_3CN/H_2O$ of varied compositions. Conditions: 0.2 mM $[Ir(ppy)_2(dtbpy)]Cl$, 0.3 M TEA, 10 μM Co complex.

**Table S3.** Photocatalytic control experiments with specific absent part, a typical complete system including 0.3 M TEA, 0.2 mM $[Ir(ppy)_2(dtbpy)]Cl$, 10 μM **C1** and irradiation of 6 hours, the solvent was a mixture of $CH_3CN/H_2O$ (8:2,v/v).

| Absent Part | PS | Cat | SD | Light |
|---|---|---|---|---|
| $H_2$ μmol | 0 | 0.628 | 0 | 0 |

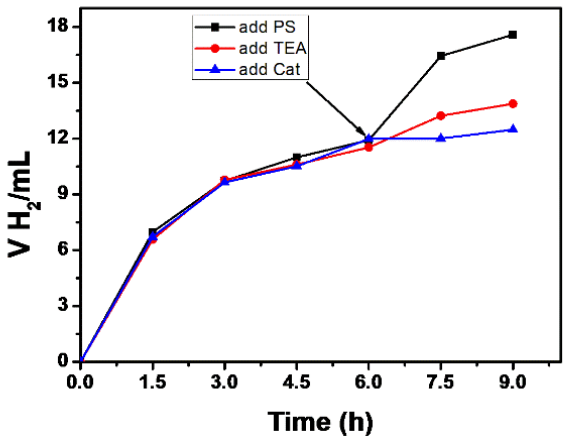


**Figure S24.** Consecutive photocatalytic $H_2$ production by adding 0.3 M TEA, 0.2 mM PS, 10 μM **C1** after 6 h irradiation. Initial condition: 0.2 mM $[Ir(ppy)_2(dtbpy)]Cl$, 0.3 M TEA, $MeCN/H_2O$ (8:2), 10 μM **C1**.

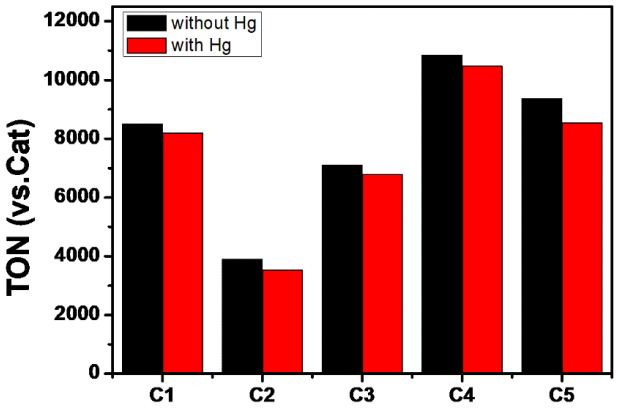


**Figure S25.** Photocatalytic $H_2$ production with or without Hg (10% volume) after 6 h irradiation. Conditions: 0.2 mM $[Ir(ppy)_2(dtbpy)]Cl$, $CH_3CN/H_2O$ (8:2,v/v), 10 μM Co complex, 0.3 M TEA.

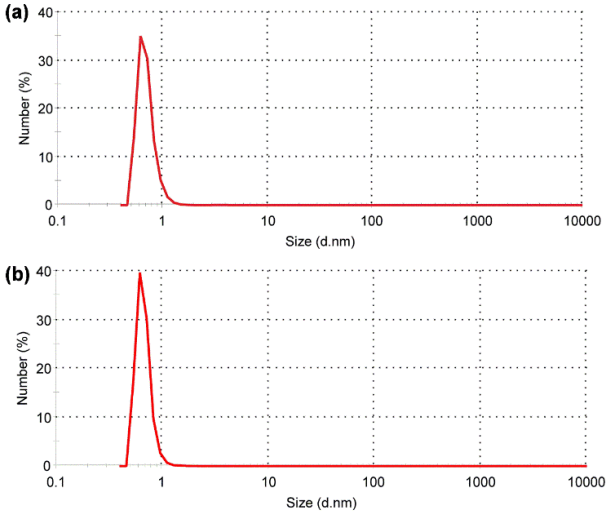


**Figure S26.** Size distribution by number obtained by dynamic light scattering for 10 μM **C2** (**a**) and **C4** (**b**) in $CH_3CN/H_2O$ (8:2,v/v) containing 0.2 mM $[Ir(ppy)_2(dtbpy)]Cl$ and 0.3 M TEA after 6 h of irradiation.

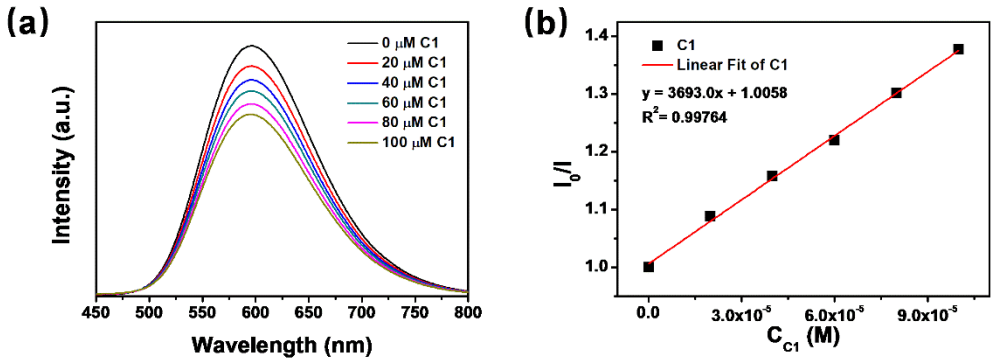


**Figure S27.** (a) Emission quenching of $[Ir(ppy)_2(dtbpy)]Cl$ by **C1**. (b) Stern-Volmer plot of the emission quenching.

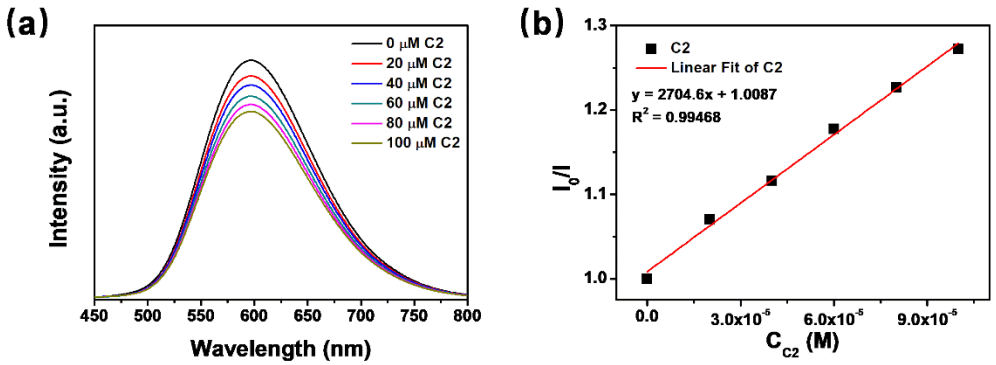


**Figure S28.** (a) Emission quenching of $[Ir(ppy)_2(dtbpy)]Cl$ by **C2**. (b) Stern-Volmer plot of the emission quenching.

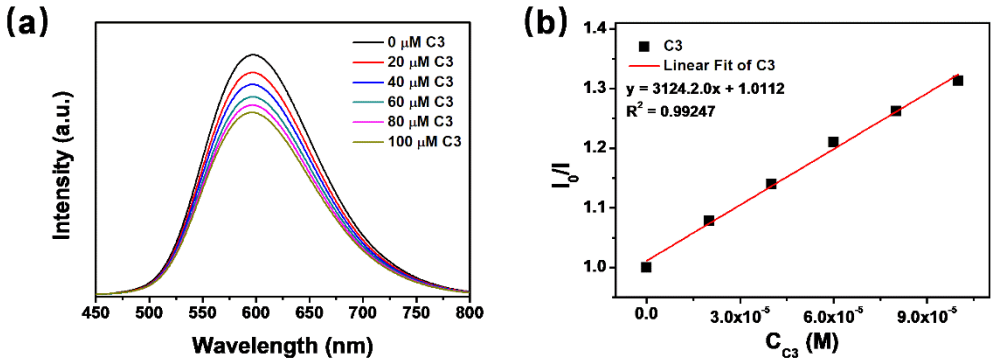


**Figure S29.** (a) Emission quenching of $[Ir(ppy)_2(dtbpy)]Cl$ by **C3**. (b) Stern-Volmer plot of the emission quenching.

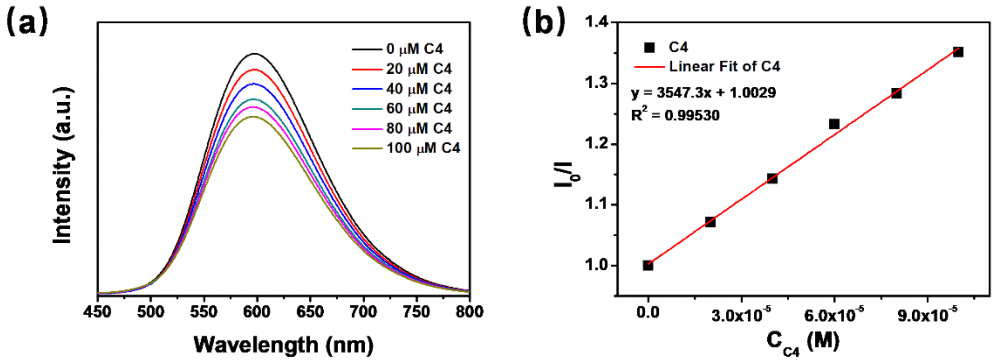


**Figure S30.** (a) Emission quenching of $[Ir(ppy)_2(dtbpy)]Cl$ by **C4**. (b) Stern-Volmer plot of the emission quenching.

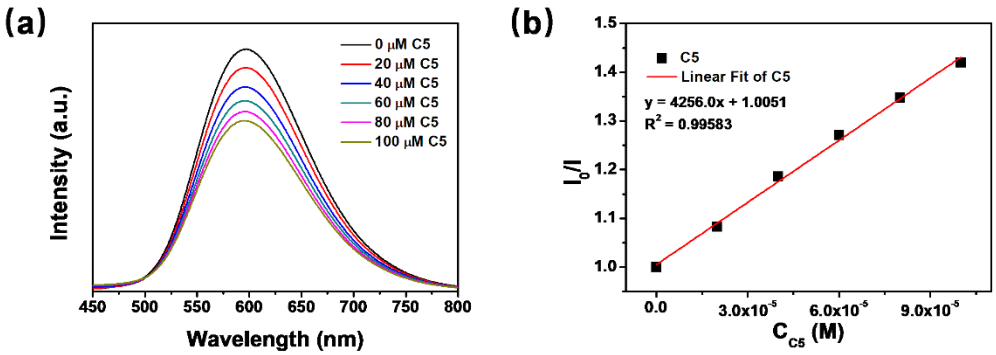


**Figure S31.** (a) Emission quenching of $[Ir(ppy)_2(dtbpy)]Cl$ by **C5**. (b) Stern-Volmer plot of the emission quenching.

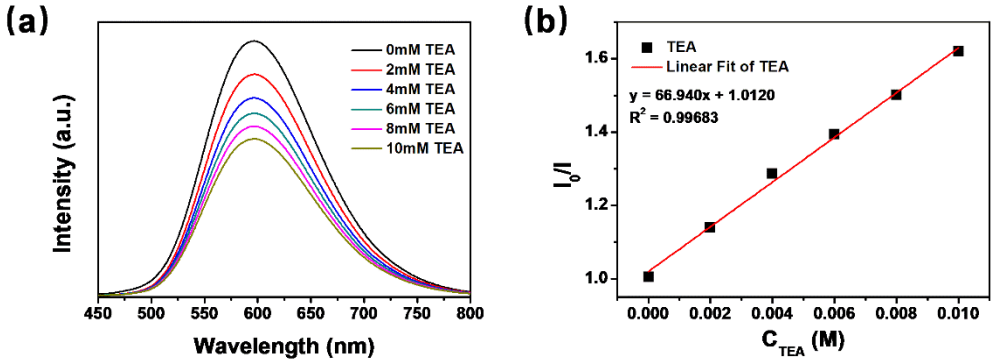


**Figure S32.** (a) Emission quenching of $[Ir(ppy)_2(dtbpy)]Cl$ by TEA. (b) Stern-Volmer plot of the emission quenching.

**Table S4.** Slopes of the Stern-Volmer plots and their quenching rate constants.

| | TEA | C1 | C2 | C3 | C4 | C5 |
|---|---|---|---|---|---|---|
| slope | 66.94 | 3693 | 2704 | 3124 | 3547 | 4256 |
| $k_q$ ($10^9$ $M^{-1}s^{-1}$) | 0.12 | 6.63 | 4.86 | 5.61 | 6.37 | 7.64 |

## 8. Computation results

**Table S5.** Selected bond lengths (Å) and angles (°) of optimized $[Co^{II}(TPA)Cl]Cl$ and crystal data of $[Co^{II}(TPA)Cl]ClO_4$ (CCDC 1529343).

| | Co-N1/Å | Co-N2/Å | Co-N3/Å | Co-Namine/Å | Co-Cl/Å | N1-Co-Cl/° |
|---|---|---|---|---|---|---|
| **CCDC 1529343** | 2.056 | 2.069 | 2.060 | 2.201 | 2.285 | 104.46 |
| **$[Co^{II}(TPA)Cl]Cl$** | 2.08830 | 2.08863 | 2.08933 | 2.28014 | 2.33279 | 102.44549 |

**Table S6.** Calculated Gibbs free energies of **C1-C5** in high-spin states or low-spin states (in Hartree), and their difference (the energy of low-spin states minus high-spin states, in kcal/mol)

| Gsol / Hartree | C1 | C2 | C3 | C4 | C5 |
|---|---|---|---|---|---|
| High-spin states | -1521.035155 | -1635.567768 | -1635.564391 | -1635.570052 | -1560.340956 |
| Low-spin states | -1521.015277 | -1635.549582 | -1635.54287 | -1635.549365 | -1560.321824 |
| ΔGsol / (kcal/mol) | 12.47380693 | 11.41162076 | 13.50468664 | 12.98123662 | 12.00542092 |

**Table S7.** Selected bond lengths (Å) and angles (°) of optimized **C1-C5**.

| | C1 | C2 | C3 | C4 | C5 |
|---|---|---|---|---|---|
| **Co-N1/Å** | 2.08830 | 2.12408 | 2.09123 | 2.07529 | 2.08203 |
| **Cl-Co-N1/°** | 102.44549 | 114.69198 | 103.02949 | 102.63419 | 102.76455 |

**Table S8.** Selected bond lengths (Å) of optimized Co(II)-Cl and Co(I)-Cl intermediates.

| | | C1 | C2 | C3 | C4 | C5 |
|---|---|---|---|---|---|---|
| **Co-Cl /Å** | **Co(II)-Cl** | 2.33279 | 2.33896 | 2.33146 | 2.33733 | 2.33431 |
| | **Co(I)-Cl** | 2.40166 | 2.41324 | 2.40136 | 2.40517 | 2.40224 |

**Table S9.** The Calculated Gibbs free energy changes (in kcal/mol) during selected bond dissociation from Co(I)-Cl intermediates of C1-C5.

| | C1 | C2 | C3 | C4 | C5 |
|---|---|---|---|---|---|
| **Co-N1** | 2.26812862 | 0.756871187 | 0.885586037 | 2.044954689 | 4.63889905 |
| **Co-N2** | \ | 0.663936955 | 1.184600827 | 2.362393172 | 2.39799809 |
| **Co-Cl** | -0.214200539 | -3.982730669 | -0.312763534 | -0.190229656 | -0.199378752 |

**Table S10.** Calculated Gibbs free energies of Co(I) and Co(III)-H intermediates (in Hartrees) and corresponding energy changes (in kJ/mol).

| | $G_{sol}$ ($Co^{I}$) /Hartree | $G_{sol}$ ($Co^{III}$-H) /Hartree | $\Delta G_{sol}$ / kJ/mol |
|---|---|---|---|
| **C1** | -1060.773042 | -1061.183652 | 8.026328403 |
| **C2** | -1175.314739 | -1175.724695 | 9.740991145 |
| **C3** | -1175.305128 | -1175.71545 | 8.780897632 |
| **C4** | -1175.310251 | -1175.722339 | 4.145364093 |
| **C5** | -1100.081766 | -1100.493129 | 6.048459095 |

**Table S11.** Selected bond lengths (Å) and angles (°) of optimized Co(III)-H intermediates, N1 is the N atom of pyridine with substituent.

| | C1 | C2 | C3 | C4 | C5 |
|---|---|---|---|---|---|
| **Co-N1 /Å** | 1.99171 | 2.00587 | 1.99178 | 1.96663 | 1.98153 |
| **N1-Co-H /°** | 96.83926 | 98.21885 | 96.87186 | 96.01514 | 96.48975 |

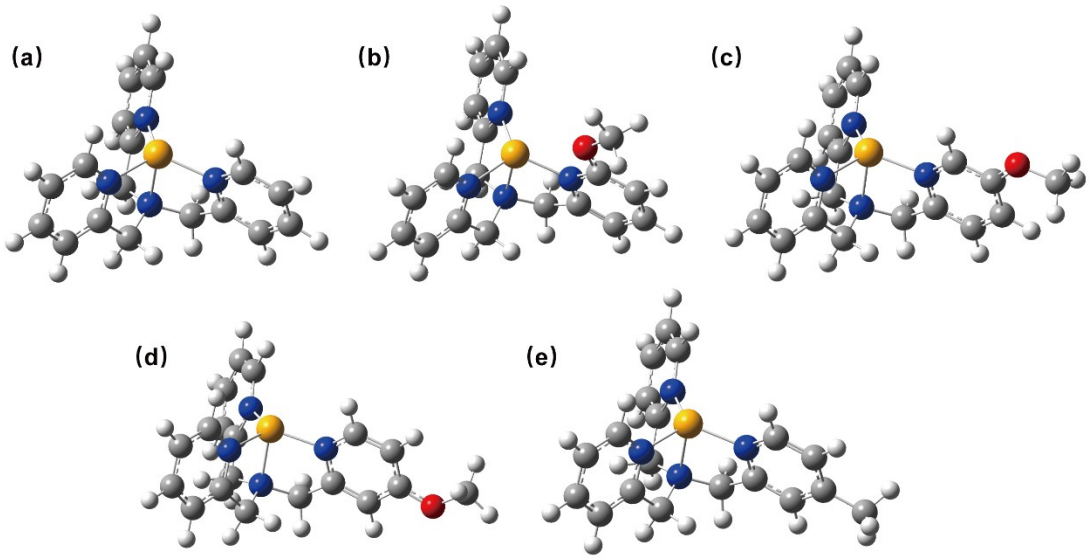


**Figure S33.** Optimized structures of the Co(II) species derived from **C1**-**C5** (**a**-**e**).

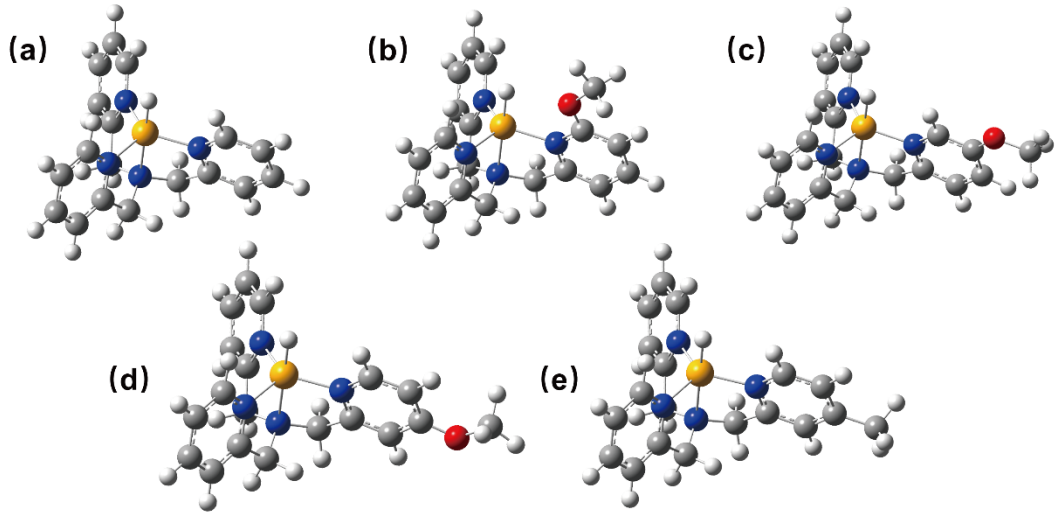


**Figure S34.** Optimized structures of the Co(III)-H intermediates of **C1**-**C5** (**a**-**e**).

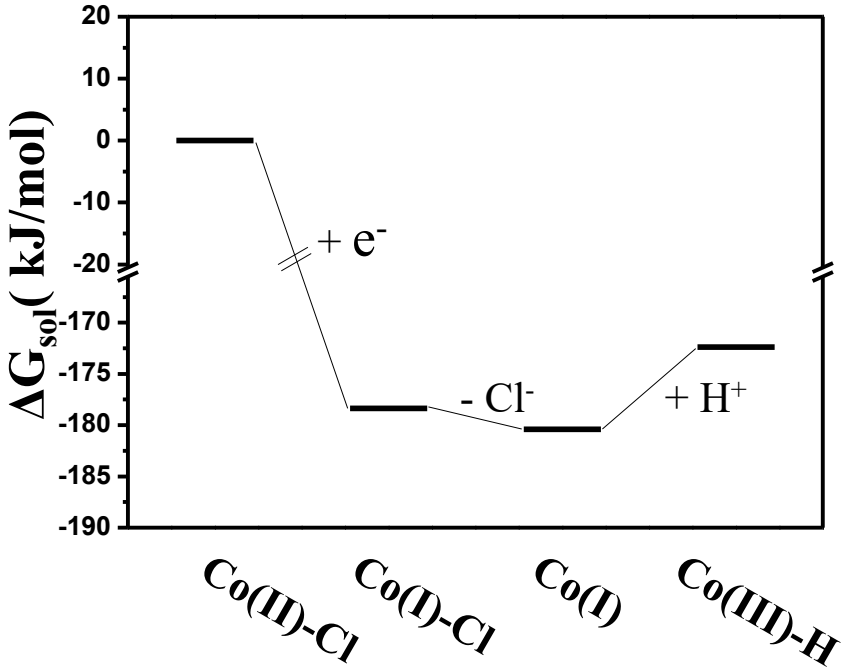


**Figure S35.** DFT-calculated free energy profile for the key intermediates of **C1**.

## References

1. J. Wang, C. Li, Q. Zhou, W. Wang, Y. Hou, B. Zhang and X. Wang, *Dalton Trans*, 2016, **45**, 5439-5443.
2. D. A. Quist, M. A. Ehudin and K. D. Karlin, *Inorg. Chim. Acta*, 2019, **485**, 155-161.
3. M. A. Ehudin, A. W. Schaefer, S. M. Adam, D. A. Quist, D. E. Diaz, J. A. Tang, E. I. Solomon and K. D. Karlin, *Chem. Sci.*, 2019, **10**, 2893-2905.

## Appendix：Cartesian coordinates of the optimized geometries

**C1**

**$Co^{II}$(TPA)Cl (High-spin state)**

| | | | |
|---|---|---|---|
| Co | -0.000000 | 0.001000 | 0.700000 |
| N | 0.000000 | 0.002000 | -1.580000 |
| C | -3.605000 | 2.438000 | 0.855000 |
| H | -4.130000 | 2.995000 | 1.621000 |
| C | -2.210000 | 0.980000 | -1.036000 |
| N | 1.765000 | 1.024000 | 0.251000 |
| N | 0.003000 | -2.038000 | 0.250000 |
| C | 1.955000 | 1.423000 | -1.034000 |
| C | -2.451000 | 1.726000 | 1.183000 |
| H | -2.046000 | 1.695000 | 2.188000 |
| C | -1.431000 | 0.088000 | -1.980000 |
| H | -1.846000 | -0.926000 | -1.929000 |
| H | -1.543000 | 0.430000 | -3.019000 |
| N | -1.769000 | 1.016000 | 0.249000 |
| C | 4.130000 | 2.296000 | -0.468000 |
| H | 5.053000 | 2.787000 | -0.753000 |
| C | -3.352000 | 1.681000 | -1.426000 |
| H | -3.684000 | 1.649000 | -2.458000 |
| C | -0.273000 | -2.983000 | 1.183000 |
| C | 3.136000 | 2.056000 | -1.426000 |
| H | 3.275000 | 2.359000 | -2.457000 |
| C | 0.256000 | -2.402000 | -1.035000 |
| C | 3.919000 | 1.894000 | 0.855000 |
| H | 4.665000 | 2.068000 | 1.621000 |
| C | -0.315000 | -4.338000 | 0.855000 |
| C | 0.217000 | -3.741000 | -1.426000 |
| H | 0.412000 | -4.013000 | -2.457000 |
| C | 2.723000 | 1.255000 | 1.185000 |
| H | 2.492000 | 0.922000 | 2.189000 |
| C | 0.643000 | -1.281000 | -1.977000 |
| H | 1.728000 | -1.133000 | -1.920000 |
| H | 0.408000 | -1.549000 | -3.017000 |
| C | -4.059000 | 2.419000 | -0.468000 |
| H | -4.949000 | 2.968000 | -0.752000 |
| C | -0.071000 | -4.722000 | -0.468000 |
| H | -0.104000 | -5.767000 | -0.753000 |
| C | 0.792000 | 1.199000 | -1.976000 |
| H | 0.122000 | 2.066000 | -1.919000 |
| H | 1.141000 | 1.130000 | -3.017000 |
| Cl | -0.000000 | 0.001000 | 3.033000 |
| H | -0.448000 | -2.616000 | 2.188000 |
| H | -0.537000 | -5.071000 | 1.620000 |

**$Co^{II}$(TPA)Cl (Low-spin state)**

| | | | |
|---|---|---|---|
| Co | -0.056000 | -0.334000 | 0.517000 |
| N | -0.121000 | -0.192000 | -1.494000 |
| C | 3.879000 | -2.032000 | 0.880000 |
| H | 4.527000 | -2.381000 | 1.677000 |
| C | 2.166000 | -1.106000 | -1.057000 |
| N | -2.033000 | -0.612000 | 0.294000 |
| N | 0.223000 | 1.784000 | 0.339000 |
| C | -2.334000 | -1.078000 | -0.942000 |
| C | 2.674000 | -1.410000 | 1.196000 |
| H | 2.339000 | -1.273000 | 2.218000 |
| C | 1.232000 | -0.474000 | -2.066000 |
| H | 1.668000 | 0.480000 | -2.380000 |
| H | 1.144000 | -1.091000 | -2.969000 |
| N | 1.834000 | -0.951000 | 0.245000 |
| C | -4.645000 | -1.319000 | -0.338000 |
| H | -5.666000 | -1.595000 | -0.587000 |
| C | 3.344000 | -1.740000 | -1.447000 |
| H | 3.576000 | -1.860000 | -2.501000 |
| C | 0.672000 | 2.639000 | 1.271000 |
| C | -3.632000 | -1.435000 | -1.295000 |
| H | -3.847000 | -1.800000 | -2.295000 |
| C | 0.029000 | 2.220000 | -0.919000 |
| C | -4.327000 | -0.843000 | 0.934000 |
| H | -5.085000 | -0.739000 | 1.703000 |
| C | 0.948000 | 3.975000 | 0.976000 |
| C | 0.295000 | 3.534000 | -1.300000 |
| H | 0.136000 | 3.856000 | -2.326000 |
| C | -3.006000 | -0.499000 | 1.216000 |
| H | -2.689000 | -0.144000 | 2.190000 |
| C | -0.575000 | 1.191000 | -1.852000 |
| H | -1.664000 | 1.220000 | -1.743000 |
| H | -0.348000 | 1.407000 | -2.904000 |
| C | 4.217000 | -2.208000 | -0.463000 |
| H | 5.142000 | -2.704000 | -0.742000 |
| C | 0.762000 | 4.427000 | -0.331000 |
| H | 0.976000 | 5.458000 | -0.595000 |
| C | -1.148000 | -1.202000 | -1.879000 |
| H | -0.692000 | -2.194000 | -1.772000 |
| H | -1.450000 | -1.087000 | -2.929000 |
| Cl | -0.075000 | -0.555000 | 2.752000 |

| | | | |
|---|---|---|---|
| H | 0.802000 | 2.224000 | 2.266000 |
| H | 1.306000 | 4.639000 | 1.757000 |

**$Co^{I}$(TPA)Cl**

| | | | |
|---|---|---|---|
| Co | -0.064000 | -0.016000 | 0.709000 |
| N | -0.034000 | 0.034000 | -1.609000 |
| C | 2.617000 | 3.472000 | 0.863000 |
| H | 3.219000 | 3.958000 | 1.625000 |
| C | 1.051000 | 2.168000 | -0.985000 |
| N | 1.006000 | -1.738000 | 0.223000 |
| N | -2.078000 | -0.244000 | 0.285000 |
| C | 1.363000 | -1.940000 | -1.067000 |
| C | 1.899000 | 2.320000 | 1.176000 |
| H | 1.899000 | 1.880000 | 2.170000 |
| C | 0.089000 | 1.458000 | -1.925000 |
| H | -0.908000 | 1.903000 | -1.799000 |
| H | 0.384000 | 1.635000 | -2.975000 |
| N | 1.142000 | 1.672000 | 0.270000 |
| C | 2.225000 | -4.132000 | -0.561000 |
| H | 2.688000 | -5.065000 | -0.870000 |
| C | 1.755000 | 3.308000 | -1.377000 |
| H | 1.674000 | 3.671000 | -2.399000 |
| C | -3.033000 | 0.029000 | 1.206000 |
| C | 1.959000 | -3.124000 | -1.495000 |
| H | 2.215000 | -3.254000 | -2.544000 |
| C | -2.425000 | -0.198000 | -1.030000 |
| C | 1.879000 | -3.910000 | 0.776000 |
| H | 2.069000 | -4.658000 | 1.540000 |
| C | -4.344000 | 0.343000 | 0.859000 |
| C | -3.713000 | 0.118000 | -1.449000 |
| H | -3.943000 | 0.148000 | -2.512000 |
| C | 1.270000 | -2.707000 | 1.125000 |
| H | 0.972000 | -2.477000 | 2.145000 |
| C | -1.319000 | -0.568000 | -2.000000 |
| H | -1.183000 | -1.655000 | -1.970000 |
| H | -1.605000 | -0.305000 | -3.033000 |
| C | 2.552000 | 3.972000 | -0.441000 |
| H | 3.107000 | 4.863000 | -0.724000 |
| C | -4.701000 | 0.392000 | -0.492000 |
| H | -5.714000 | 0.641000 | -0.797000 |
| C | 1.134000 | -0.764000 | -2.003000 |
| H | 2.013000 | -0.111000 | -1.947000 |
| H | 1.064000 | -1.112000 | -3.048000 |
| Cl | -0.015000 | 0.022000 | 3.110000 |

| | | | |
|---|---|---|---|
| H | -2.698000 | -0.013000 | 2.239000 |
| H | -5.071000 | 0.546000 | 1.641000 |

**$Co^{I}$(TPA)**

| | | | |
|---|---|---|---|
| Co | -0.025000 | 0.121000 | 0.844000 |
| N | 0.030000 | 0.153000 | -1.306000 |
| C | -3.891000 | 2.082000 | 1.212000 |
| H | -4.511000 | 2.490000 | 2.004000 |
| C | -2.250000 | 0.990000 | -0.711000 |
| N | 1.871000 | 0.908000 | 0.617000 |
| N | 0.043000 | -1.939000 | 0.533000 |
| C | 2.049000 | 1.422000 | -0.626000 |
| C | -2.765000 | 1.327000 | 1.531000 |
| H | -2.496000 | 1.136000 | 2.565000 |
| C | -1.374000 | 0.281000 | -1.736000 |
| H | -1.769000 | -0.734000 | -1.860000 |
| H | -1.461000 | 0.775000 | -2.715000 |
| N | -1.952000 | 0.787000 | 0.598000 |
| C | 4.270000 | 2.171000 | -0.066000 |
| H | 5.202000 | 2.659000 | -0.337000 |
| C | -3.354000 | 1.745000 | -1.105000 |
| H | -3.558000 | 1.893000 | -2.162000 |
| C | -0.230000 | -2.931000 | 1.403000 |
| C | 3.239000 | 2.047000 | -0.999000 |
| H | 3.353000 | 2.435000 | -2.007000 |
| C | 0.264000 | -2.266000 | -0.763000 |
| C | 4.084000 | 1.649000 | 1.215000 |
| H | 4.858000 | 1.716000 | 1.973000 |
| C | -0.293000 | -4.273000 | 1.032000 |
| C | 0.201000 | -3.584000 | -1.214000 |
| H | 0.372000 | -3.805000 | -2.264000 |
| C | 2.875000 | 1.023000 | 1.510000 |
| H | 2.694000 | 0.591000 | 2.489000 |
| C | 0.654000 | -1.128000 | -1.695000 |
| H | 1.740000 | -0.997000 | -1.635000 |
| H | 0.426000 | -1.394000 | -2.738000 |
| C | -4.190000 | 2.300000 | -0.133000 |
| H | -5.055000 | 2.890000 | -0.423000 |
| C | -0.077000 | -4.607000 | -0.305000 |
| H | -0.127000 | -5.640000 | -0.636000 |
| C | 0.871000 | 1.328000 | -1.590000 |
| H | 0.242000 | 2.218000 | -1.463000 |
| H | 1.235000 | 1.341000 | -2.630000 |
| H | -0.407000 | -2.628000 | 2.431000 |

| | | | |
|---|---|---|---|
| H | -0.513000 | -5.031000 | 1.777000 |

**$Co^{III}$-H(TPA)**

| | | | |
|---|---|---|---|
| Co | -0.002000 | -0.000000 | -0.760000 |
| N | -0.001000 | -0.002000 | 1.307000 |
| C | 0.935000 | 4.159000 | -1.210000 |
| H | 0.930000 | 4.897000 | -2.006000 |
| C | 0.922000 | 2.215000 | 0.749000 |
| N | -1.925000 | -0.462000 | -0.523000 |
| N | 1.361000 | -1.435000 | -0.524000 |
| C | -2.383000 | -0.311000 | 0.749000 |
| C | 0.568000 | 2.846000 | -1.484000 |
| H | 0.272000 | 2.533000 | -2.479000 |
| C | 0.959000 | 1.060000 | 1.726000 |
| H | 1.965000 | 0.623000 | 1.721000 |
| H | 0.757000 | 1.392000 | 2.752000 |
| N | 0.564000 | 1.895000 | -0.523000 |
| C | -4.548000 | -1.126000 | 0.093000 |
| H | -5.573000 | -1.388000 | 0.338000 |
| C | 1.287000 | 3.514000 | 1.089000 |
| H | 1.562000 | 3.754000 | 2.112000 |
| C | 2.185000 | -1.912000 | -1.485000 |
| C | -3.691000 | -0.643000 | 1.088000 |
| H | -4.037000 | -0.523000 | 2.110000 |
| C | 1.461000 | -1.907000 | 0.748000 |
| C | -4.072000 | -1.270000 | -1.212000 |
| H | -4.708000 | -1.641000 | -2.009000 |
| C | 3.142000 | -2.883000 | -1.211000 |
| C | 2.406000 | -2.869000 | 1.088000 |
| H | 2.476000 | -3.228000 | 2.110000 |
| C | -2.751000 | -0.932000 | -1.485000 |
| H | -2.331000 | -1.032000 | -2.479000 |
| C | 0.439000 | -1.366000 | 1.724000 |
| H | -0.443000 | -2.018000 | 1.713000 |
| H | 0.823000 | -1.359000 | 2.751000 |
| C | 1.296000 | 4.499000 | 0.096000 |
| H | 1.581000 | 5.518000 | 0.341000 |
| C | 3.256000 | -3.366000 | 0.094000 |
| H | 3.999000 | -4.120000 | 0.340000 |
| C | -1.402000 | 0.297000 | 1.727000 |
| H | -1.526000 | 1.386000 | 1.726000 |
| H | -1.587000 | -0.047000 | 2.753000 |
| H | 2.060000 | -1.499000 | -2.480000 |
| H | 3.784000 | -3.245000 | -2.007000 |

| | | | |
|---|---|---|---|
| H | -0.003000 | 0.001000 | -2.263000 |

**$Co^{II}$-H(TPA)**

| | | | |
|---|---|---|---|
| Co | -0.000000 | 0.001000 | -1.082000 |
| N | -0.002000 | 0.001000 | 1.300000 |
| C | 1.039000 | -4.250000 | -1.080000 |
| H | 1.385000 | -4.945000 | -1.838000 |
| C | 0.153000 | -2.407000 | 0.764000 |
| N | 1.590000 | 1.304000 | -0.516000 |
| N | -1.925000 | 0.724000 | -0.517000 |
| C | 2.010000 | 1.336000 | 0.765000 |
| C | 0.767000 | -2.926000 | -1.420000 |
| H | 0.885000 | -2.553000 | -2.433000 |
| C | -0.416000 | -1.354000 | 1.697000 |
| H | -1.511000 | -1.398000 | 1.635000 |
| H | -0.149000 | -1.579000 | 2.741000 |
| N | 0.336000 | -2.027000 | -0.516000 |
| C | 3.599000 | 3.067000 | 0.246000 |
| H | 4.380000 | 3.757000 | 0.549000 |
| C | 0.415000 | -3.712000 | 1.183000 |
| H | 0.268000 | -3.991000 | 2.223000 |
| C | -2.919000 | 0.801000 | -1.421000 |
| C | 3.010000 | 2.215000 | 1.184000 |
| H | 3.324000 | 2.229000 | 2.224000 |
| C | -2.164000 | 1.072000 | 0.764000 |
| C | 3.167000 | 3.020000 | -1.081000 |
| H | 3.599000 | 3.664000 | -1.839000 |
| C | -4.202000 | 1.225000 | -1.082000 |
| C | -3.426000 | 1.495000 | 1.182000 |
| H | -3.595000 | 1.761000 | 2.222000 |
| C | 2.155000 | 2.124000 | -1.420000 |
| H | 1.774000 | 2.039000 | -2.433000 |
| C | -0.968000 | 1.037000 | 1.698000 |
| H | -0.459000 | 2.007000 | 1.639000 |
| H | -1.298000 | 0.916000 | 2.741000 |
| C | 0.863000 | -4.647000 | 0.247000 |
| H | 1.072000 | -5.669000 | 0.550000 |
| C | -4.459000 | 1.575000 | 0.245000 |
| H | -5.449000 | 1.904000 | 0.548000 |
| C | 1.379000 | 0.320000 | 1.700000 |
| H | 1.964000 | -0.606000 | 1.644000 |
| H | 1.437000 | 0.667000 | 2.743000 |
| H | -2.654000 | 0.513000 | -2.434000 |
| H | -4.976000 | 1.274000 | -1.840000 |

| | | | |
|---|---|---|---|
| H | 0.000000 | 0.002000 | -2.721000 |

**$Co^{II}$(TPA)**

| | | | |
|---|---|---|---|
| Co | 0.000000 | -0.002000 | -0.822000 |
| N | 0.001000 | -0.002000 | 1.310000 |
| C | 4.019000 | -1.587000 | -1.197000 |
| H | 4.761000 | -1.706000 | -1.979000 |
| C | 2.065000 | -1.247000 | 0.725000 |
| N | -0.155000 | 2.008000 | -0.556000 |
| N | -1.664000 | -1.138000 | -0.555000 |
| C | 0.049000 | 2.408000 | 0.726000 |
| C | 2.778000 | -1.037000 | -1.496000 |
| H | 2.535000 | -0.716000 | -2.504000 |
| C | 0.914000 | -1.104000 | 1.706000 |
| H | 0.335000 | -2.035000 | 1.702000 |
| H | 1.288000 | -0.966000 | 2.729000 |
| N | 1.818000 | -0.872000 | -0.556000 |
| C | -0.432000 | 4.689000 | 0.123000 |
| H | -0.542000 | 5.735000 | 0.393000 |
| C | 3.292000 | -1.791000 | 1.094000 |
| H | 3.473000 | -2.076000 | 2.126000 |
| C | -2.290000 | -1.884000 | -1.494000 |
| C | -0.091000 | 3.744000 | 1.095000 |
| H | 0.067000 | 4.042000 | 2.127000 |
| C | -2.112000 | -1.163000 | 0.727000 |
| C | -0.633000 | 4.272000 | -1.195000 |
| H | -0.901000 | 4.974000 | -1.977000 |
| C | -3.390000 | -2.679000 | -1.196000 |
| C | -3.200000 | -1.949000 | 1.095000 |
| H | -3.538000 | -1.962000 | 2.127000 |
| C | -0.491000 | 2.922000 | -1.494000 |
| H | -0.649000 | 2.551000 | -2.503000 |
| C | -1.409000 | -0.241000 | 1.709000 |
| H | -1.925000 | 0.726000 | 1.710000 |
| H | -1.475000 | -0.638000 | 2.730000 |
| C | 4.281000 | -1.968000 | 0.122000 |
| H | 5.243000 | -2.393000 | 0.392000 |
| C | -3.851000 | -2.714000 | 0.123000 |
| H | -4.703000 | -3.331000 | 0.393000 |
| C | 0.499000 | 1.340000 | 1.707000 |
| H | 1.595000 | 1.304000 | 1.705000 |
| H | 0.191000 | 1.595000 | 2.729000 |
| H | -1.891000 | -1.834000 | -2.503000 |
| H | -3.866000 | -3.260000 | -1.979000 |

**C2**

**$Co^{II}$(6-MeOTPA)Cl (High-spin state)**

| | | | |
|---|---|---|---|
| Co | 0.081000 | 0.025000 | 0.575000 |
| N | 0.687000 | 0.029000 | -1.640000 |
| C | 3.406000 | -2.696000 | 1.490000 |
| H | 3.679000 | -3.326000 | 2.327000 |
| C | 2.636000 | -1.052000 | -0.591000 |
| N | -1.589000 | -0.808000 | -0.440000 |
| N | 0.271000 | 2.066000 | 0.139000 |
| C | -1.377000 | -1.328000 | -1.678000 |
| C | 2.231000 | -1.944000 | 1.545000 |
| H | 1.576000 | -1.942000 | 2.407000 |
| C | 2.169000 | -0.076000 | -1.647000 |
| H | 2.569000 | 0.919000 | -1.415000 |
| H | 2.555000 | -0.358000 | -2.638000 |
| N | 1.853000 | -1.143000 | 0.517000 |
| C | -3.637000 | -2.142000 | -1.763000 |
| H | -4.433000 | -2.670000 | -2.275000 |
| C | 3.820000 | -1.783000 | -0.706000 |
| H | 4.425000 | -1.699000 | -1.602000 |
| C | 0.337000 | 3.007000 | 1.115000 |
| C | -2.382000 | -1.996000 | -2.373000 |
| H | -2.192000 | -2.396000 | -3.362000 |
| C | 0.343000 | 2.433000 | -1.167000 |
| C | -3.870000 | -1.589000 | -0.506000 |
| H | -4.839000 | -1.669000 | -0.034000 |
| C | 0.479000 | 4.362000 | 0.809000 |
| C | 0.499000 | 3.771000 | -1.533000 |
| H | 0.565000 | 4.044000 | -2.580000 |
| C | -2.820000 | -0.899000 | 0.123000 |
| C | 0.187000 | 1.320000 | -2.182000 |
| H | -0.879000 | 1.192000 | -2.403000 |
| H | 0.684000 | 1.584000 | -3.127000 |
| C | 4.210000 | -2.616000 | 0.349000 |
| H | 5.127000 | -3.191000 | 0.280000 |
| C | 0.564000 | 4.748000 | -0.532000 |
| H | 0.682000 | 5.793000 | -0.797000 |
| C | 0.022000 | -1.163000 | -2.228000 |
| H | 0.621000 | -2.039000 | -1.953000 |
| H | -0.001000 | -1.119000 | -3.327000 |
| Cl | -0.108000 | 0.058000 | 2.906000 |
| H | 0.270000 | 2.637000 | 2.130000 |

| | | | |
|---|---|---|---|
| H | 0.526000 | 5.091000 | 1.608000 |
| O | -2.912000 | -0.239000 | 1.300000 |
| C | -4.076000 | -0.407000 | 2.177000 |
| H | -4.963000 | 0.049000 | 1.727000 |
| H | -4.245000 | -1.467000 | 2.386000 |
| H | -3.798000 | 0.115000 | 3.089000 |

**$Co^{II}$(6-MeOTPA)Cl (Low-spin state)**

| | | | |
|---|---|---|---|
| Co | -0.000000 | -0.423000 | -0.604000 |
| N | -0.000000 | -1.280000 | 1.383000 |
| C | 4.244000 | -0.136000 | -1.005000 |
| H | 4.956000 | 0.345000 | -1.668000 |
| C | 2.350000 | -1.337000 | 0.595000 |
| N | 0.000000 | 1.297000 | 0.429000 |
| N | -1.957000 | -0.551000 | -0.432000 |
| C | 0.000000 | 1.210000 | 1.770000 |
| C | 2.878000 | 0.029000 | -1.218000 |
| H | 2.495000 | 0.628000 | -2.038000 |
| C | 1.251000 | -2.067000 | 1.349000 |
| H | 1.044000 | -2.992000 | 0.800000 |
| H | 1.595000 | -2.344000 | 2.357000 |
| N | 1.956000 | -0.551000 | -0.432000 |
| C | 0.001000 | 3.599000 | 1.958000 |
| H | 0.001000 | 4.505000 | 2.558000 |
| C | 3.702000 | -1.533000 | 0.877000 |
| H | 3.996000 | -2.162000 | 1.712000 |
| C | -2.878000 | 0.030000 | -1.218000 |
| C | 0.001000 | 2.348000 | 2.576000 |
| H | 0.001000 | 2.256000 | 3.658000 |
| C | -2.351000 | -1.337000 | 0.595000 |
| C | 0.001000 | 3.694000 | 0.568000 |
| H | 0.001000 | 4.659000 | 0.077000 |
| C | -4.244000 | -0.134000 | -1.005000 |
| C | -3.703000 | -1.532000 | 0.877000 |
| H | -3.996000 | -2.161000 | 1.712000 |
| C | 0.000000 | 2.503000 | -0.168000 |
| C | -1.252000 | -2.067000 | 1.349000 |
| H | -1.595000 | -2.344000 | 2.356000 |
| H | -1.044000 | -2.992000 | 0.800000 |
| C | 4.663000 | -0.926000 | 0.066000 |
| H | 5.721000 | -1.073000 | 0.264000 |
| C | -4.663000 | -0.925000 | 0.066000 |
| H | -5.721000 | -1.071000 | 0.265000 |
| C | -0.000000 | -0.188000 | 2.379000 |
| H | 0.876000 | -0.283000 | 3.032000 |
| H | -0.877000 | -0.283000 | 3.032000 |
| Cl | -0.000000 | -2.161000 | -2.037000 |
| H | -2.495000 | 0.628000 | -2.038000 |
| H | -4.956000 | 0.346000 | -1.668000 |
| O | 0.000000 | 2.412000 | -1.512000 |
| C | 0.001000 | 3.617000 | -2.296000 |
| H | -0.899000 | 4.210000 | -2.096000 |
| H | 0.900000 | 4.209000 | -2.096000 |
| H | 0.000000 | 3.285000 | -3.334000 |

**$Co^{I}$(6-MeOTPA)Cl**

| | | | |
|---|---|---|---|
| Co | 0.077000 | 0.059000 | 0.584000 |
| N | 0.699000 | 0.064000 | -1.656000 |
| C | 3.077000 | -3.130000 | 1.339000 |
| H | 3.282000 | -3.830000 | 2.143000 |
| C | 2.474000 | -1.306000 | -0.624000 |
| N | -1.627000 | -0.712000 | -0.427000 |
| N | 0.172000 | 2.117000 | 0.172000 |
| C | -1.501000 | -1.059000 | -1.729000 |
| C | 1.962000 | -2.297000 | 1.410000 |
| H | 1.290000 | -2.295000 | 2.264000 |
| C | 2.135000 | -0.214000 | -1.628000 |
| H | 2.641000 | 0.711000 | -1.319000 |
| H | 2.533000 | -0.478000 | -2.624000 |
| N | 1.655000 | -1.414000 | 0.442000 |
| C | -3.836000 | -1.582000 | -1.911000 |
| H | -4.696000 | -1.914000 | -2.485000 |
| C | 3.604000 | -2.113000 | -0.775000 |
| H | 4.233000 | -2.008000 | -1.655000 |
| C | 0.278000 | 3.045000 | 1.151000 |
| C | -2.573000 | -1.486000 | -2.506000 |
| H | -2.423000 | -1.740000 | -3.552000 |
| C | 0.555000 | 2.468000 | -1.083000 |
| C | -3.983000 | -1.237000 | -0.566000 |
| H | -4.950000 | -1.294000 | -0.082000 |
| C | 0.748000 | 4.335000 | 0.919000 |
| C | 1.051000 | 3.733000 | -1.386000 |
| H | 1.356000 | 3.964000 | -2.404000 |
| C | -2.852000 | -0.799000 | 0.137000 |
| C | 0.353000 | 1.406000 | -2.147000 |
| H | -0.710000 | 1.385000 | -2.414000 |
| H | 0.908000 | 1.667000 | -3.064000 |
| C | 3.911000 | -3.042000 | 0.221000 |

| | | | |
|---|---|---|---|
| H | 4.786000 | -3.680000 | 0.128000 |
| C | 1.147000 | 4.695000 | -0.372000 |
| H | 1.529000 | 5.689000 | -0.585000 |
| C | -0.088000 | -1.007000 | -2.279000 |
| H | 0.405000 | -1.957000 | -2.041000 |
| H | -0.108000 | -0.922000 | -3.379000 |
| Cl | 0.121000 | 0.140000 | 2.995000 |
| H | -0.013000 | 2.702000 | 2.140000 |
| H | 0.806000 | 5.040000 | 1.744000 |
| O | -2.852000 | -0.415000 | 1.422000 |
| C | -4.044000 | -0.501000 | 2.192000 |
| H | -4.823000 | 0.162000 | 1.794000 |
| H | -4.416000 | -1.533000 | 2.231000 |
| H | -3.757000 | -0.176000 | 3.193000 |

**$Co^{I}$(6-MeOTPA)**

| | | | |
|---|---|---|---|
| Co | 0.105000 | -0.114000 | 0.615000 |
| N | 0.558000 | -0.079000 | -1.499000 |
| C | 3.461000 | -2.639000 | 1.734000 |
| H | 3.812000 | -3.157000 | 2.621000 |
| C | 2.495000 | -1.257000 | -0.443000 |
| N | -1.753000 | -0.664000 | -0.111000 |
| N | 0.422000 | 1.931000 | 0.423000 |
| C | -1.714000 | -1.073000 | -1.400000 |
| C | 2.411000 | -1.728000 | 1.831000 |
| H | 1.935000 | -1.526000 | 2.786000 |
| C | 1.995000 | -0.398000 | -1.597000 |
| H | 2.542000 | 0.552000 | -1.562000 |
| H | 2.246000 | -0.870000 | -2.558000 |
| N | 1.926000 | -1.046000 | 0.772000 |
| C | -4.071000 | -1.505000 | -1.381000 |
| H | -4.981000 | -1.830000 | -1.877000 |
| C | 3.541000 | -2.161000 | -0.619000 |
| H | 3.966000 | -2.311000 | -1.607000 |
| C | 0.628000 | 2.842000 | 1.394000 |
| C | -2.857000 | -1.491000 | -2.075000 |
| H | -2.802000 | -1.801000 | -3.113000 |
| C | 0.553000 | 2.328000 | -0.866000 |
| C | -4.118000 | -1.100000 | -0.050000 |
| C | 0.970000 | 4.168000 | 1.134000 |
| C | 0.910000 | 3.633000 | -1.206000 |
| H | 1.019000 | 3.910000 | -2.251000 |
| C | -2.922000 | -0.679000 | 0.552000 |
| C | 0.226000 | 1.293000 | -1.932000 |
| H | -0.854000 | 1.325000 | -2.117000 |
| H | 0.718000 | 1.552000 | -2.882000 |
| C | 4.037000 | -2.864000 | 0.483000 |
| H | 4.852000 | -3.571000 | 0.365000 |
| C | 1.118000 | 4.572000 | -0.193000 |
| H | 1.394000 | 5.594000 | -0.437000 |
| C | -0.338000 | -1.104000 | -2.058000 |
| H | 0.119000 | -2.082000 | -1.858000 |
| H | -0.443000 | -1.019000 | -3.152000 |
| H | 0.515000 | 2.484000 | 2.413000 |
| H | 1.122000 | 4.859000 | 1.957000 |
| H | -5.053000 | -1.105000 | 0.497000 |
| O | -2.803000 | -0.253000 | 1.824000 |
| C | -3.968000 | -0.219000 | 2.661000 |
| H | -3.620000 | 0.152000 | 3.624000 |
| H | -4.721000 | 0.465000 | 2.253000 |
| H | -4.390000 | -1.222000 | 2.782000 |

**$Co^{III}$-H(6-MeOTPA)**

| | | | |
|---|---|---|---|
| Co | 0.101000 | -0.008000 | 0.556000 |
| N | 0.639000 | 0.004000 | -1.453000 |
| C | 2.775000 | -3.165000 | 1.698000 |
| H | 2.921000 | -3.815000 | 2.554000 |
| C | 2.335000 | -1.463000 | -0.430000 |
| N | -1.682000 | -0.534000 | -0.198000 |
| N | 0.633000 | 1.920000 | 0.446000 |
| C | -1.656000 | -0.895000 | -1.514000 |
| C | 1.763000 | -2.212000 | 1.719000 |
| H | 1.104000 | -2.100000 | 2.572000 |
| C | 2.062000 | -0.434000 | -1.506000 |
| H | 2.691000 | 0.445000 | -1.324000 |
| H | 2.322000 | -0.815000 | -2.502000 |
| N | 1.549000 | -1.378000 | 0.676000 |
| C | -4.025000 | -1.227000 | -1.501000 |
| H | -4.945000 | -1.498000 | -2.010000 |
| C | 3.356000 | -2.404000 | -0.518000 |
| H | 3.968000 | -2.463000 | -1.413000 |
| C | 0.858000 | 2.741000 | 1.496000 |
| C | -2.806000 | -1.237000 | -2.200000 |
| H | -2.764000 | -1.514000 | -3.248000 |
| C | 0.806000 | 2.381000 | -0.821000 |
| C | -4.062000 | -0.866000 | -0.162000 |
| H | -4.998000 | -0.850000 | 0.380000 |
| C | 1.265000 | 4.059000 | 1.320000 |

| | | | |
|---|---|---|---|
| C | 1.223000 | 3.686000 | -1.063000 |
| H | 1.363000 | 4.034000 | -2.082000 |
| C | -2.860000 | -0.508000 | 0.474000 |
| C | 0.455000 | 1.405000 | -1.925000 |
| H | -0.601000 | 1.533000 | -2.188000 |
| H | 1.039000 | 1.598000 | -2.834000 |
| C | 3.582000 | -3.264000 | 0.562000 |
| H | 4.376000 | -4.003000 | 0.513000 |
| C | 1.452000 | 4.538000 | 0.022000 |
| H | 1.776000 | 5.561000 | -0.147000 |
| C | -0.277000 | -0.955000 | -2.133000 |
| H | 0.133000 | -1.962000 | -1.991000 |
| H | -0.315000 | -0.770000 | -3.213000 |
| H | 0.705000 | 2.318000 | 2.482000 |
| H | 1.435000 | 4.690000 | 2.186000 |
| O | -2.749000 | -0.114000 | 1.740000 |
| C | -3.926000 | -0.053000 | 2.584000 |
| H | -4.644000 | 0.667000 | 2.182000 |
| H | -4.374000 | -1.045000 | 2.682000 |
| H | -3.559000 | 0.287000 | 3.551000 |
| H | -0.268000 | -0.023000 | 2.011000 |

**$Co^{II}$-H(6-MeOTPA)**

| | | | |
|---|---|---|---|
| Co | -0.072000 | 0.005000 | -0.909000 |
| N | -0.648000 | 0.015000 | 1.408000 |
| C | 4.022000 | -1.287000 | 0.275000 |
| C | 1.535000 | -1.143000 | 1.441000 |
| N | -0.427000 | 2.053000 | -0.409000 |
| N | -1.807000 | -1.258000 | -0.705000 |
| C | -0.528000 | 2.425000 | 0.883000 |
| C | 2.907000 | -0.756000 | -0.396000 |
| C | 0.128000 | -1.083000 | 2.003000 |
| H | -0.383000 | -2.022000 | 1.757000 |
| H | 0.161000 | -1.019000 | 3.102000 |
| N | 1.686000 | -0.706000 | 0.174000 |
| C | -0.972000 | 4.700000 | 0.239000 |
| H | -1.190000 | 5.733000 | 0.496000 |
| C | 2.592000 | -1.660000 | 2.183000 |
| H | 2.438000 | -1.992000 | 3.205000 |
| C | -2.173000 | -2.074000 | -1.709000 |
| C | -0.808000 | 3.743000 | 1.243000 |
| H | -0.895000 | 4.015000 | 2.291000 |
| C | -2.537000 | -1.230000 | 0.427000 |
| C | -0.857000 | 4.310000 | -1.097000 |
| H | -0.980000 | 5.021000 | -1.907000 |
| C | -3.285000 | -2.910000 | -1.620000 |
| C | -3.658000 | -2.043000 | 0.596000 |
| H | -4.223000 | -2.008000 | 1.523000 |
| C | -0.587000 | 2.972000 | -1.378000 |
| H | -0.492000 | 2.601000 | -2.394000 |
| C | -2.098000 | -0.220000 | 1.471000 |
| H | -2.600000 | 0.732000 | 1.261000 |
| H | -2.423000 | -0.536000 | 2.475000 |
| C | 3.850000 | -1.741000 | 1.577000 |
| C | -4.038000 | -2.895000 | -0.444000 |
| H | -4.908000 | -3.536000 | -0.336000 |
| C | -0.260000 | 1.341000 | 1.912000 |
| H | 0.817000 | 1.320000 | 2.117000 |
| H | -0.758000 | 1.583000 | 2.864000 |
| H | -1.549000 | -2.033000 | -2.597000 |
| H | -3.548000 | -3.555000 | -2.451000 |
| H | 4.697000 | -2.147000 | 2.123000 |
| H | 4.993000 | -1.330000 | -0.203000 |
| O | 2.933000 | -0.243000 | -1.631000 |
| C | 4.149000 | -0.269000 | -2.390000 |
| H | 3.892000 | 0.174000 | -3.351000 |
| H | 4.927000 | 0.327000 | -1.900000 |
| H | 4.492000 | -1.299000 | -2.538000 |
| H | 0.100000 | -0.013000 | -2.532000 |

**$Co^{II}$(6-MeOTPA)**

| | | | |
|---|---|---|---|
| Co | -0.052000 | 0.002000 | -0.595000 |
| N | -0.629000 | -0.018000 | 1.482000 |
| C | 4.140000 | -0.457000 | 0.133000 |
| C | 1.766000 | -0.657000 | 1.550000 |
| N | -0.822000 | 1.889000 | -0.494000 |
| N | -1.383000 | -1.541000 | -0.682000 |
| C | -1.089000 | 2.313000 | 0.768000 |
| C | 2.894000 | -0.269000 | -0.478000 |
| C | 0.400000 | -0.824000 | 2.192000 |
| H | 0.108000 | -1.878000 | 2.117000 |
| H | 0.435000 | -0.577000 | 3.261000 |
| N | 1.747000 | -0.373000 | 0.224000 |
| C | -2.014000 | 4.366000 | -0.082000 |
| H | -2.484000 | 5.331000 | 0.083000 |
| C | 2.963000 | -0.840000 | 2.225000 |
| H | 2.974000 | -1.061000 | 3.287000 |
| C | -1.519000 | -2.419000 | -1.701000 |

| | | | |
|---|---|---|---|
| C | -1.692000 | 3.546000 | 1.002000 |
| H | -1.904000 | 3.863000 | 2.019000 |
| C | -2.124000 | -1.704000 | 0.444000 |
| C | -1.729000 | 3.928000 | -1.378000 |
| H | -1.965000 | 4.535000 | -2.246000 |
| C | -2.403000 | -3.490000 | -1.644000 |
| C | -3.017000 | -2.765000 | 0.572000 |
| H | -3.594000 | -2.882000 | 1.484000 |
| C | -1.137000 | 2.682000 | -1.543000 |
| H | -0.906000 | 2.296000 | -2.532000 |
| C | -1.978000 | -0.636000 | 1.514000 |
| H | -2.713000 | 0.154000 | 1.318000 |
| H | -2.209000 | -1.045000 | 2.506000 |
| C | 4.158000 | -0.741000 | 1.496000 |
| C | -3.163000 | -3.667000 | -0.485000 |
| H | -3.857000 | -4.499000 | -0.403000 |
| C | -0.632000 | 1.407000 | 1.898000 |
| H | 0.397000 | 1.677000 | 2.166000 |
| H | -1.246000 | 1.562000 | 2.794000 |
| H | -0.898000 | -2.249000 | -2.577000 |
| H | -2.485000 | -4.170000 | -2.486000 |
| H | 5.111000 | -0.885000 | 1.998000 |
| H | 5.062000 | -0.378000 | -0.431000 |
| O | 2.668000 | 0.027000 | -1.766000 |
| C | 3.792000 | 0.168000 | -2.674000 |
| H | 3.349000 | 0.397000 | -3.642000 |
| H | 4.435000 | 0.992000 | -2.352000 |
| H | 4.350000 | -0.770000 | -2.730000 |

**C3**

**$Co^{II}$(5-MeOTPA)Cl (High-spin state)**

| | | | |
|---|---|---|---|
| Co | 0.357000 | -0.006000 | 0.639000 |
| N | 0.738000 | 0.006000 | -1.608000 |
| C | 2.681000 | -3.655000 | 1.160000 |
| H | 2.816000 | -4.380000 | 1.953000 |
| C | 2.289000 | -1.750000 | -0.806000 |
| N | -1.566000 | -0.261000 | -0.142000 |
| N | 1.191000 | 1.886000 | 0.330000 |
| C | -1.669000 | -0.543000 | -1.471000 |
| C | 1.846000 | -2.555000 | 1.361000 |
| H | 1.320000 | -2.379000 | 2.291000 |
| C | 2.077000 | -0.617000 | -1.787000 |
| H | 2.827000 | 0.160000 | -1.594000 |
| H | 2.231000 | -0.963000 | -2.820000 |
| N | 1.655000 | -1.627000 | 0.390000 |
| C | -4.082000 | -0.475000 | -1.309000 |
| H | -5.053000 | -0.555000 | -1.779000 |
| C | 3.128000 | -2.834000 | -1.069000 |
| H | 3.619000 | -2.922000 | -2.031000 |
| C | 1.638000 | 2.653000 | 1.357000 |
| C | -2.921000 | -0.644000 | -2.074000 |
| H | -2.998000 | -0.860000 | -3.134000 |
| C | 1.311000 | 2.324000 | -0.951000 |
| C | -3.956000 | -0.201000 | 0.060000 |
| C | 2.235000 | 3.894000 | 1.130000 |
| C | 1.911000 | 3.551000 | -1.240000 |
| H | 2.007000 | 3.880000 | -2.269000 |
| C | -2.667000 | -0.096000 | 0.615000 |
| H | -2.527000 | 0.113000 | 1.668000 |
| C | 0.699000 | 1.437000 | -2.014000 |
| H | -0.356000 | 1.711000 | -2.135000 |
| H | 1.188000 | 1.598000 | -2.985000 |
| C | 3.328000 | -3.798000 | -0.072000 |
| H | 3.977000 | -4.646000 | -0.257000 |
| C | 2.377000 | 4.346000 | -0.186000 |
| H | 2.843000 | 5.303000 | -0.391000 |
| C | -0.368000 | -0.802000 | -2.196000 |
| H | -0.092000 | -1.857000 | -2.079000 |
| H | -0.477000 | -0.615000 | -3.275000 |
| Cl | -0.004000 | -0.018000 | 2.942000 |
| H | 1.492000 | 2.244000 | 2.349000 |
| H | 2.580000 | 4.486000 | 1.968000 |
| O | -4.989000 | -0.014000 | 0.937000 |
| C | -6.370000 | -0.122000 | 0.466000 |
| H | -6.978000 | 0.055000 | 1.351000 |
| H | -6.582000 | 0.639000 | -0.292000 |
| H | -6.567000 | -1.123000 | 0.070000 |

**$Co^{II}$(5-MeOTPA)Cl (Low-spin state)**

| | | | |
|---|---|---|---|
| Co | 0.322000 | -0.262000 | -0.416000 |
| N | 0.729000 | -0.001000 | 1.540000 |
| C | 0.844000 | 4.061000 | -1.301000 |
| H | 0.630000 | 4.747000 | -2.114000 |
| C | 1.358000 | 2.244000 | 0.688000 |
| N | -1.610000 | -0.175000 | 0.143000 |
| N | 2.085000 | -1.231000 | -0.375000 |
| C | -1.761000 | -0.127000 | 1.491000 |

| | | | |
|---|---|---|---|
| C | 0.581000 | 2.699000 | -1.452000 |
| H | 0.163000 | 2.283000 | -2.364000 |
| C | 1.688000 | 1.142000 | 1.672000 |
| H | 2.690000 | 0.761000 | 1.446000 |
| H | 1.705000 | 1.507000 | 2.707000 |
| N | 0.834000 | 1.815000 | -0.475000 |
| C | -4.121000 | -0.585000 | 1.283000 |
| H | -5.087000 | -0.754000 | 1.745000 |
| C | 1.635000 | 3.590000 | 0.926000 |
| H | 2.050000 | 3.910000 | 1.877000 |
| C | 2.887000 | -1.558000 | -1.403000 |
| C | -3.000000 | -0.343000 | 2.081000 |
| H | -3.102000 | -0.316000 | 3.163000 |
| C | 2.374000 | -1.683000 | 0.869000 |
| C | -3.960000 | -0.607000 | -0.108000 |
| C | 4.022000 | -2.348000 | -1.226000 |
| C | 3.493000 | -2.471000 | 1.121000 |
| H | 3.706000 | -2.815000 | 2.129000 |
| C | -2.670000 | -0.412000 | -0.637000 |
| H | -2.494000 | -0.465000 | -1.706000 |
| C | 1.373000 | -1.285000 | 1.937000 |
| H | 0.583000 | -2.042000 | 2.008000 |
| H | 1.848000 | -1.206000 | 2.925000 |
| C | 1.374000 | 4.513000 | -0.092000 |
| H | 1.581000 | 5.568000 | 0.061000 |
| C | 4.329000 | -2.812000 | 0.054000 |
| H | 5.207000 | -3.429000 | 0.222000 |
| C | -0.540000 | 0.282000 | 2.282000 |
| H | -0.582000 | 1.364000 | 2.450000 |
| H | -0.519000 | -0.192000 | 3.271000 |
| Cl | -0.061000 | -0.631000 | -2.598000 |
| H | 2.581000 | -1.183000 | -2.374000 |
| H | 4.646000 | -2.591000 | -2.079000 |
| O | -4.933000 | -0.815000 | -1.015000 |
| C | -6.273000 | -1.034000 | -0.562000 |
| H | -6.866000 | -1.169000 | -1.466000 |
| H | -6.333000 | -1.937000 | 0.057000 |
| H | -6.643000 | -0.166000 | -0.004000 |

**$Co^{I}$(5-MeOTPA)Cl**

| | | | |
|---|---|---|---|
| Co | 0.403000 | -0.040000 | 0.652000 |
| N | 0.723000 | -0.010000 | -1.641000 |
| C | 2.969000 | -3.456000 | 1.172000 |
| H | 3.183000 | -4.139000 | 1.989000 |
| C | 2.380000 | -1.649000 | -0.812000 |
| N | -1.575000 | -0.239000 | -0.121000 |
| N | 1.061000 | 1.902000 | 0.308000 |
| C | -1.668000 | -0.601000 | -1.423000 |
| C | 2.259000 | -2.285000 | 1.425000 |
| H | 1.896000 | -2.026000 | 2.416000 |
| C | 2.071000 | -0.566000 | -1.828000 |
| H | 2.779000 | 0.257000 | -1.677000 |
| H | 2.227000 | -0.942000 | -2.854000 |
| N | 1.965000 | -1.384000 | 0.457000 |
| C | -4.081000 | -0.644000 | -1.278000 |
| H | -5.045000 | -0.797000 | -1.749000 |
| C | 3.083000 | -2.804000 | -1.139000 |
| H | 3.389000 | -2.976000 | -2.168000 |
| C | 1.460000 | 2.723000 | 1.304000 |
| C | -2.906000 | -0.793000 | -2.026000 |
| H | -2.964000 | -1.068000 | -3.077000 |
| C | 1.181000 | 2.331000 | -0.970000 |
| C | -3.967000 | -0.297000 | 0.073000 |
| C | 2.003000 | 3.982000 | 1.064000 |
| C | 1.733000 | 3.570000 | -1.289000 |
| H | 1.828000 | 3.869000 | -2.330000 |
| C | -2.684000 | -0.100000 | 0.611000 |
| H | -2.545000 | 0.167000 | 1.656000 |
| C | 0.611000 | 1.402000 | -2.030000 |
| H | -0.457000 | 1.628000 | -2.140000 |
| H | 1.079000 | 1.600000 | -3.009000 |
| C | 3.393000 | -3.730000 | -0.133000 |
| H | 3.941000 | -4.638000 | -0.365000 |
| C | 2.154000 | 4.417000 | -0.257000 |
| H | 2.586000 | 5.388000 | -0.481000 |
| C | -0.359000 | -0.853000 | -2.155000 |
| H | -0.057000 | -1.897000 | -1.990000 |
| H | -0.505000 | -0.734000 | -3.244000 |
| Cl | -0.048000 | -0.081000 | 3.010000 |
| H | 1.323000 | 2.326000 | 2.306000 |
| H | 2.308000 | 4.604000 | 1.900000 |
| O | -5.005000 | -0.118000 | 0.932000 |
| C | -6.329000 | -0.316000 | 0.449000 |
| H | -6.984000 | -0.131000 | 1.301000 |
| H | -6.568000 | 0.390000 | -0.358000 |
| H | -6.472000 | -1.345000 | 0.094000 |

**$Co^{I}$(5-MeOTPA)**

| | | | |
|---|---|---|---|
| Co | -0.486000 | 0.049000 | -0.778000 |
| N | -0.868000 | 0.034000 | 1.338000 |
| C | -2.616000 | -3.741000 | -1.441000 |
| H | -2.694000 | -4.503000 | -2.210000 |
| C | -2.338000 | -1.750000 | 0.440000 |
| N | 1.463000 | -0.350000 | -0.150000 |
| N | -0.844000 | 2.066000 | -0.617000 |
| C | 1.533000 | -0.589000 | 1.185000 |
| C | -1.756000 | -2.661000 | -1.618000 |
| H | -1.149000 | -2.569000 | -2.514000 |
| C | -2.198000 | -0.592000 | 1.423000 |
| H | -2.938000 | 0.177000 | 1.166000 |
| H | -2.435000 | -0.935000 | 2.443000 |
| N | -1.612000 | -1.679000 | -0.704000 |
| C | 3.952000 | -0.600000 | 1.110000 |
| H | 4.904000 | -0.693000 | 1.619000 |
| C | -3.207000 | -2.811000 | 0.694000 |
| H | -3.762000 | -2.844000 | 1.628000 |
| C | -1.087000 | 2.943000 | -1.614000 |
| C | 2.758000 | -0.704000 | 1.832000 |
| H | 2.790000 | -0.881000 | 2.904000 |
| C | -1.201000 | 2.412000 | 0.646000 |
| C | 3.873000 | -0.371000 | -0.267000 |
| C | -1.688000 | 4.182000 | -1.407000 |
| C | -1.817000 | 3.631000 | 0.928000 |
| H | -2.097000 | 3.872000 | 1.949000 |
| C | 2.598000 | -0.245000 | -0.849000 |
| H | 2.519000 | -0.047000 | -1.914000 |
| C | -0.822000 | 1.445000 | 1.760000 |
| H | 0.213000 | 1.662000 | 2.048000 |
| H | -1.443000 | 1.629000 | 2.650000 |
| C | -3.356000 | -3.819000 | -0.260000 |
| H | -4.032000 | -4.651000 | -0.082000 |
| C | -2.065000 | 4.533000 | -0.111000 |
| H | -2.544000 | 5.486000 | 0.091000 |
| C | 0.213000 | -0.795000 | 1.910000 |
| H | -0.088000 | -1.843000 | 1.796000 |
| H | 0.336000 | -0.617000 | 2.990000 |
| H | -0.780000 | 2.630000 | -2.608000 |
| H | -1.857000 | 4.849000 | -2.247000 |
| O | 4.918000 | -0.246000 | -1.115000 |
| C | 6.245000 | -0.366000 | -0.595000 |
| H | 6.906000 | -0.238000 | -1.452000 |
| H | 6.448000 | 0.417000 | 0.146000 |
| H | 6.403000 | -1.355000 | -0.151000 |

**$Co^{III}$-H(5-MeOTPA)**

| | | | |
|---|---|---|---|
| Co | -0.367000 | -0.008000 | -0.661000 |
| N | -0.745000 | 0.002000 | 1.371000 |
| C | -2.586000 | -3.577000 | -1.512000 |
| H | -2.690000 | -4.274000 | -2.336000 |
| C | -2.263000 | -1.749000 | 0.531000 |
| N | 1.521000 | -0.241000 | -0.071000 |
| N | -1.163000 | 1.819000 | -0.573000 |
| C | 1.654000 | -0.528000 | 1.254000 |
| C | -1.744000 | -2.478000 | -1.639000 |
| H | -1.178000 | -2.295000 | -2.546000 |
| C | -2.074000 | -0.649000 | 1.553000 |
| H | -2.845000 | 0.115000 | 1.400000 |
| H | -2.192000 | -1.025000 | 2.577000 |
| N | -1.588000 | -1.582000 | -0.638000 |
| C | 4.059000 | -0.478000 | 1.030000 |
| H | 5.042000 | -0.571000 | 1.480000 |
| C | -3.111000 | -2.834000 | 0.724000 |
| H | -3.636000 | -2.955000 | 1.667000 |
| C | -1.578000 | 2.554000 | -1.630000 |
| C | 2.918000 | -0.642000 | 1.819000 |
| H | 3.022000 | -0.864000 | 2.878000 |
| C | -1.318000 | 2.300000 | 0.689000 |
| C | 3.910000 | -0.191000 | -0.337000 |
| C | -2.164000 | 3.804000 | -1.464000 |
| C | -1.908000 | 3.538000 | 0.921000 |
| H | -2.031000 | 3.902000 | 1.937000 |
| C | 2.603000 | -0.073000 | -0.848000 |
| H | 2.451000 | 0.159000 | -1.895000 |
| C | -0.748000 | 1.432000 | 1.790000 |
| H | 0.292000 | 1.727000 | 1.973000 |
| H | -1.293000 | 1.566000 | 2.733000 |
| C | -3.278000 | -3.759000 | -0.312000 |
| H | -3.938000 | -4.612000 | -0.181000 |
| C | -2.334000 | 4.302000 | -0.170000 |
| H | -2.795000 | 5.272000 | -0.009000 |
| C | 0.364000 | -0.777000 | 2.000000 |
| H | 0.098000 | -1.839000 | 1.933000 |
| H | 0.457000 | -0.535000 | 3.066000 |
| H | -1.430000 | 2.120000 | -2.612000 |
| H | -2.482000 | 4.369000 | -2.334000 |
| O | 4.891000 | -0.007000 | -1.222000 |

| | | | |
|---|---|---|---|
| C | 6.268000 | -0.118000 | -0.803000 |
| H | 6.853000 | 0.064000 | -1.703000 |
| H | 6.500000 | 0.640000 | -0.048000 |
| H | 6.471000 | -1.125000 | -0.423000 |
| H | -0.095000 | -0.015000 | -2.140000 |

**$Co^{II}$-H(5-MeOTPA)**

| | | | |
|---|---|---|---|
| Co | -0.341000 | -0.008000 | -0.992000 |
| N | -0.722000 | 0.001000 | 1.360000 |
| C | 3.978000 | -0.200000 | -0.296000 |
| C | 1.681000 | -0.537000 | 1.213000 |
| N | -1.200000 | 1.898000 | -0.563000 |
| N | -1.673000 | -1.634000 | -0.626000 |
| C | -1.314000 | 2.312000 | 0.716000 |
| C | 2.685000 | -0.103000 | -0.845000 |
| H | 2.549000 | 0.108000 | -1.901000 |
| C | 0.376000 | -0.793000 | 1.939000 |
| H | 0.110000 | -1.852000 | 1.826000 |
| H | 0.491000 | -0.610000 | 3.019000 |
| N | 1.584000 | -0.267000 | -0.108000 |
| C | -2.404000 | 4.337000 | 0.008000 |
| H | -2.878000 | 5.287000 | 0.236000 |
| C | 2.926000 | -0.632000 | 1.827000 |
| H | 2.995000 | -0.840000 | 2.892000 |
| C | -1.889000 | -2.566000 | -1.572000 |
| C | -1.920000 | 3.527000 | 1.038000 |
| H | -2.009000 | 3.833000 | 2.076000 |
| C | -2.274000 | -1.755000 | 0.574000 |
| C | -2.272000 | 3.908000 | -1.314000 |
| H | -2.634000 | 4.508000 | -2.142000 |
| C | -2.714000 | -3.667000 | -1.357000 |
| C | -3.106000 | -2.835000 | 0.869000 |
| H | -3.571000 | -2.915000 | 1.847000 |
| C | -1.666000 | 2.677000 | -1.556000 |
| H | -1.534000 | 2.285000 | -2.560000 |
| C | -2.042000 | -0.618000 | 1.553000 |
| H | -2.802000 | 0.152000 | 1.368000 |
| H | -2.190000 | -0.964000 | 2.588000 |
| C | 4.093000 | -0.467000 | 1.074000 |
| C | -3.331000 | -3.804000 | -0.112000 |
| H | -3.977000 | -4.653000 | 0.095000 |
| C | -0.686000 | 1.414000 | 1.766000 |
| H | 0.367000 | 1.701000 | 1.876000 |
| H | -1.161000 | 1.576000 | 2.746000 |
| H | -1.379000 | -2.401000 | -2.518000 |
| H | -2.864000 | -4.397000 | -2.146000 |
| H | 5.061000 | -0.544000 | 1.556000 |
| O | 4.996000 | -0.017000 | -1.159000 |
| C | 6.341000 | -0.112000 | -0.676000 |
| H | 6.974000 | 0.062000 | -1.546000 |
| H | 6.539000 | 0.653000 | 0.083000 |
| H | 6.540000 | -1.111000 | -0.269000 |
| H | -0.090000 | -0.014000 | -2.611000 |

**$Co^{II}$(5-MeOTPA)**

| | | | |
|---|---|---|---|
| Co | -0.341000 | -0.008000 | -0.992000 |
| N | -0.722000 | 0.001000 | 1.360000 |
| C | 3.978000 | -0.200000 | -0.296000 |
| C | 1.681000 | -0.537000 | 1.213000 |
| N | -1.200000 | 1.898000 | -0.563000 |
| N | -1.673000 | -1.634000 | -0.626000 |
| C | -1.314000 | 2.312000 | 0.716000 |
| C | 2.685000 | -0.103000 | -0.845000 |
| H | 2.549000 | 0.108000 | -1.901000 |
| C | 0.376000 | -0.793000 | 1.939000 |
| H | 0.110000 | -1.852000 | 1.826000 |
| H | 0.491000 | -0.610000 | 3.019000 |
| N | 1.584000 | -0.267000 | -0.108000 |
| C | -2.404000 | 4.337000 | 0.008000 |
| H | -2.878000 | 5.287000 | 0.236000 |
| C | 2.926000 | -0.632000 | 1.827000 |
| H | 2.995000 | -0.840000 | 2.892000 |
| C | -1.889000 | -2.566000 | -1.572000 |
| C | -1.920000 | 3.527000 | 1.038000 |
| H | -2.009000 | 3.833000 | 2.076000 |
| C | -2.274000 | -1.755000 | 0.574000 |
| C | -2.272000 | 3.908000 | -1.314000 |
| H | -2.634000 | 4.508000 | -2.142000 |
| C | -2.714000 | -3.667000 | -1.357000 |
| C | -3.106000 | -2.835000 | 0.869000 |
| H | -3.571000 | -2.915000 | 1.847000 |
| C | -1.666000 | 2.677000 | -1.556000 |
| H | -1.534000 | 2.285000 | -2.560000 |
| C | -2.042000 | -0.618000 | 1.553000 |
| H | -2.802000 | 0.152000 | 1.368000 |
| H | -2.190000 | -0.964000 | 2.588000 |
| C | 4.093000 | -0.467000 | 1.074000 |
| C | -3.331000 | -3.804000 | -0.112000 |

| | | | |
|---|---|---|---|
| H | -3.977000 | -4.653000 | 0.095000 |
| C | -0.686000 | 1.414000 | 1.766000 |
| H | 0.367000 | 1.701000 | 1.876000 |
| H | -1.161000 | 1.576000 | 2.746000 |
| H | -1.379000 | -2.401000 | -2.518000 |
| H | -2.864000 | -4.397000 | -2.146000 |
| H | 5.061000 | -0.544000 | 1.556000 |
| O | 4.996000 | -0.017000 | -1.159000 |
| C | 6.341000 | -0.112000 | -0.676000 |
| H | 6.974000 | 0.062000 | -1.546000 |
| H | 6.539000 | 0.653000 | 0.083000 |
| H | 6.540000 | -1.111000 | -0.269000 |
| H | -0.090000 | -0.014000 | -2.611000 |

**C4**

**$Co^{II}$(4-MeOTPA)Cl (High-spin state)**

| | | | |
|---|---|---|---|
| Co | 0.518000 | 0.000000 | 0.712000 |
| N | 0.445000 | -0.003000 | -1.569000 |
| C | -3.818000 | 0.116000 | 1.017000 |
| H | -4.522000 | 0.302000 | 1.817000 |
| C | -1.924000 | -0.363000 | -0.942000 |
| N | 1.442000 | 1.810000 | 0.226000 |
| N | 1.620000 | -1.708000 | 0.229000 |
| C | 1.338000 | 2.250000 | -1.056000 |
| C | -2.454000 | 0.125000 | 1.292000 |
| H | -2.072000 | 0.310000 | 2.289000 |
| C | -0.820000 | -0.705000 | -1.920000 |
| H | -0.621000 | -1.782000 | -1.859000 |
| H | -1.132000 | -0.491000 | -2.953000 |
| N | -1.520000 | -0.103000 | 0.336000 |
| C | 2.712000 | 4.162000 | -0.538000 |
| H | 3.210000 | 5.076000 | -0.840000 |
| C | -3.264000 | -0.374000 | -1.294000 |
| H | -3.586000 | -0.571000 | -2.309000 |
| C | 1.937000 | -2.647000 | 1.155000 |
| C | 1.972000 | 3.423000 | -1.469000 |
| H | 1.886000 | 3.754000 | -2.498000 |
| C | 1.980000 | -1.883000 | -1.070000 |
| C | 2.802000 | 3.708000 | 0.783000 |
| H | 3.363000 | 4.257000 | 1.528000 |
| C | 2.625000 | -3.810000 | 0.806000 |
| C | 2.658000 | -3.032000 | -1.482000 |
| H | 2.929000 | -3.160000 | -2.524000 |
| C | 2.155000 | 2.522000 | 1.134000 |
| H | 2.178000 | 2.115000 | 2.138000 |
| C | 1.663000 | -0.737000 | -2.007000 |
| H | 2.498000 | -0.026000 | -1.985000 |
| H | 1.572000 | -1.095000 | -3.043000 |
| C | -4.237000 | -0.133000 | -0.302000 |
| C | 2.986000 | -4.007000 | -0.531000 |
| H | 3.514000 | -4.905000 | -0.832000 |
| C | 0.450000 | 1.431000 | -1.969000 |
| H | -0.580000 | 1.798000 | -1.882000 |
| H | 0.749000 | 1.559000 | -3.019000 |
| Cl | 0.606000 | 0.011000 | 3.048000 |
| H | 1.630000 | -2.429000 | 2.171000 |
| H | 2.867000 | -4.542000 | 1.566000 |
| O | -5.531000 | -0.164000 | -0.720000 |
| C | -6.621000 | 0.062000 | 0.236000 |
| H | -6.546000 | 1.061000 | 0.674000 |
| H | -7.528000 | -0.020000 | -0.358000 |
| H | -6.611000 | -0.704000 | 1.017000 |

**$Co^{II}$(4-MeOTPA)Cl (Low-spin state)**

| | | | |
|---|---|---|---|
| Co | -0.432000 | -0.219000 | 0.542000 |
| N | -0.482000 | -0.157000 | -1.472000 |
| C | 3.837000 | -0.475000 | 1.021000 |
| H | 4.529000 | -0.577000 | 1.847000 |
| C | 1.962000 | -0.195000 | -0.968000 |
| N | -2.152000 | -1.232000 | 0.284000 |
| N | -0.992000 | 1.835000 | 0.302000 |
| C | -2.204000 | -1.812000 | -0.939000 |
| C | 2.488000 | -0.275000 | 1.291000 |
| H | 2.113000 | -0.237000 | 2.308000 |
| C | 0.894000 | 0.089000 | -2.001000 |
| H | 0.959000 | 1.150000 | -2.268000 |
| H | 1.061000 | -0.481000 | -2.923000 |
| N | 1.559000 | -0.132000 | 0.327000 |
| C | -4.267000 | -2.907000 | -0.382000 |
| H | -5.094000 | -3.561000 | -0.644000 |
| C | 3.280000 | -0.415000 | -1.328000 |
| H | 3.583000 | -0.472000 | -2.369000 |
| C | -0.943000 | 2.815000 | 1.216000 |
| C | -3.251000 | -2.651000 | -1.309000 |
| H | -3.272000 | -3.099000 | -2.298000 |
| C | -1.298000 | 2.135000 | -0.974000 |
| C | -4.204000 | -2.309000 | 0.877000 |
| H | -4.972000 | -2.484000 | 1.623000 |

| | | | |
|---|---|---|---|
| C | -1.201000 | 4.146000 | 0.888000 |
| C | -1.553000 | 3.442000 | -1.389000 |
| H | -1.788000 | 3.656000 | -2.428000 |
| C | -3.127000 | -1.477000 | 1.177000 |
| H | -3.007000 | -1.000000 | 2.144000 |
| C | -1.417000 | 0.936000 | -1.891000 |
| H | -2.437000 | 0.544000 | -1.822000 |
| H | -1.243000 | 1.204000 | -2.941000 |
| C | 4.252000 | -0.556000 | -0.318000 |
| C | -1.505000 | 4.464000 | -0.437000 |
| H | -1.702000 | 5.492000 | -0.728000 |
| C | -1.028000 | -1.494000 | -1.842000 |
| H | -0.229000 | -2.230000 | -1.687000 |
| H | -1.312000 | -1.532000 | -2.903000 |
| Cl | -0.433000 | -0.373000 | 2.786000 |
| H | -0.694000 | 2.502000 | 2.227000 |
| H | -1.157000 | 4.912000 | 1.655000 |
| O | 5.508000 | -0.762000 | -0.731000 |
| C | 6.556000 | -0.920000 | 0.241000 |
| H | 6.367000 | -1.794000 | 0.873000 |
| H | 7.465000 | -1.072000 | -0.340000 |
| H | 6.653000 | -0.017000 | 0.853000 |

**$Co^{I}$(4-MeOTPA)Cl**

| | | | |
|---|---|---|---|
| Co | -0.585000 | 0.025000 | 0.720000 |
| N | -0.431000 | 0.036000 | -1.590000 |
| C | 3.834000 | -0.151000 | 1.010000 |
| H | 4.539000 | -0.362000 | 1.806000 |
| C | 1.922000 | 0.374000 | -0.898000 |
| N | -1.403000 | -1.810000 | 0.200000 |
| N | -1.873000 | 1.557000 | 0.261000 |
| C | -1.294000 | -2.230000 | -1.084000 |
| C | 2.466000 | -0.202000 | 1.277000 |
| H | 2.085000 | -0.437000 | 2.268000 |
| C | 0.816000 | 0.745000 | -1.878000 |
| H | 0.612000 | 1.819000 | -1.770000 |
| H | 1.162000 | 0.590000 | -2.915000 |
| N | 1.527000 | 0.042000 | 0.352000 |
| C | -2.626000 | -4.188000 | -0.633000 |
| H | -3.108000 | -5.104000 | -0.962000 |
| C | 3.261000 | 0.435000 | -1.260000 |
| H | 3.563000 | 0.690000 | -2.271000 |
| C | -2.226000 | 2.499000 | 1.173000 |
| C | -1.901000 | -3.400000 | -1.535000 |
| H | -1.805000 | -3.692000 | -2.578000 |
| C | -2.002000 | 1.870000 | -1.059000 |
| C | -2.712000 | -3.765000 | 0.698000 |
| H | -3.257000 | -4.343000 | 1.439000 |
| C | -2.711000 | 3.751000 | 0.812000 |
| C | -2.469000 | 3.106000 | -1.491000 |
| H | -2.548000 | 3.310000 | -2.556000 |
| C | -2.095000 | -2.576000 | 1.072000 |
| H | -2.130000 | -2.193000 | 2.088000 |
| C | -1.648000 | 0.749000 | -2.017000 |
| H | -2.463000 | 0.016000 | -2.007000 |
| H | -1.565000 | 1.130000 | -3.049000 |
| C | 4.243000 | 0.170000 | -0.292000 |
| C | -2.839000 | 4.074000 | -0.544000 |
| H | -3.208000 | 5.046000 | -0.859000 |
| C | -0.412000 | -1.379000 | -1.983000 |
| H | 0.621000 | -1.734000 | -1.883000 |
| H | -0.693000 | -1.518000 | -3.041000 |
| Cl | -0.560000 | -0.025000 | 3.124000 |
| H | -2.099000 | 2.201000 | 2.211000 |
| H | -2.984000 | 4.462000 | 1.587000 |
| O | 5.530000 | 0.249000 | -0.705000 |
| C | 6.572000 | -0.001000 | 0.239000 |
| H | 6.509000 | -1.022000 | 0.633000 |
| H | 7.503000 | 0.122000 | -0.314000 |
| H | 6.535000 | 0.720000 | 1.064000 |

**$Co^{I}$(4-MeOTPA)**

| | | | |
|---|---|---|---|
| Co | 0.469000 | -0.033000 | -0.854000 |
| N | 0.476000 | -0.090000 | 1.296000 |
| C | -3.888000 | -0.068000 | -1.227000 |
| H | -4.613000 | -0.165000 | -2.027000 |
| C | -1.927000 | 0.203000 | 0.690000 |
| N | 1.760000 | -1.624000 | -0.615000 |
| N | 1.547000 | 1.717000 | -0.540000 |
| C | 1.665000 | -2.159000 | 0.629000 |
| C | -2.544000 | 0.109000 | -1.540000 |
| H | -2.232000 | 0.151000 | -2.579000 |
| C | -0.827000 | 0.460000 | 1.711000 |
| H | -0.707000 | 1.546000 | 1.802000 |
| H | -1.134000 | 0.091000 | 2.701000 |
| N | -1.566000 | 0.243000 | -0.624000 |
| C | 3.288000 | -3.859000 | 0.093000 |
| H | 3.882000 | -4.724000 | 0.373000 |

| | | | |
|---|---|---|---|
| C | -3.238000 | 0.018000 | 1.094000 |
| H | -3.504000 | -0.017000 | 2.146000 |
| C | 1.812000 | 2.708000 | -1.413000 |
| C | 2.422000 | -3.265000 | 1.014000 |
| H | 2.333000 | -3.657000 | 2.024000 |
| C | 1.855000 | 1.915000 | 0.765000 |
| C | 3.377000 | -3.315000 | -1.190000 |
| H | 4.039000 | -3.738000 | -1.939000 |
| C | 2.382000 | 3.923000 | -1.038000 |
| C | 2.411000 | 3.110000 | 1.221000 |
| H | 2.632000 | 3.237000 | 2.277000 |
| C | 2.603000 | -2.199000 | -1.496000 |
| H | 2.655000 | -1.735000 | -2.477000 |
| C | 1.627000 | 0.740000 | 1.704000 |
| H | 2.519000 | 0.104000 | 1.670000 |
| H | 1.530000 | 1.092000 | 2.742000 |
| C | -4.253000 | -0.119000 | 0.127000 |
| C | 2.684000 | 4.132000 | 0.308000 |
| H | 3.120000 | 5.069000 | 0.642000 |
| C | 0.655000 | -1.524000 | 1.578000 |
| H | -0.319000 | -2.009000 | 1.429000 |
| H | 0.948000 | -1.713000 | 2.623000 |
| H | 1.549000 | 2.513000 | -2.449000 |
| H | 2.575000 | 4.685000 | -1.787000 |
| O | -5.498000 | -0.292000 | 0.592000 |
| C | -6.584000 | -0.440000 | -0.335000 |
| H | -6.441000 | -1.327000 | -0.961000 |
| H | -7.474000 | -0.563000 | 0.282000 |
| H | -6.686000 | 0.455000 | -0.958000 |

**$Co^{III}$-H(4-MeOTPA)**

| | | | |
|---|---|---|---|
| Co | 0.513000 | 0.003000 | -0.758000 |
| N | 0.536000 | -0.001000 | 1.308000 |
| C | -3.737000 | -0.110000 | -1.192000 |
| H | -4.441000 | -0.289000 | -1.996000 |
| C | -1.841000 | 0.346000 | 0.766000 |
| N | 1.447000 | -1.750000 | -0.530000 |
| N | 1.604000 | 1.661000 | -0.531000 |
| C | 1.415000 | -2.233000 | 0.740000 |
| C | -2.382000 | -0.122000 | -1.466000 |
| H | -2.022000 | -0.313000 | -2.470000 |
| C | -0.725000 | 0.673000 | 1.734000 |
| H | -0.546000 | 1.754000 | 1.718000 |
| H | -0.989000 | 0.402000 | 2.764000 |
| N | -1.437000 | 0.098000 | -0.519000 |
| C | 2.741000 | -4.127000 | 0.080000 |
| H | 3.250000 | -5.056000 | 0.322000 |
| C | -3.170000 | 0.359000 | 1.122000 |
| H | -3.482000 | 0.549000 | 2.145000 |
| C | 1.874000 | 2.571000 | -1.494000 |
| C | 2.061000 | -3.419000 | 1.076000 |
| H | 2.032000 | -3.786000 | 2.097000 |
| C | 2.041000 | 1.870000 | 0.739000 |
| C | 2.763000 | -3.627000 | -1.224000 |
| H | 3.280000 | -4.149000 | -2.022000 |
| C | 2.598000 | 3.727000 | -1.225000 |
| C | 2.758000 | 3.014000 | 1.075000 |
| H | 3.093000 | 3.168000 | 2.097000 |
| C | 2.107000 | -2.431000 | -1.493000 |
| H | 2.098000 | -1.995000 | -2.486000 |
| C | 1.755000 | 0.753000 | 1.719000 |
| H | 2.599000 | 0.053000 | 1.714000 |
| H | 1.657000 | 1.131000 | 2.745000 |
| C | -4.160000 | 0.133000 | 0.133000 |
| C | 3.044000 | 3.953000 | 0.079000 |
| H | 3.605000 | 4.851000 | 0.322000 |
| C | 0.586000 | -1.433000 | 1.721000 |
| H | -0.441000 | -1.818000 | 1.717000 |
| H | 0.964000 | -1.535000 | 2.746000 |
| H | 1.497000 | 2.352000 | -2.487000 |
| H | 2.800000 | 4.434000 | -2.023000 |
| O | -5.413000 | 0.166000 | 0.547000 |
| C | -6.507000 | -0.049000 | -0.378000 |
| H | -6.439000 | -1.049000 | -0.817000 |
| H | -7.407000 | 0.032000 | 0.229000 |
| H | -6.504000 | 0.724000 | -1.151000 |
| H | 0.488000 | 0.001000 | -2.259000 |

**$Co^{II}$-H(4-MeOTPA)**

| | | | |
|---|---|---|---|
| Co | -0.549000 | 0.000000 | -1.095000 |
| N | -0.519000 | -0.000000 | 1.292000 |
| C | 3.823000 | 0.094000 | -1.152000 |
| H | 4.551000 | 0.278000 | -1.932000 |
| C | 1.856000 | -0.368000 | 0.721000 |
| N | -1.470000 | 1.835000 | -0.510000 |
| N | -1.679000 | -1.715000 | -0.512000 |
| C | -1.390000 | 2.253000 | 0.770000 |
| C | 2.468000 | 0.098000 | -1.466000 |

| | | | |
|---|---|---|---|
| H | 2.129000 | 0.281000 | -2.482000 |
| C | 0.718000 | -0.703000 | 1.668000 |
| H | 0.522000 | -1.780000 | 1.597000 |
| H | 1.009000 | -0.500000 | 2.710000 |
| N | 1.499000 | -0.123000 | -0.562000 |
| C | -2.741000 | 4.180000 | 0.270000 |
| H | -3.240000 | 5.093000 | 0.580000 |
| C | 3.178000 | -0.377000 | 1.130000 |
| H | 3.451000 | -0.566000 | 2.164000 |
| C | -1.989000 | -2.665000 | -1.413000 |
| C | -2.022000 | 3.421000 | 1.196000 |
| H | -1.950000 | 3.732000 | 2.235000 |
| C | -2.049000 | -1.873000 | 0.775000 |
| C | -2.812000 | 3.746000 | -1.055000 |
| H | -3.360000 | 4.307000 | -1.806000 |
| C | -2.682000 | -3.823000 | -1.064000 |
| C | -2.733000 | -3.012000 | 1.203000 |
| H | -3.010000 | -3.121000 | 2.247000 |
| C | -2.162000 | 2.564000 | -1.403000 |
| H | -2.179000 | 2.171000 | -2.416000 |
| C | -1.735000 | -0.717000 | 1.707000 |
| H | -2.571000 | -0.008000 | 1.665000 |
| H | -1.672000 | -1.070000 | 2.749000 |
| C | 4.194000 | -0.145000 | 0.182000 |
| C | -3.056000 | -3.999000 | 0.269000 |
| H | -3.590000 | -4.892000 | 0.580000 |
| C | -0.524000 | 1.415000 | 1.693000 |
| H | 0.507000 | 1.784000 | 1.627000 |
| H | -0.839000 | 1.547000 | 2.740000 |
| H | -1.667000 | -2.468000 | -2.431000 |
| H | -2.914000 | -4.565000 | -1.820000 |
| O | 5.452000 | -0.172000 | 0.642000 |
| C | 6.543000 | 0.053000 | -0.264000 |
| H | 6.475000 | 1.050000 | -0.711000 |
| H | 7.443000 | -0.018000 | 0.347000 |
| H | 6.563000 | -0.716000 | -1.044000 |
| H | -0.585000 | 0.006000 | -2.735000 |

**$Co^{II}$(4-MeOTPA)**

| | | | |
|---|---|---|---|
| Co | -0.529000 | -0.003000 | -0.824000 |
| N | -0.538000 | -0.002000 | 1.308000 |
| C | 3.780000 | 0.078000 | -1.203000 |
| H | 4.497000 | 0.252000 | -1.996000 |
| C | 1.844000 | -0.357000 | 0.723000 |
| N | -1.442000 | 1.800000 | -0.558000 |
| N | -1.657000 | -1.679000 | -0.561000 |
| C | -1.402000 | 2.247000 | 0.724000 |
| C | 2.428000 | 0.090000 | -1.495000 |
| H | 2.093000 | 0.278000 | -2.511000 |
| C | 0.726000 | -0.678000 | 1.700000 |
| H | 0.544000 | -1.759000 | 1.680000 |
| H | 1.017000 | -0.421000 | 2.727000 |
| N | 1.462000 | -0.123000 | -0.569000 |
| C | -2.708000 | 4.179000 | 0.122000 |
| H | -3.205000 | 5.106000 | 0.393000 |
| C | 3.168000 | -0.369000 | 1.102000 |
| H | 3.461000 | -0.548000 | 2.132000 |
| C | -1.960000 | -2.604000 | -1.501000 |
| C | -2.035000 | 3.432000 | 1.093000 |
| H | -1.999000 | 3.769000 | 2.125000 |
| C | -2.059000 | -1.873000 | 0.721000 |
| C | -2.740000 | 3.716000 | -1.196000 |
| H | -3.255000 | 4.265000 | -1.977000 |
| C | -2.681000 | -3.754000 | -1.203000 |
| C | -2.771000 | -3.011000 | 1.090000 |
| H | -3.075000 | -3.152000 | 2.123000 |
| C | -2.100000 | 2.519000 | -1.495000 |
| H | -2.107000 | 2.116000 | -2.503000 |
| C | -1.752000 | -0.758000 | 1.706000 |
| H | -2.595000 | -0.056000 | 1.710000 |
| H | -1.661000 | -1.153000 | 2.726000 |
| C | 4.177000 | -0.154000 | 0.132000 |
| C | -3.091000 | -3.962000 | 0.116000 |
| H | -3.649000 | -4.854000 | 0.386000 |
| C | -0.584000 | 1.427000 | 1.705000 |
| H | 0.445000 | 1.807000 | 1.705000 |
| H | -0.967000 | 1.547000 | 2.727000 |
| H | -1.610000 | -2.406000 | -2.510000 |
| H | -2.907000 | -4.469000 | -1.986000 |
| O | 5.424000 | -0.187000 | 0.569000 |
| C | 6.533000 | 0.017000 | -0.339000 |
| H | 6.476000 | 1.013000 | -0.787000 |
| H | 7.423000 | -0.062000 | 0.284000 |
| H | 6.541000 | -0.763000 | -1.106000 |

**C5**

**$Co^{II}$(4-MeTPA)Cl (High-spin state)**

| | | | |
|---|---|---|---|
| Co | 0.292000 | -0.000000 | 0.719000 |

| | | | |
|---|---|---|---|
| Cl | 0.457000 | 0.001000 | 3.047000 |
| N | -1.765000 | -0.042000 | 0.403000 |
| N | 0.144000 | 0.001000 | -1.558000 |
| N | 1.324000 | -1.742000 | 0.200000 |
| N | 1.250000 | 1.784000 | 0.204000 |
| C | 2.010000 | 2.475000 | 1.090000 |
| H | 2.053000 | 2.067000 | 2.093000 |
| C | 2.679000 | 3.642000 | 0.718000 |
| H | 3.278000 | 4.174000 | 1.445000 |
| C | 2.562000 | 4.098000 | -0.600000 |
| H | 3.076000 | 4.998000 | -0.917000 |
| C | 1.773000 | 3.381000 | -1.507000 |
| H | 1.664000 | 3.715000 | -2.533000 |
| C | 1.118000 | 2.227000 | -1.074000 |
| C | 0.178000 | 1.434000 | -1.957000 |
| H | 0.446000 | 1.555000 | -3.017000 |
| H | -0.837000 | 1.830000 | -1.836000 |
| C | 1.327000 | -0.767000 | -2.034000 |
| H | 2.182000 | -0.080000 | -2.036000 |
| H | 1.195000 | -1.119000 | -3.067000 |
| C | 1.639000 | -1.924000 | -1.109000 |
| C | 2.270000 | -3.092000 | -1.543000 |
| H | 2.506000 | -3.225000 | -2.592000 |
| C | 2.597000 | -4.078000 | -0.604000 |
| H | 3.089000 | -4.990000 | -0.921000 |
| C | 2.282000 | -3.874000 | 0.744000 |
| H | 2.524000 | -4.614000 | 1.496000 |
| C | 1.640000 | -2.692000 | 1.116000 |
| H | 1.370000 | -2.466000 | 2.140000 |
| C | -1.151000 | -0.664000 | -1.870000 |
| H | -0.979000 | -1.747000 | -1.827000 |
| H | -1.491000 | -0.432000 | -2.889000 |
| C | -2.212000 | -0.300000 | -0.853000 |
| C | -3.573000 | -0.288000 | -1.155000 |
| H | -3.901000 | -0.489000 | -2.169000 |
| C | -4.519000 | -0.023000 | -0.148000 |
| C | -4.031000 | 0.228000 | 1.148000 |
| H | -4.715000 | 0.435000 | 1.963000 |
| C | -2.661000 | 0.215000 | 1.392000 |
| H | -2.241000 | 0.399000 | 2.373000 |
| C | -5.996000 | -0.004000 | -0.442000 |
| H | -6.530000 | -0.720000 | 0.194000 |
| H | -6.205000 | -0.254000 | -1.484000 |
| H | -6.423000 | 0.985000 | -0.237000 |

**$Co^{II}$(4-MeTPA)Cl (Low-spin state)**

| | | | |
|---|---|---|---|
| Co | 0.174000 | -0.274000 | 0.546000 |
| Cl | 0.224000 | -0.437000 | 2.786000 |
| N | -1.826000 | -0.285000 | 0.405000 |
| N | 0.047000 | -0.167000 | -1.465000 |
| N | 1.950000 | -1.153000 | 0.220000 |
| N | 0.733000 | 1.782000 | 0.299000 |
| C | 1.325000 | 2.589000 | 1.192000 |
| H | 1.438000 | 2.180000 | 2.192000 |
| C | 1.761000 | 3.872000 | 0.855000 |
| H | 2.233000 | 4.499000 | 1.605000 |
| C | 1.583000 | 4.318000 | -0.455000 |
| H | 1.919000 | 5.307000 | -0.753000 |
| C | 0.965000 | 3.475000 | -1.384000 |
| H | 0.807000 | 3.795000 | -2.410000 |
| C | 0.546000 | 2.214000 | -0.961000 |
| C | -0.226000 | 1.257000 | -1.845000 |
| H | -0.010000 | 1.416000 | -2.909000 |
| H | -1.296000 | 1.438000 | -1.701000 |
| C | 1.323000 | -0.647000 | -2.079000 |
| H | 1.876000 | 0.231000 | -2.433000 |
| H | 1.115000 | -1.263000 | -2.963000 |
| C | 2.201000 | -1.382000 | -1.090000 |
| C | 3.259000 | -2.188000 | -1.507000 |
| H | 3.426000 | -2.364000 | -2.566000 |
| C | 4.099000 | -2.753000 | -0.546000 |
| H | 4.932000 | -3.382000 | -0.847000 |
| C | 3.848000 | -2.498000 | 0.803000 |
| H | 4.474000 | -2.917000 | 1.584000 |
| C | 2.758000 | -1.704000 | 1.148000 |
| H | 2.491000 | -1.496000 | 2.179000 |
| C | -1.124000 | -1.033000 | -1.784000 |
| H | -0.803000 | -2.076000 | -1.669000 |
| H | -1.451000 | -0.899000 | -2.825000 |
| C | -2.241000 | -0.728000 | -0.804000 |
| C | -3.587000 | -0.913000 | -1.101000 |
| H | -3.881000 | -1.261000 | -2.088000 |
| C | -4.561000 | -0.651000 | -0.123000 |
| C | -4.107000 | -0.195000 | 1.123000 |
| H | -4.810000 | 0.028000 | 1.921000 |
| C | -2.746000 | -0.027000 | 1.353000 |
| H | -2.354000 | 0.303000 | 2.309000 |
| C | -6.026000 | -0.867000 | -0.393000 |

| | | | |
|---|---|---|---|
| H | -6.368000 | -1.794000 | 0.085000 |
| H | -6.234000 | -0.947000 | -1.464000 |
| H | -6.629000 | -0.050000 | 0.018000 |

**$Co^{I}$(4-MeTPA)Cl**

| | | | |
|---|---|---|---|
| Co | -0.349000 | 0.025000 | 0.723000 |
| Cl | -0.430000 | -0.019000 | 3.124000 |
| N | 1.757000 | -0.035000 | 0.415000 |
| N | -0.137000 | 0.038000 | -1.583000 |
| N | -1.599000 | 1.591000 | 0.228000 |
| N | -1.181000 | -1.800000 | 0.175000 |
| C | -1.911000 | -2.553000 | 1.027000 |
| H | -1.959000 | -2.174000 | 2.045000 |
| C | -2.550000 | -3.724000 | 0.632000 |
| H | -3.125000 | -4.293000 | 1.357000 |
| C | -2.445000 | -4.140000 | -0.700000 |
| H | -2.942000 | -5.042000 | -1.045000 |
| C | -1.682000 | -3.365000 | -1.581000 |
| H | -1.571000 | -3.653000 | -2.624000 |
| C | -1.057000 | -2.213000 | -1.108000 |
| C | -0.136000 | -1.376000 | -1.982000 |
| H | -0.393000 | -1.505000 | -3.047000 |
| H | 0.887000 | -1.752000 | -1.856000 |
| C | -1.322000 | 0.779000 | -2.044000 |
| H | -2.155000 | 0.066000 | -2.061000 |
| H | -1.201000 | 1.160000 | -3.072000 |
| C | -1.679000 | 1.907000 | -1.095000 |
| C | -2.102000 | 3.155000 | -1.538000 |
| H | -2.145000 | 3.362000 | -2.605000 |
| C | -2.476000 | 4.129000 | -0.601000 |
| H | -2.811000 | 5.110000 | -0.925000 |
| C | -2.396000 | 3.804000 | 0.758000 |
| H | -2.673000 | 4.521000 | 1.526000 |
| C | -1.953000 | 2.538000 | 1.131000 |
| H | -1.863000 | 2.235000 | 2.171000 |
| C | 1.136000 | 0.720000 | -1.824000 |
| H | 0.950000 | 1.798000 | -1.722000 |
| H | 1.513000 | 0.560000 | -2.850000 |
| C | 2.198000 | 0.321000 | -0.809000 |
| C | 3.559000 | 0.384000 | -1.114000 |
| H | 3.872000 | 0.661000 | -2.118000 |
| C | 4.514000 | 0.100000 | -0.130000 |
| C | 4.035000 | -0.245000 | 1.144000 |
| H | 4.723000 | -0.474000 | 1.953000 |
| C | 2.665000 | -0.301000 | 1.374000 |
| H | 2.245000 | -0.554000 | 2.344000 |
| C | 5.993000 | 0.167000 | -0.419000 |
| H | 6.475000 | 0.947000 | 0.184000 |
| H | 6.189000 | 0.388000 | -1.473000 |
| H | 6.487000 | -0.781000 | -0.172000 |

**$Co^{I}$(4-MeTPA)**

| | | | |
|---|---|---|---|
| Co | 0.235000 | -0.050000 | -0.867000 |
| N | -1.816000 | 0.034000 | -0.688000 |
| N | 0.195000 | -0.118000 | 1.283000 |
| N | 1.068000 | 1.826000 | -0.514000 |
| N | 1.690000 | -1.487000 | -0.599000 |
| C | 2.610000 | -1.963000 | -1.463000 |
| H | 2.638000 | -1.485000 | -2.438000 |
| C | 3.486000 | -2.997000 | -1.146000 |
| H | 4.206000 | -3.342000 | -1.881000 |
| C | 3.419000 | -3.561000 | 0.129000 |
| H | 4.091000 | -4.364000 | 0.417000 |
| C | 2.475000 | -3.069000 | 1.033000 |
| H | 2.401000 | -3.480000 | 2.036000 |
| C | 1.618000 | -2.042000 | 0.637000 |
| C | 0.526000 | -1.524000 | 1.567000 |
| H | 0.819000 | -1.682000 | 2.617000 |
| H | -0.385000 | -2.114000 | 1.401000 |
| C | 1.239000 | 0.832000 | 1.716000 |
| H | 2.198000 | 0.303000 | 1.682000 |
| H | 1.092000 | 1.154000 | 2.758000 |
| C | 1.336000 | 2.040000 | 0.797000 |
| C | 1.742000 | 3.285000 | 1.275000 |
| H | 1.935000 | 3.421000 | 2.336000 |
| C | 1.902000 | 4.346000 | 0.379000 |
| H | 2.220000 | 5.322000 | 0.732000 |
| C | 1.640000 | 4.123000 | -0.973000 |
| H | 1.748000 | 4.913000 | -1.708000 |
| C | 1.220000 | 2.855000 | -1.371000 |
| H | 0.992000 | 2.646000 | -2.412000 |
| C | -1.170000 | 0.285000 | 1.668000 |
| H | -1.163000 | 1.374000 | 1.792000 |
| H | -1.466000 | -0.142000 | 2.638000 |
| C | -2.211000 | -0.049000 | 0.607000 |
| C | -3.526000 | -0.344000 | 0.961000 |
| H | -3.795000 | -0.406000 | 2.013000 |
| C | -4.501000 | -0.554000 | -0.025000 |

| | | | |
|---|---|---|---|
| C | -4.079000 | -0.457000 | -1.359000 |
| H | -4.779000 | -0.607000 | -2.177000 |
| C | -2.749000 | -0.170000 | -1.642000 |
| H | -2.404000 | -0.093000 | -2.669000 |
| C | -5.931000 | -0.870000 | 0.326000 |
| H | -6.606000 | -0.098000 | -0.065000 |
| H | -6.078000 | -0.933000 | 1.407000 |
| H | -6.242000 | -1.823000 | -0.118000 |

**$Co^{III}$-H(4-MeTPA)**

| | | | |
|---|---|---|---|
| Co | 0.284000 | 0.001000 | -0.773000 |
| N | -1.689000 | 0.029000 | -0.593000 |
| N | 0.229000 | -0.001000 | 1.292000 |
| N | 1.300000 | 1.697000 | -0.508000 |
| N | 1.253000 | -1.723000 | -0.510000 |
| C | 1.963000 | -2.387000 | -1.450000 |
| H | 1.977000 | -1.952000 | -2.443000 |
| C | 2.641000 | -3.565000 | -1.158000 |
| H | 3.199000 | -4.073000 | -1.937000 |
| C | 2.590000 | -4.065000 | 0.145000 |
| H | 3.114000 | -4.980000 | 0.405000 |
| C | 1.858000 | -3.375000 | 1.117000 |
| H | 1.804000 | -3.743000 | 2.138000 |
| C | 1.192000 | -2.207000 | 0.759000 |
| C | 0.308000 | -1.431000 | 1.710000 |
| H | 0.654000 | -1.519000 | 2.748000 |
| H | -0.706000 | -1.846000 | 1.673000 |
| C | 1.410000 | 0.790000 | 1.745000 |
| H | 2.276000 | 0.117000 | 1.763000 |
| H | 1.268000 | 1.161000 | 2.768000 |
| C | 1.689000 | 1.919000 | 0.776000 |
| C | 2.353000 | 3.087000 | 1.137000 |
| H | 2.648000 | 3.251000 | 2.169000 |
| C | 2.636000 | 4.039000 | 0.151000 |
| H | 3.156000 | 4.956000 | 0.412000 |
| C | 2.241000 | 3.799000 | -1.167000 |
| H | 2.444000 | 4.514000 | -1.958000 |
| C | 1.569000 | 2.618000 | -1.461000 |
| H | 1.233000 | 2.388000 | -2.466000 |
| C | -1.066000 | 0.634000 | 1.674000 |
| H | -0.918000 | 1.721000 | 1.673000 |
| H | -1.358000 | 0.350000 | 2.693000 |
| C | -2.137000 | 0.282000 | 0.665000 |
| C | -3.492000 | 0.276000 | 0.968000 |
| H | -3.816000 | 0.474000 | 1.986000 |
| C | -4.443000 | 0.021000 | -0.037000 |
| C | -3.953000 | -0.231000 | -1.332000 |
| H | -4.635000 | -0.436000 | -2.152000 |
| C | -2.590000 | -0.224000 | -1.574000 |
| H | -2.187000 | -0.422000 | -2.561000 |
| C | -5.916000 | 0.013000 | 0.253000 |
| H | -6.429000 | 0.770000 | -0.353000 |
| H | -6.128000 | 0.213000 | 1.306000 |
| H | -6.356000 | -0.956000 | -0.012000 |
| H | 0.318000 | 0.001000 | -2.275000 |

**$Co^{II}$-H(4-MeTPA)**

| | | | |
|---|---|---|---|
| Co | -0.312000 | -0.000000 | -1.103000 |
| N | -0.216000 | 0.002000 | 1.281000 |
| C | 4.051000 | 0.215000 | -1.271000 |
| H | 4.764000 | 0.420000 | -2.064000 |
| C | 2.153000 | -0.298000 | 0.641000 |
| N | -1.277000 | 1.802000 | -0.495000 |
| N | -1.365000 | -1.752000 | -0.491000 |
| C | -1.176000 | 2.224000 | 0.782000 |
| C | 2.692000 | 0.196000 | -1.559000 |
| H | 2.314000 | 0.378000 | -2.562000 |
| C | 1.055000 | -0.657000 | 1.626000 |
| H | 0.891000 | -1.741000 | 1.576000 |
| H | 1.370000 | -0.432000 | 2.656000 |
| N | 1.757000 | -0.053000 | -0.623000 |
| C | -2.604000 | 4.104000 | 0.319000 |
| H | -3.125000 | 5.001000 | 0.643000 |
| C | 3.499000 | -0.283000 | 1.005000 |
| H | 3.780000 | -0.476000 | 2.037000 |
| C | -1.667000 | -2.712000 | -1.383000 |
| C | -1.835000 | 3.371000 | 1.226000 |
| H | -1.746000 | 3.684000 | 2.262000 |
| C | -1.695000 | -1.922000 | 0.805000 |
| C | -2.696000 | 3.668000 | -1.003000 |
| H | -3.282000 | 4.209000 | -1.739000 |
| C | -2.311000 | -3.893000 | -1.016000 |
| C | -2.330000 | -3.082000 | 1.251000 |
| H | -2.576000 | -3.199000 | 2.303000 |
| C | -2.017000 | 2.507000 | -1.369000 |
| H | -2.047000 | 2.114000 | -2.381000 |
| C | -1.396000 | -0.755000 | 1.729000 |
| H | -2.255000 | -0.073000 | 1.708000 |

| | | | |
|---|---|---|---|
| H | -1.294000 | -1.103000 | 2.769000 |
| C | 4.486000 | -0.025000 | 0.042000 |
| C | -2.644000 | -4.080000 | 0.326000 |
| H | -3.140000 | -4.990000 | 0.651000 |
| C | -0.256000 | 1.417000 | 1.681000 |
| H | 0.759000 | 1.821000 | 1.584000 |
| H | -0.545000 | 1.540000 | 2.737000 |
| H | -1.379000 | -2.506000 | -2.410000 |
| H | -2.538000 | -4.643000 | -1.766000 |
| H | -0.390000 | -0.000000 | -2.741000 |
| C | 5.950000 | 0.001000 | 0.396000 |
| H | 6.373000 | 0.998000 | 0.223000 |
| H | 6.119000 | -0.262000 | 1.444000 |
| H | 6.514000 | -0.701000 | -0.229000 |

**$Co^{II}$(4-MeTPA)**

| | | | |
|---|---|---|---|
| Co | -0.294000 | -0.001000 | -0.838000 |
| N | -0.229000 | -0.002000 | 1.293000 |
| C | 4.003000 | 0.194000 | -1.334000 |
| H | 4.701000 | 0.390000 | -2.143000 |
| C | 2.142000 | -0.293000 | 0.631000 |
| N | -1.250000 | 1.771000 | -0.540000 |
| N | -1.348000 | -1.717000 | -0.539000 |
| C | -1.184000 | 2.220000 | 0.740000 |
| C | 2.644000 | 0.189000 | -1.597000 |
| H | 2.268000 | 0.383000 | -2.598000 |
| C | 1.067000 | -0.635000 | 1.647000 |
| H | 0.917000 | -1.722000 | 1.646000 |
| H | 1.383000 | -0.358000 | 2.661000 |
| N | 1.719000 | -0.053000 | -0.636000 |
| C | -2.566000 | 4.110000 | 0.181000 |
| H | -3.082000 | 5.023000 | 0.468000 |
| C | 3.493000 | -0.287000 | 0.959000 |
| H | 3.795000 | -0.474000 | 1.986000 |
| C | -1.646000 | -2.652000 | -1.469000 |
| C | -1.840000 | 3.385000 | 1.130000 |
| H | -1.782000 | 3.723000 | 2.160000 |
| C | -1.703000 | -1.923000 | 0.755000 |
| C | -2.626000 | 3.646000 | -1.136000 |
| H | -3.181000 | 4.179000 | -1.900000 |
| C | -2.316000 | -3.827000 | -1.149000 |
| C | -2.363000 | -3.085000 | 1.146000 |
| H | -2.631000 | -3.235000 | 2.187000 |
| C | -1.959000 | 2.470000 | -1.456000 |
| H | -1.986000 | 2.066000 | -2.464000 |
| C | -1.407000 | -0.795000 | 1.728000 |
| H | -2.272000 | -0.121000 | 1.754000 |
| H | -1.275000 | -1.183000 | 2.747000 |
| C | 4.465000 | -0.046000 | -0.026000 |
| C | -2.677000 | -4.048000 | 0.183000 |
| H | -3.194000 | -4.959000 | 0.469000 |
| C | -0.309000 | 1.426000 | 1.694000 |
| H | 0.707000 | 1.839000 | 1.662000 |
| H | -0.663000 | 1.533000 | 2.727000 |
| H | -1.335000 | -2.444000 | -2.489000 |
| H | -2.540000 | -4.551000 | -1.925000 |
| C | 5.932000 | -0.041000 | 0.294000 |
| H | 6.454000 | -0.811000 | -0.287000 |
| H | 6.384000 | 0.921000 | 0.022000 |
| H | 6.121000 | -0.224000 | 1.354000 |