Supplementary Information for

Asymmetric hydrogenation of ketones with planar chiral manganese(I) complexes

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Experimental Details

General methods

All reactions were carried out using conventional Schlenk tube techniques under an inert atmosphere of argon, unless otherwise stated. (Dimethylaminomethyl)ferrocene (Strem Chemicals), 2-(methylamino)methylpyridine (Sigma-Aldrich), 6-methoxy-2-pyridinemethanamine (BLDPharm), 2-picolylamine and methyl 2-bromobenzoate (TCI Chemicals) were used as received. Rac-, (*S*)- and (*R*)-ferrocenyl thiophosphinoalcohol **1** were prepared according to previously reported procedures.[1] Thin-layer chromatography (TLC) and column chromatography were carried out on Merck Kieselgel 60F254 recoated aluminum plates and Merck Kieselgel 60, respectively. Solvents for all syntheses were either dried by standard methods and distilled under argon before use, or purified on an Innovative PURESOLV Solvent Purification System equipped with 4 Å MS columns, unless otherwise stated. NMR analyses were performed on Bruker AV400 or AV300 spectrometers. The spectra were referenced internally using the residual signals of the deuterated solvent for ^{1}H and ^{13}C, and externally using 85% H_3PO_4 for ^{31}P. Chemical shifts (δ) for all nuclei and coupling constants are given in ppm and Hertz, respectively. Peaks are labelled as singlet (s), doublet (d), triplet (t), multiplet (m) and broad (br). Mass spectra analyses [GCT 1er Waters for DCI, CH_4; UPLC Xevo G2 Q TOF (waters) for ES^+] were performed by the 'Service Commun de Spectrométrie de masse' of the ICT-Université de Toulouse (France). The chromatographic analyses were obtained on a Shimadzu GC2010 Pro equipped with a chiral Supelco BETA DEX 225 column.

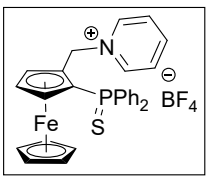
X-ray structural analyses details

Data were collected on a Rigaku XtaLAB Synergy Dualflex diffractometer using a PhotonJet X-ray source (CuK_α, λ = 1.54184 Å). An Oxford Cryosystems Cryostream cooling device was used to collect data at low temperature (100(2) K). Omega scans were performed for data collection. Absorption corrections were applied [2,3] and the structures were solved by intrinsic phasing method (ShelXT).[4] All non-hydrogen atoms were refined anisotropically by means of least-squares procedures on F^2 with ShelXL.[5] All the hydrogen atoms were refined isotropically at calculated positions using a riding model, except for the hydrogen atom attached to nitrogen, which was located on difference Fourier maps and refined freely. For complex **5a**, the absolute configuration was determined by refining the Flack parameter.[6] For **5b**, the SQUEEZE [7] tool in PLATON was used to remove the electron density contribution of the highly disordered dichloromethane molecules from the model. Crystal data and refinement parameters, bond distances, bond angles and hydrogen bond parameters are provided here.

Deposition Numbers CCDC 2490601-2490602 (for **5a** and **5b**) contain the supplementary crystallographic data for this paper. These data are provided free of charge by the joint Cambridge Crystallographic Data Centre and Fachinformationszentrum Karlsruhe Access Structures service.

Syntheses

Synthesis of pyridinium salt 2



In a dry Schlenk tube under argon, (2-diphenylthiophosphinoferrocenyl) methanol **1** (200 mg, 0.46 mmol, 1 equiv.) was dissolved in dry dichloromethane (2mL). $HBF_4.OEt_2$ (0.2 mL, 1.38 mmol, 54% wt.

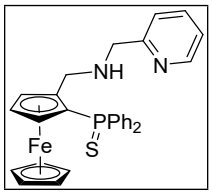
in Et_2O, 3 equiv.) was added at room temperature and the mixture was stirred for 5 min. Pyridine (0.22 mL, 2.77 mmol, 6 equiv.) was added and the mixture was stirred for 10 minutes. It was then washed successively with 1M aq. HCl, H_2O and sat. aq. $NaHCO_3$, dried (Na_2SO_4) and filtered. Dichloromethane was concentrated to the minimum and an excess of diethyl ether was added to precipitate the product. It was filtered, washed with Et_2O and dried in vacuo to give a yellow powder (220 mg, 82% yield).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.78 (2H, m, Py), 8.06 (1H, m, Py), 7.75-7.70 (2H, m, Ph), 7.60-7.13 (10H, m, 8H Ph + 2H Py), 6.74 (1H, m (AB system), CH_2N), 5.75 (1H, m (AB system), CH_2N), 5.36 (m, 1H, *subst*. Cp), 4.60 (m, 1H, *subst*. Cp), 4.49 (s, 5H, Cp), 3.87 (m, 1H, subst Cp).
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ 145.22 (s, Py), 144.06 (s, Py), 133.83 (d, J_{PC} = 85 Hz, *quat*. Ph), 132.07 (d, J_{PC} = 3.1 Hz, Ph), 131.89-131.77 (2 x Ph), 131.48 (d, J_{PC} = 90 Hz, *quat.* Ph), 131.32 (d, J_{PC} = 10.5 Hz, Ph), 128.71 (d, J_{PC} = 12.3 Hz, Ph), 128.43 (d, J_{PC} = 12.7 Hz, Ph), 127.53 (s, Py), 82.45 (d, J_{PC} = 12.1 Hz, *quat.* Cp), 77.59 (d, J_{PC} = 8.6 Hz, *subst.* Cp), 76.9 (*subst.* Cp, under $CDCl_3$), 75.01 (d, J_{PC} = 93.6Hz, *quat.* Cp), 71.7 (*subst.* Cp, under Cp), 71.67 (s, Cp), 59.71 (s, CH_2Py).
^{31}P{^{1}H} NMR (162 MHz, $CDCl_3$): δ 40.53 (s, PPh_2).

Synthesis of thiophosphines 3a-b

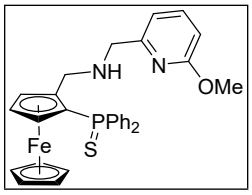
In a dry Schlenk tube under argon, pyridinium salt **2** (220 mg, 0.38 mmol, 1 equiv.), K_2CO_3 (127 mg, 0.92 mmol, 2 equiv.) and either 2-picolylamine (0.29 mL, 2.76 mmol, 6 equiv., for **3a**) or 6-methoxy-2-pyridinemethanamine (380 mg, 1.85 mmol, 4 equiv., for **3b**) were added, followed by dry, degassed acetonitrile (3 mL). The reaction mixture was heated to reflux for 24 hours. The resulting dark orange solution was concentrated *in vacuo* and the residue was purified by column chromatography on silicagel (eluent: diethyl ether + 1.5% NEt_3).

1-(diphenylthiophosphino)-2-[[(2-pyridinylmethyl)amino]methyl]ferrocene 3a



Yellow-orange powder (165 mg, 68% yield from **1**).
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.48 (1H, app. d, *J*= 4 Hz, Py), 7.86-7.79 (2H, m, Ph), 7.72-7.64 (2H, m, Ph), 7.58-7.45 (4H, m, Ph), 7.40-7.32 (3H, m, 2H Ph + 1H Py); 7.13-7.11 (1H, m, Py), 7.05 (1H, app. d, *J* = 7.8 Hz, Py), 4.65 (m, 1H, *subst*. Cp), 4.34 (s, 5H, Cp), 4.34-4.27 (2H, m, 1H CH_2Cp + 1H *subst.* Cp), 3.79 (1H, d (AB system), *J* = 14.6 Hz, CH_2Py), 3.79 (m, 1H, subst Cp), 3.70 (1H, d (AB system), *J* = 14.6 Hz, CH_2Py), 3.67 (1H, d (AB system), *J* = 13.4 Hz, CH_2Cp).
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ 159.09 (s, *quat.* Py), 148.96 (s, Py), 136.36 (s, Py), 134.87 (d, J_{PC} = 86 Hz, *quat*. Ph), 133.31 (d, J_{PC} = 86 Hz, *quat.* Ph), 132.02 (d, J_{PC} = 11.0 Hz, Ph), 131.82 (d, J_{PC} = 10.6 Hz, Ph), 131.33 (d, J_{PC} = 3.1Hz, Ph), 131.24 (d, J_{PC} = 3.1 Hz, Ph), 128.35 (d, J_{PC} = 12.5 Hz, Ph), 128.08 (d, J_{PC} = 12.5 Hz, Ph), 121.80 (s, Py), 121.75 (s, Py), 90.34 (m, *quat.* Cp), 74.64 (d, J_{PC} = 12.2 Hz, *subst.* Cp), ca. 74.6 (d, *subst.* Cp, under 74.64 signal), 74.26 (d, J_{PC} = 95.1Hz, *quat.* Cp), 70.66 (s, Cp); 69.09 (d, J_{PC} = 10.6 Hz, *subst.* Cp), 53.76 (s, CH_2Py), 46.49 (s, CH_2Cp).
^{31}P{^{1}H} NMR (162 MHz, $CDCl_3$): δ 41.32 (s, PPh_2).
HRMS (DCI-CH_4): m/z $[M]^+$ (100%, calcd. for $C_{29}H_{27}FeN_2PS$ 522.0979, found 522.0956).

1-(diphenylthiophosphino)-2-[[(2-4-(methoxyl)pyridinylmethyl)amino]methyl]ferrocene 3b



Yellow-orange powder (138 mg, 54% yield from **1**).

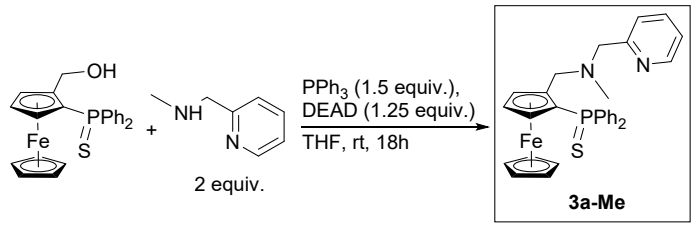
^{1}H NMR (400 MHz, $CDCl_3$): *δ* 7.85-7.80 (2H, m, Ph), 7.69-7.64 (2H, m, Ph), 7.54-7.32 (7H, m, Py + 6xPh), 6.62 (1H, app. d, *J* = 7.3 Hz, Py); 6.56 (1H, app. d, *J* = 8.2 Hz, Py), 4.68 (1H, m, *subst*. Cp), 4.34 (5H, s, Cp), 4.35-4.31 (1H, m, *subst*. Cp), 4.14 (1H, d (AB system), *J* = 13.5 Hz, CH_2Cp), 3.87 (3H, s, CH_3O), 3.80-3.79 (1H, m, *subst*. Cp), 3.73 (1H, d (AB system), *J* = 13.5 Hz, CH_2Cp), 3.68 (1H, d (AB system), *J* = 14.3 Hz, CH_2Py), 3.62 (1H, d (AB system), *J* = 14.3 Hz, CH_2Py).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ 163.60 (s, *quat.* Py), 157.27 (s, *quat.* Py), 138.70 (s, Py), 134.94 (d, J_{PC} = 86.4 Hz, *quat*. Ph), 133.53 (d, J_{PC} = 85.9 Hz, *quat.* Ph), 132.03 (d, J_{PC} = 10.8 Hz, Ph), 131.80 (d, J_{PC} = 10.6 Hz, Ph), 131.27 (d, J_{PC} = 3.1Hz, Ph), 131.19 (d, J_{PC} = 2.9 Hz, Ph), 128.28 (d, J_{PC} = 12.4 Hz, Ph), 128.04 (d, J_{PC} = 12.4 Hz, Ph), 114.25 (s, Py), 108.47 (s, Py), 91.15 (d, J_{PC} = 12.5 Hz, *quat.* Cp), 74.57 (d, J_{PC} = 12.7 Hz, *subst.* Cp), 74.20 (d, J_{PC} = 95.1Hz, *quat.* Cp), 74.11 (d, J_{PC} = 9.8 Hz, *subst.* Cp), 70.58 (s, Cp), 68.91 (d, J_{PC} = 10.4 Hz, *subst.* Cp), 54.01 (s, CH_2Py), 53.24 (s, OMe), 46.00 (s, CH_2Cp).

^{31}P{^{1}H} NMR (162 MHz, $CDCl_3$): *δ* 41.43 (s, PPh_2).

HRMS (ESI, pos.): m/z $[M+H]^+$ (100%, calcd. for $C_{30}H_{30}FeN_2OPS$ 553.1166, found 553.1172).

Synthesis of thiophosphine 3a-Me



1-(diphenylthiophosphino)-2-[[methyl(2-pyridinylmethyl)amino]methyl]ferrocene 3a-Me

In a dry Schlenk tube under argon, a solution of racemic (2-diphenylthiophosphinoferrocenyl) methanol (500 mg, 1.16 mmol, 1 equiv.) was dissolved in dry THF (30 mL). PPh_3 (460 mg, 1.74 mmol, 1.5 equiv.) was added, followed by 2-(N-methylaminomethyl)pyridine (290 μL, 2.32 mmol, 2 equiv.). Finally, a solution of diethylazadicarboxylate (DEAD) in hexane (660 μL, 1.45 mmol, 1.25 equiv.) was slowly added and the reaction mixture was stirred at room temperature for 18h under argon. The solvent was evaporated *in vacuo* and the crude reddish-orange oil was purified by column chromatography on silicagel (eluent: *n*-hexane/EtOAc 1:1 + 1% NEt_3). **3a-Me** was obtained as a yellow-orange solid (300 mg, 49% yield).

^{1}H NMR (400 MHz, $CDCl_3$): *δ* 8.41-8.39 (1H, m, Py), 7.85-7.80 (2H, m, Ph), 7.71-7.65 (2H, m, Ph), 7.53-7.42 (4H, m, Ph), 7.37-7.32 (2H, m, Ph), 7.28-7.24 (1H, m, Py), 7.02-6.99 (1H, m, Py), 6.48 (1H, app. d, *J* = 7.9 Hz, Py), 4.61-4.60 (1H, m, *subst.* Cp), 4.52 (1H, d (AB system), *J* = 12.8 Hz, CH_2Cp), 4.30 (5H, s, Cp), 4.33-4.28 (1H, m, *subst*. Cp), 3.81-3.79 (1H, m, *subst.* Cp), 3.71 (1H, d (AB system), *J* = 14.0 Hz, CH_2Py), 3.42 (1H, d (AB system), *J* = 14.0 Hz, CH_2Py), 3.21 (1H, d (AB system), *J* = 12.8 Hz, CH_2Cp), 1.87 (3H, s, NCH_3).

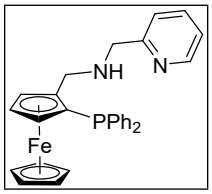
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): *δ* 160.0 (s, *quat.* Py), 148.30 (s, Py), 136.09 (s, Py), 135.30 (d, J_{PC} = 88.1 Hz, *quat*. Ph), 134.12 (d, J_{PC} = 85.8 Hz, *quat.* Ph), 132.21 (d, J_{PC} = 10.5 Hz, Ph), 132.06 (d, J_{PC} = 10.7 Hz, Ph), 131.09 (d, J_{PC} = 3.0Hz, Ph), 130.82 (d, J_{PC} = 3.0 Hz, Ph), 127.91 (d, J_{PC} = 12.5 Hz, 2C, Ph), 122.87 (s,

Py), 121.43 (s, Py), 89.71 (d, J_{PC} = 11.9 Hz, *quat.* Cp), 75.48 (d, J_{PC} = 9.8 Hz, *subst.* Cp), 75.14 (d, J_{PC} = 12.6 Hz, *subst.* Cp), 73.89 (d, J_{PC} = 95.6 Hz, *quat.* Cp), 70.75 (s, Cp); 68.83 (d, J_{PC} = 10.5 Hz, *subst.* Cp), 63.67 (s, $\underline{C}H_2Py$), 56.41 (s, $\underline{C}H_2Cp$), 40.84 (s, $N\underline{C}H_3$).
$^{31}P\{^1H\}$ NMR (162 MHz, $CDCl_3$): δ 41.90 (s, PPh_2).
HRMS (DCI-CH_4): m/z $[M+H]^+$ (100%, calcd. for $C_{30}H_{30}FeN_2PS$ 537.1217, found 537.1205).

Synthesis of phosphines 4a-b and 4a-Me

In a dry Schlenk tube under argon, **3a**, **3b** or **3a-Me** (1 equiv.) was dissolved in dry, degassed toluene. Degassed tris-(dimethylamino)phosphine (10 equiv.) was added to the solution and the mixture was refluxed overnight. After cooling to room temperature, the solvent was evaporated *in vacuo*. The orange residue was purified by flash column chromatography on silicagel under argon (eluent: degassed *n*-pentane/dichloromethane 60:40 + 1% NEt_3).

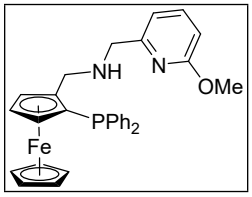
1-(diphenylphosphino)-2-[[(2-pyridinylmethyl)amino]methyl]ferrocene 4a



Obtained from 300 mg (0.58 mmol) of **3a** and 1.2 mL (5.89 mmol) of $P(NMe_2)_3$ in 10 mL toluene as a yellow solid (225 mg, 80% yield).

^1H NMR (400 MHz, $CDCl_3$): δ 8.49 (1H, app. d, *J* = 4 Hz, Py), 7.56-7.52 (3H, m, 2H Ph + 1H Py), 7.40-7.39 (3H, m, Ph), 7.28-7.24 (5H, m, Ph), 7.13-7.10 (1H, m, Py), 7.02 (1H, app. d, *J* = 7.8 Hz, Py), 4.57 (1H, m, *subst*. Cp), 4.29 (1H, m, *subst.* Cp), 4.08 (5H, s, Cp), 3.86 (1H, d (AB system), *J* = 13.0 Hz, $C\underline{H}_2Cp$), 3.80 (s, 2H, $C\underline{H}_2Py$), 3.72 (1H, m, *subst*. Cp), 3.64 (1H, d (AB system), *J* = 13.1 Hz, $C\underline{H}_2Cp$).
$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$): δ 159.82 (s, *quat.* Py), 149.06 (s, Py), 139.87 (d, J_{PC} = 10.7 Hz, *quat.*, Ph), 137.21 (d, J_{PC} = 8.4 Hz, *quat*., Ph), 136.28 (s, Py), 134.83 (d, J_{PC} = 20.6 Hz, Ph), 132.53 (d, J_{PC} = 18.4 Hz, Ph), 129.05 (s, Ph), 128.29-128.06 (m, Ph), 121.73 (Py), 121.70 (Py), 91.58 (d, J_{PC} = 24.2 Hz, *quat.* Cp), 75.83 (d, J_{PC} = 6.8 Hz, *quat,* Cp), 71.99 (d, J_{PC} = 3.0 Hz, Cp), 71.30 (d, J_{PC} = 3.4 Hz, Cp), 69.57 (s, Cp), 69.15 (s, Cp), 54.52 (s, $\underline{C}H_2Py$), 47.51 (d, J_{PC} = 9.8 Hz, $Cp\underline{C}H_2$).
$^{31}P\{^1H\}$ NMR (162 MHz, $CDCl_3$): δ -23.62 (s, PPh_2).
HRMS (DCI-CH_4): m/z $[M+H]^+$ (100%, calcd. for $C_{29}H_{28}FeN_2P$ 491.1340, found 491.1353).

1-(diphenylphosphino)-2-[[(2-4-(methoxyl)pyridinylmethyl)amino]methyl]ferrocene 4b

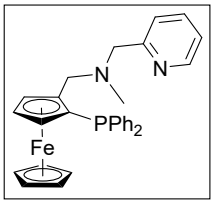


Obtained from 300 mg (0.58 mmol) of **3b** and 1.2 mL (5.89 mmol) of $P(NMe_2)_3$ in 10 mL toluene as a yellow powder (100 mg, 71% yield).

^1H NMR (400 MHz, $CDCl_3$): δ 7.59-7.52 (2H, m, Ph), 7.46-7.43 (1H, m, Py), 7.41-7.39 (3H, m, Ph), 7.24-7.23 (5H, m, Ph), 6.63 (1H, app. d, *J* = 7.2 Hz, Py); 6.58 (1H, app. d, *J* = 8.2 Hz, Py), 4.61-4.60 (1H, m, *subst*. Cp), 4.30-4.29 (1H, m, *subst*. Cp), 4.08 (5H, s, Cp), 3.86 (3H, s, $C\underline{H}_3O$), 3.83 (1H, dd (AB system), J_1 = 13.5 Hz, J_2 = 1.9 Hz, $\underline{CH}_2Cp$), 3.75-3.74 (1H, m, *subst*. Cp), 3.73 (2H, s, $C\underline{H}_2Py$), 3.68 (1H, d (AB system), *J* = 13.2 Hz, $C\underline{H}_2Cp$).

$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$): δ 163.71 (s, *quat.*, CH_2Py), 157.41 (s, *quat.* PyOMe), 139.94 (d, J_{PC} = 10.2 Hz, *quat.*, Ph), 138.74 (s, Py), 137.35 (d, J_{PC} = 9.1 Hz, *quat.*, Ph), 134.89 (d, J_{PC} = 20.8 Hz, Ph), 132.38 (d, J_{PC} = 18.3 Hz, Ph), 129.08 (s, Ph), 128.25-127.99 (m, Ph), 114.33 (s, Py), 108.58 (s, Py), 92.03 (d, J_{PC} = 23.8 Hz, *quat*., CpP), 75.82 (d, J_{PC} = 6.8 Hz, *quat*., $CpCH_2$), 71.72 (d, J_{PC} = 3.9 Hz, *subst*. Cp), 71.25 (d, J_{PC} = 3.8 Hz, *subst*. Cp), 69.52 (5C, s, Cp), 69.17 (s, *subst*. Cp), 54.42 (s, CH_2Py), 53.19 (s, OCH_3), 47.51 (d, J_{PC} = 9.9 Hz, $CpCH_2$).
$^{31}P\{^1H\}$ NMR (162 MHz, $CDCl_3$): δ -23.50 (s, PPh_2).
HRMS (ESI, pos.): m/z $[M+H]^+$ (100%, calcd. for $C_{30}H_{30}FeN_2OP$ 521.1445, found 521.1451).

1-(diphenylphosphino)-2-[[methyl(2-pyridinylmethyl)amino]methyl]ferrocene 4a-Me

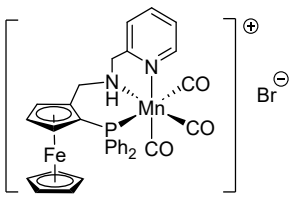


Obtained from 100 mg (0.19 mmol) of **3a-Me** and 170 µL (0.93 mmol) of $P(NMe_2)_3$ in 7 mL toluene as a yellow solid (75 mg, 80% yield). Eluent for column chromatography: degassed *n*-pentane /dichloromethane 90:10 + 0.5% NEt_3.

^1H NMR (400 MHz, $CDCl_3$): δ 8.13 (1H, app. d, *J*= 4.9 Hz, Py), 7.32-7.27 (2H, m, Ph), 7.12-7.09 (3H, m, Ph), 7.00-6.93 (6H, m, 5H Ph + 1H Py), 6.74-6.71 (1H, m, Py), 6.27 (1H, app. d, *J* = 7.9 Hz, Py), 4.23-4.22 (1H, m, *subst.* Cp), 4.02-4.01 (1H, m, *subst*. Cp), 3.76 (1H, app. d (AB system), *J* = 12.6 Hz, CH_2Py), 3.70 (5H, s, Cp), 3.56-3.55 (1H, m, *subst.* Cp), 3.34 (1H, d (AB system), *J* = 14.3 Hz, CH_2Cp), 3.24 (1H, d (AB system), *J* = 14.3 Hz, CH_2Cp), 3.03 (1H, d (AB system), *J* = 12.6 Hz, CH_2Py), 1.65 (3H, s, NCH_3).
$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$): δ 160.07 (s, *quat.* Py), 148.39 (s, Py), 140.61 (d, J_{PC} = 9.2 Hz, *quat*. Ph), 138.06 (d, J_{PC} = 8.4 Hz, *quat*. Ph), 136.17 (s, Py), 135.25 (d, J_{PC} = 21.3 Hz, Ph), 132.50 (d, J_{PC} = 18.0 Hz, Ph), 129.00 (s, Ph), 128.03 (d, J_{PC} = 7.8 Hz, Ph), 127.80 (d, J_{PC} = 6.1 Hz, Ph), 127.47 (s, Ph), 122.71 (s, Py), 121.45 (s, Py), 90.55 (d, J_{PC} = 25.8 Hz, *quat.* Cp), ca. 76.5 (*quat.* Cp, detected by 2D-HMBC), 73.58 (d, J_{PC} = 4.1 Hz, *subst.* Cp), 71.90 (d, J_{PC} = 4.8 Hz, *subst.* Cp), 69.62 (s, Cp); 69.26 (s, *subst.* Cp), 63.75 (s, CH_2Py), 57.29 (d, J_{PC} = 8.4 Hz, CH_2Cp), 41.22 (s, NCH_3).
$^{31}P\{^1H\}$ NMR (162 MHz, $CDCl_3$): δ -23.86 (s, PPh_2).

Synthesis of the manganese(I) complexes 5a-b

[1-(diphenylphosphino)-2-[[(2-pyridinylmethyl)amino]methyl]ferrocene]- κN^1-κN^2-κP-tricarbonyl manganese (I) bromide, 5a



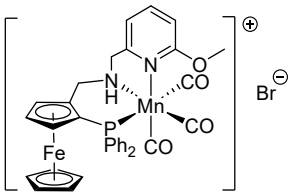
The procedure was adapted from the literature.[8] In a Schlenk tube, 1-(diphenylphosphino)-2-[[(2-pyridinylmethyl)-amino]methyl]ferrocene **4a** (50 mg, 0.102 mmol, 1.0 equiv.) and bromopentacarbonylmanganese(I) (28 mg, 0.102 mmol, 1.0 equiv.) were placed in a mixture of degassed cyclohexane (2 mL) and toluene (2 mL) and heated at 95 °C for 24 h. The system was then

cooled down to room temperature, diluted with degassed n-hexane (3 mL), filtered and washed with n-hexane (2x2 mL). After evaporation of the solvents *in vacuo*, the residue was solubilised in degassed dichloromethane (3 mL), filtered and crystallised by layering *n*-hexane (15 mL) to give the title complex **5a** as orange flake-like crystals (28 mg, 39% yield).

The ^{1}H-NMR signals appeared broad and unresolved, which may arise from partial decomposition in chlorinated solvents as well as isomeric mixtures. The ^{13}C NMR spectrum could not be exploited due to a low signal-to-noise ratio.

^{1}H NMR (400 MHz, CD_2Cl_2): δ 9.21-9.20 (m, Py), 8.63-8.62 (m, Py), 8.56-8.51 (m, Py), 7.98-7.93 (m, Ph), 7.73-7.23 (m, Ph + Py), 6.99-6.89 (m, Ph), 6.80-6.72 (m, Ph + Py), 5.23-4.03 (*subst*. Cp, CH_2Cp and CH_2Py), 3.87 (s, Cp).
^{31}P{^{1}H} NMR (162 MHz, CD_2Cl_2): δ 89.85, 56.51, 45.11.
HRMS (ESI, pos.): m/z [M-CO+MeCN]$^+$ (calcd. for $C_{33}H_{30}FeMnN_3O_2P$ 642.0806, found 642.0807); m/z [M]$^+$ (calcd. for $C_{32}H_{27}FeMnN_2O_3P$ 629.0489, found 629.0489); m/z [M-CO]$^+$ (calcd. for $C_{31}H_{27}FeMnN_2O_2P$ 601.0540, found 601.0544); m/z [M-2CO]$^+$ (calcd. for $C_{30}H_{27}FeMnN_2OP$ 573.0591, found 573.0597); m/z [M-3CO]$^+$ (calcd. for $C_{29}H_{27}FeMnN_2P$ 545.0642, found 545.0643).

[1-(diphenylphosphino)-2-[[(2-(4-methoxy)pyridinylmethyl)amino]methyl]ferrocene]- κN^1-κN^2-κP-tricarbonyl manganese (I) bromide, 5b



Prepared from **4b** (60 mg, 0.115 mmol, 1.0 equiv.) according to the procedure described for **5a** from **4a** and obtained as orange flake-like crystals (74 mg, 79% yield).

The ^{1}H-NMR and ^{13}C-NMR signals appeared broad and unresolved, which may arise from partial decomposition in chlorinated solvents as well as isomeric mixtures.

^{1}H NMR (600 MHz, CD_2Cl_2): δ 8.55 (m, Py), 7.94-6.82 (m, Ph + Py), 4.53 (m, CH_2Cp or CH_2Py), 4.47 (1H, m, *subst*. Cp), 4.30 (1H, m, *subst*. Cp), 4.28 (1H, m, *subst*. Cp), 4.13 (m, CH_2Cp or CH_2Py), 3.86 (5H, s, Cp), 3.84 (m, CH_2Cp or CH_2Py or OMe).
^{13}C{^{1}H} NMR (151 MHz, CD_2Cl_2): δ 233.18 (s, CO), 229.69 (s, CO), 223.76 (s, CO). 219.84 (s, CO),213.29 (s, CO), 165.23-158.58 (arom. C), 142.48 (arom. C), 140.87 (arom. C), 139.37 (arom. C), 135.81 (arom. C), 134.36-134.17 (arom. C), 131.38-126.79 (arom. C), 112.61 (arom. C), 105.70 (arom. C), 104.22 (arom. C), 88.85 (*quat.* Cp), 87.88 (*quat.* Cp), 75.68 (*quat.* Cp), 72.69-68.80 (*subst.* Cp), 70.75 (Cp), 57.00-51.70 (CH_2Py, CH_2Cp, OMe).
^{31}P{^{1}H} NMR (243 MHz, CD_2Cl_2): δ 90.09, 60.88, 45.43 (1:0.2:1.4), -23.47.
HRMS (ESI, pos.): m/z [M]$^+$ (calcd. for $C_{33}H_{29}FeMnN_2O_4P$ 659.0595, found 659.0615).

5b-BARF: obtained from **5b** by addition of NaBArF (20 mg, 0.022 mmol, 1.0 equiv.) in acetone-d_6, stirring for 45 min under argon and filtration on a Celite pad. The solution was directly analysed by NMR without isolation.

^{1}H NMR (600 MHz, acetone-d_6): δ 8.67 (m, Py), 8.05-7.97 (m, Py), 7.82-7.80 (BArF), 7.76 (Ph or Py), 7.69 (BArF), 7.58-7.57 (Py), 7.47-6.35 (Ph or Py), 5.21 (m, CH_2Cp or CH_2Py), 4.73-4.15 (*subst*. Cp), 4.10 (m, CH_2Cp or CH_2Py), 4.02-3.92 (*subst*. Cp), 3.86 (s, Cp), 3.83 (s, OMe).

$^{13}C\{^1H\}$ NMR (151 MHz, acetone-d_6): δ 233.78 (s, CO), 229.98 (s, CO), 167.11-159.11 (arom. C), 161.70 (q, *J* = 49.9 Hz, BArF), 141.44-126.74 (arom. C), 134.63 (m, BArF), 124.48 (q, J = 272 Hz, BArF), 117.53 (m, BArF), 112.76-104.20 (arom. C), 88.74 (m, *quat.* Cp), 87.94 (m, *quat.* Cp), 75.44 (m, *quat.* Cp), 72.54-69.49 (*subst.* Cp), 60.85 (*subst*. Cp), 56.20-51.40 (CH_2Py, CH_2Cp), 55.04 (OMe).
$^{31}P\{^1H\}$ NMR (243 MHz, acetone-d_6): δ 90.07, 73.95, 61.88, 43.91 (2.5:0.2:0.7:1.0).

Manganese-catalyzed hydrogenation with ferrocenyl ligands 4a-b and 4a-Me and [$MnBr(CO)_5$]

Typical procedure: the ligand (**4a-b** or **4a-Me**), [$MnBr(CO)_5$] and the base were placed in two vials under an argon atmosphere. The degassed solvent and ketone (0.85 mmol) were added, and the two vials were placed in an autoclave under a positive stream of argon. The vessel was then purged three times with H_2 (10 bar) before setting the right pressure and placing it in a pre-heated oil bath for a given time. After release of the H_2 pressure, an internal standard was added, the reaction mixtures were filtered on a short path of silica, rinsed with 1.5 mL of DCM and analysed by chiral GC. Each catalytic reaction was carried out at least twice to ensure reproducibility of the results.

NMR spectra

Figure S1. ^{1}H NMR spectrum of pyridinium salt **2** (400 MHz, $CDCl_3$)

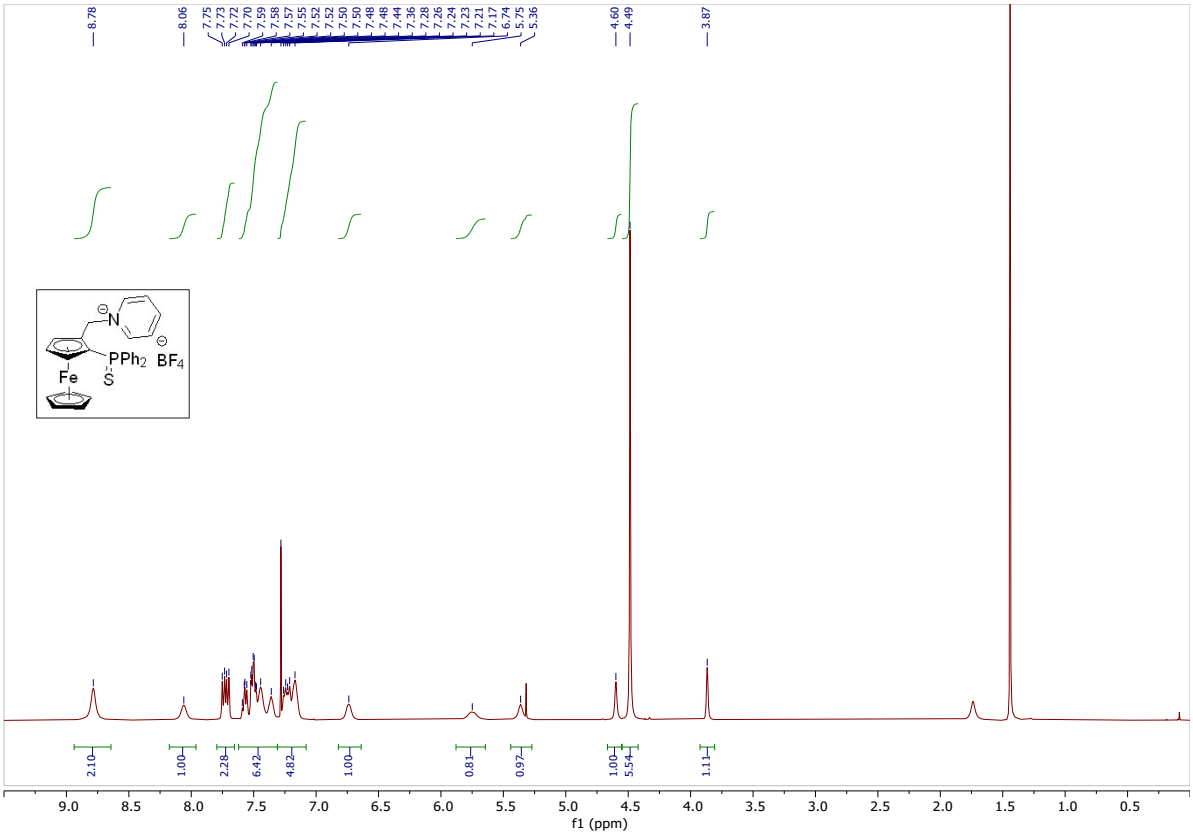


Figure S2. $^{31}P\{^{1}H\}$ NMR spectrum of pyridinium salt **2** (162 MHz, $CDCl_3$)

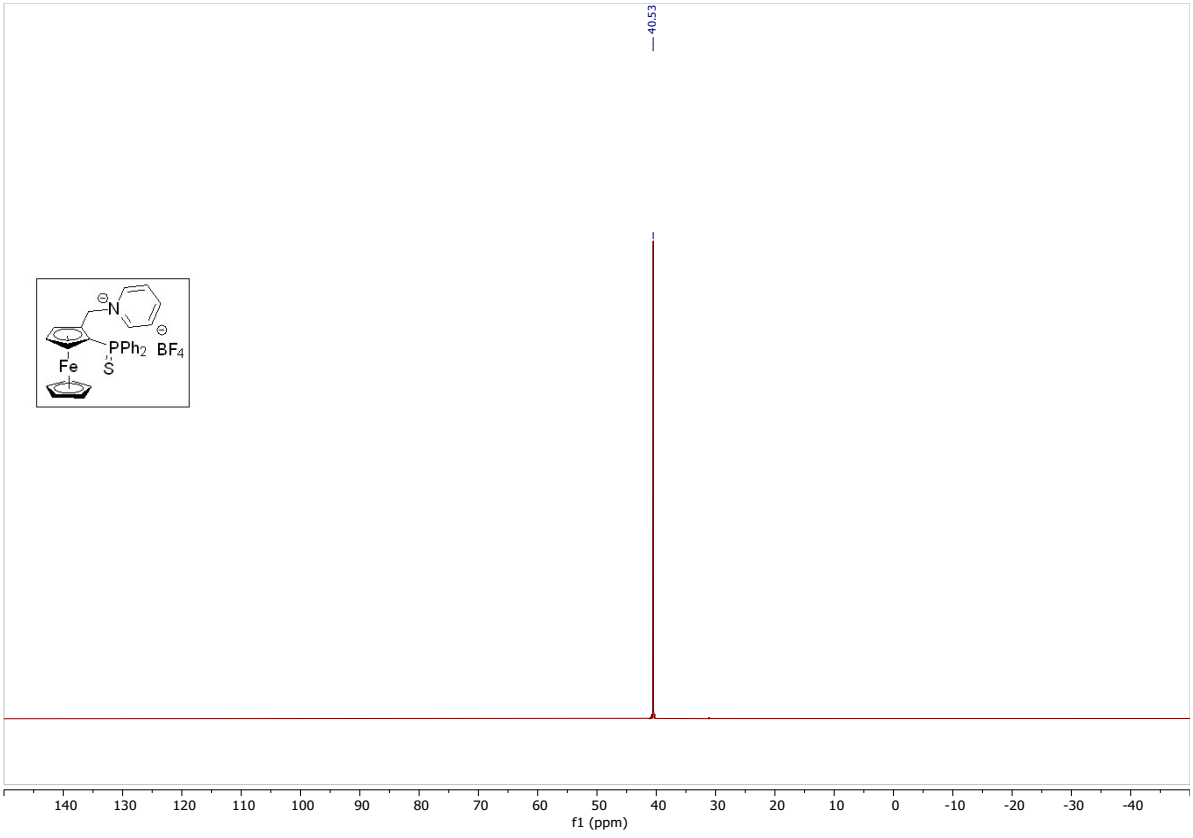


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of pyridinium salt **2** (101 MHz, $CDCl_3$)

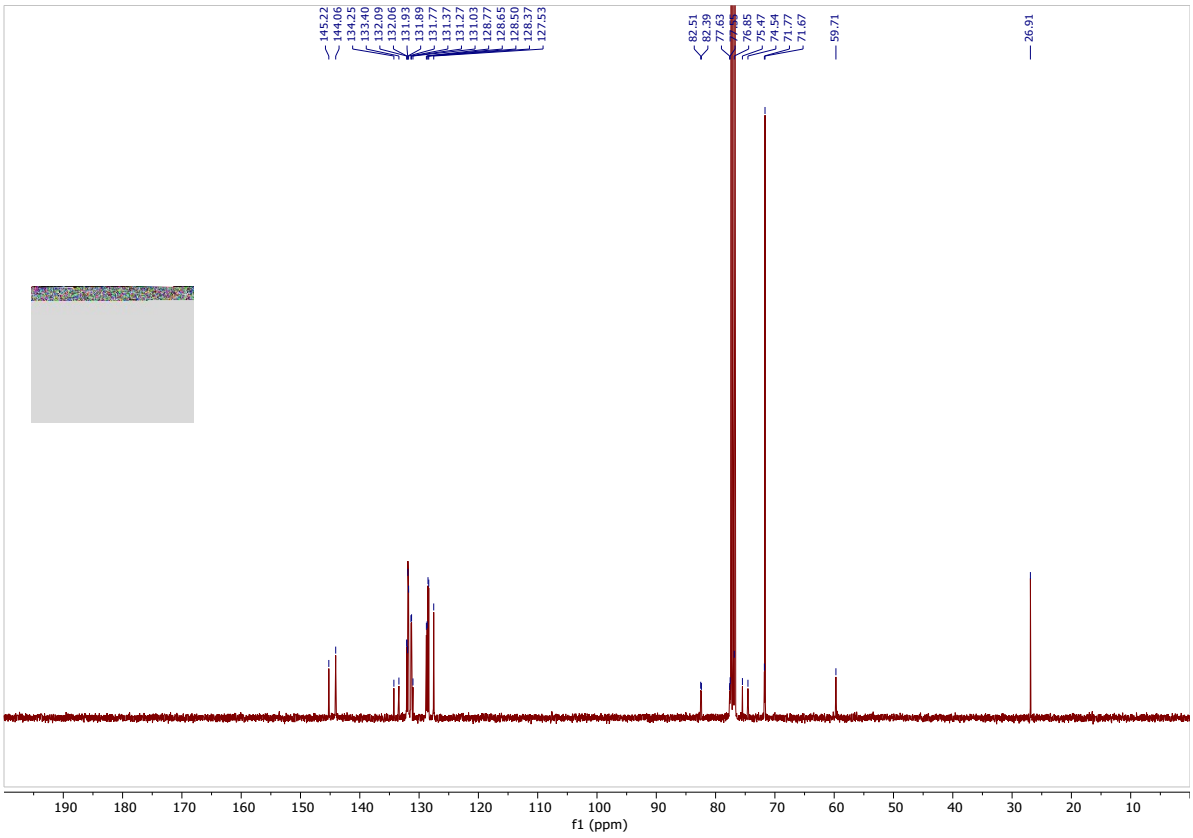


Figure S4. ^{1}H NMR spectrum of ligand **3a** (400 MHz, $CDCl_3$)

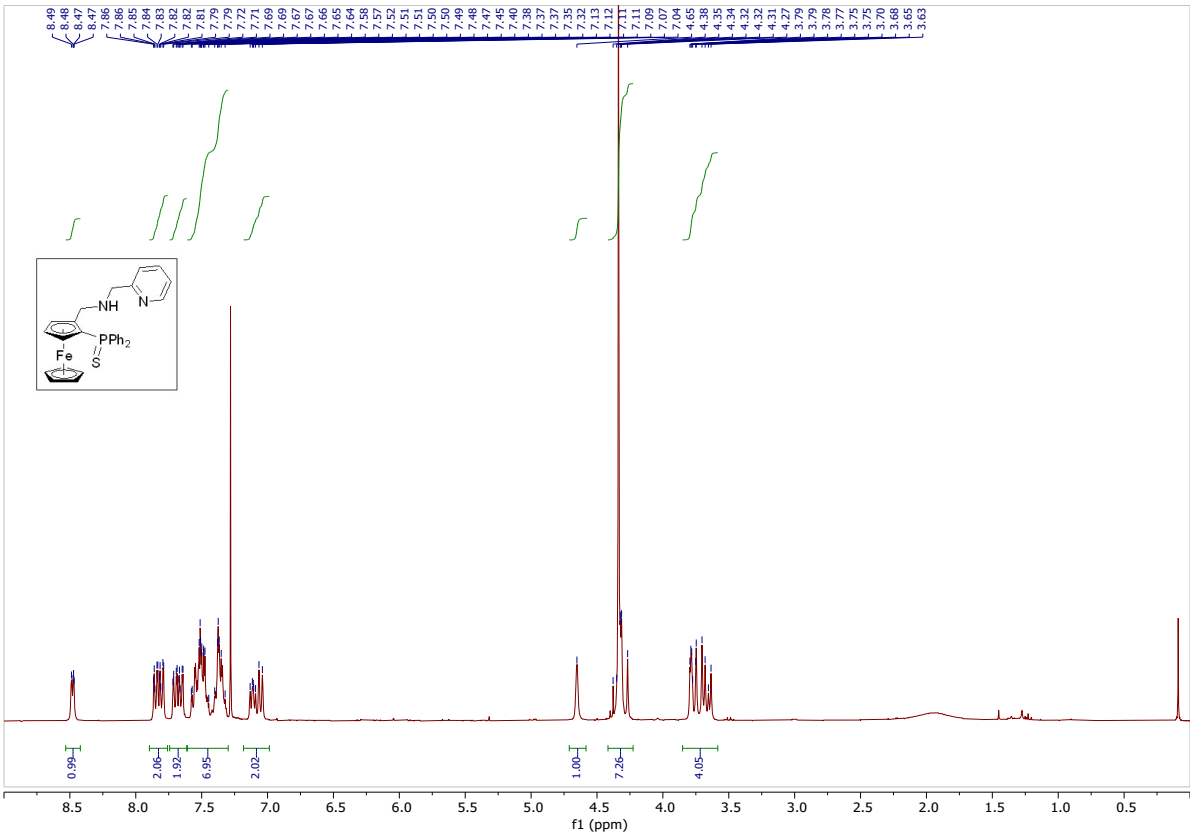


Figure S5. $^{31}P\{^{1}H\}$ NMR spectrum of ligand **3a** (162 MHz, $CDCl_3$)

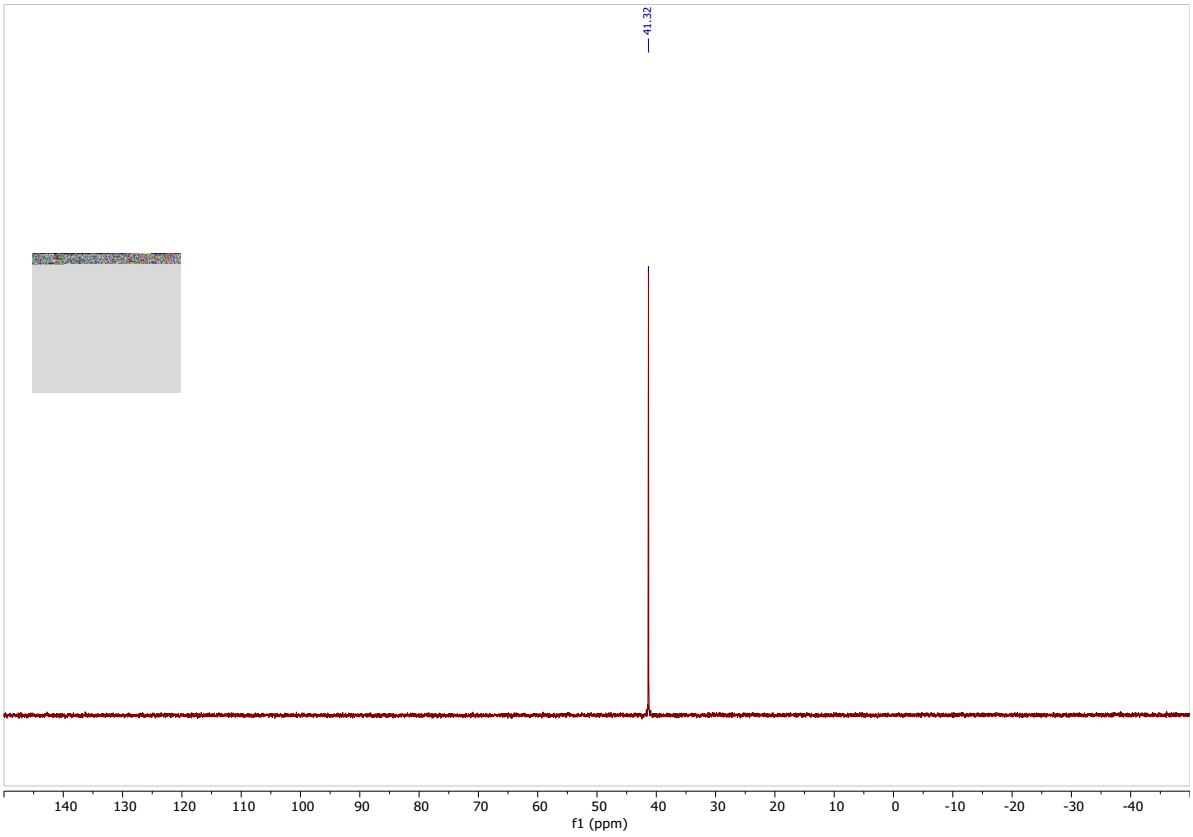


Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of ligand **3a** (101 MHz, $CDCl_3$)

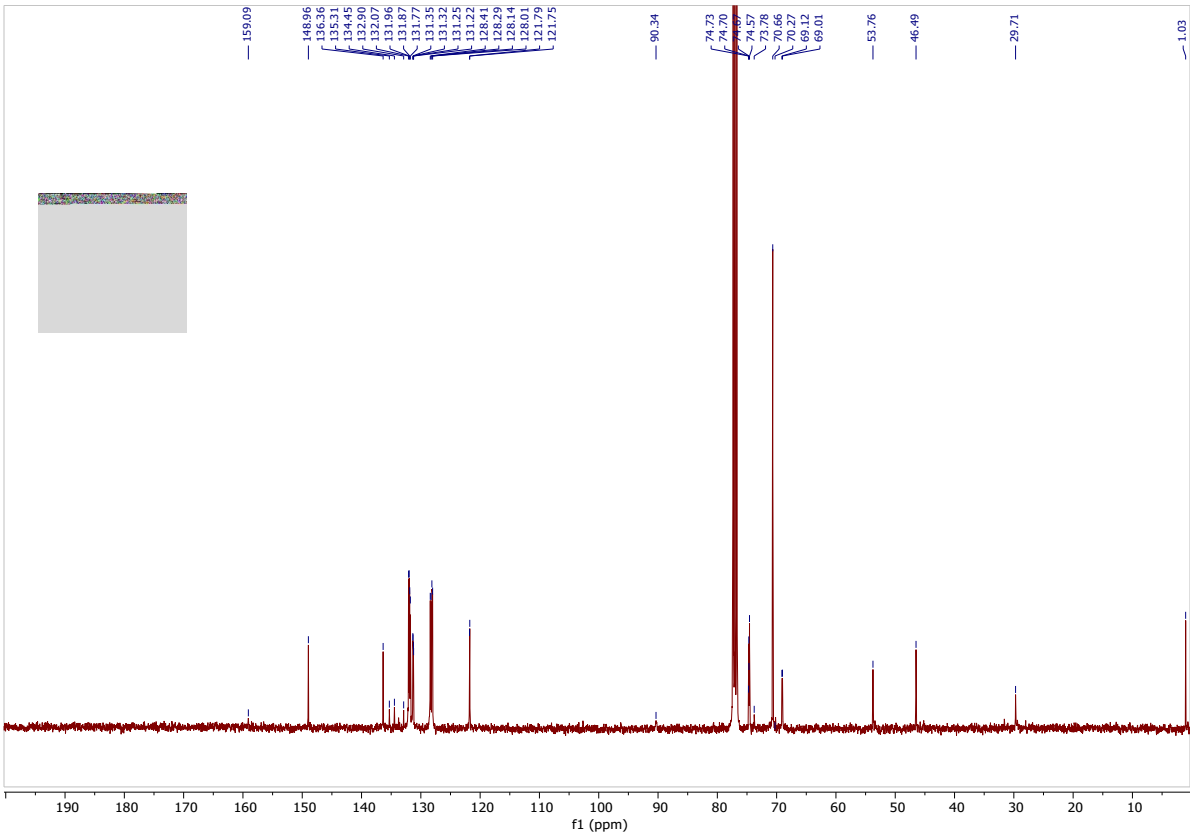


Figure S7. ^{1}H NMR spectrum of ligand **3b** (400 MHz, $CDCl_3$)

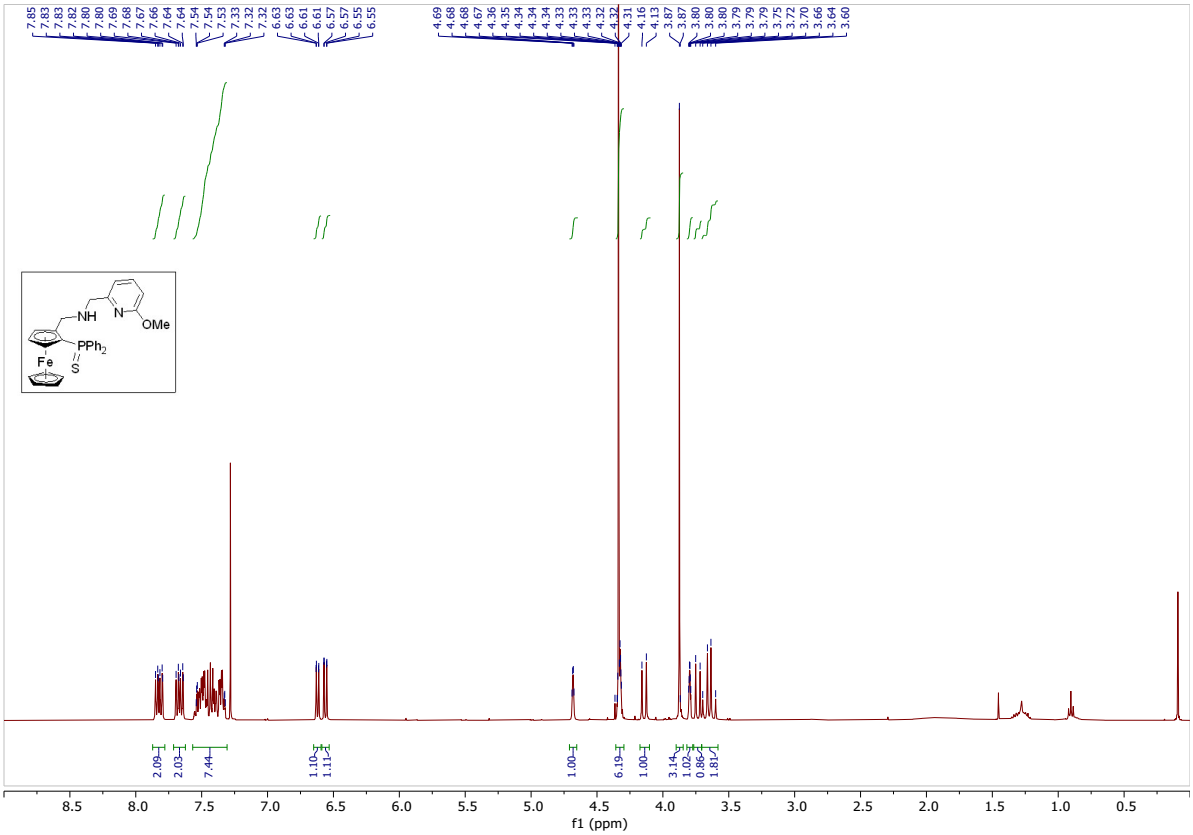


Figure S8. $^{31}P\{^{1}H\}$ NMR spectrum of ligand **3b** (162 MHz, $CDCl_3$)

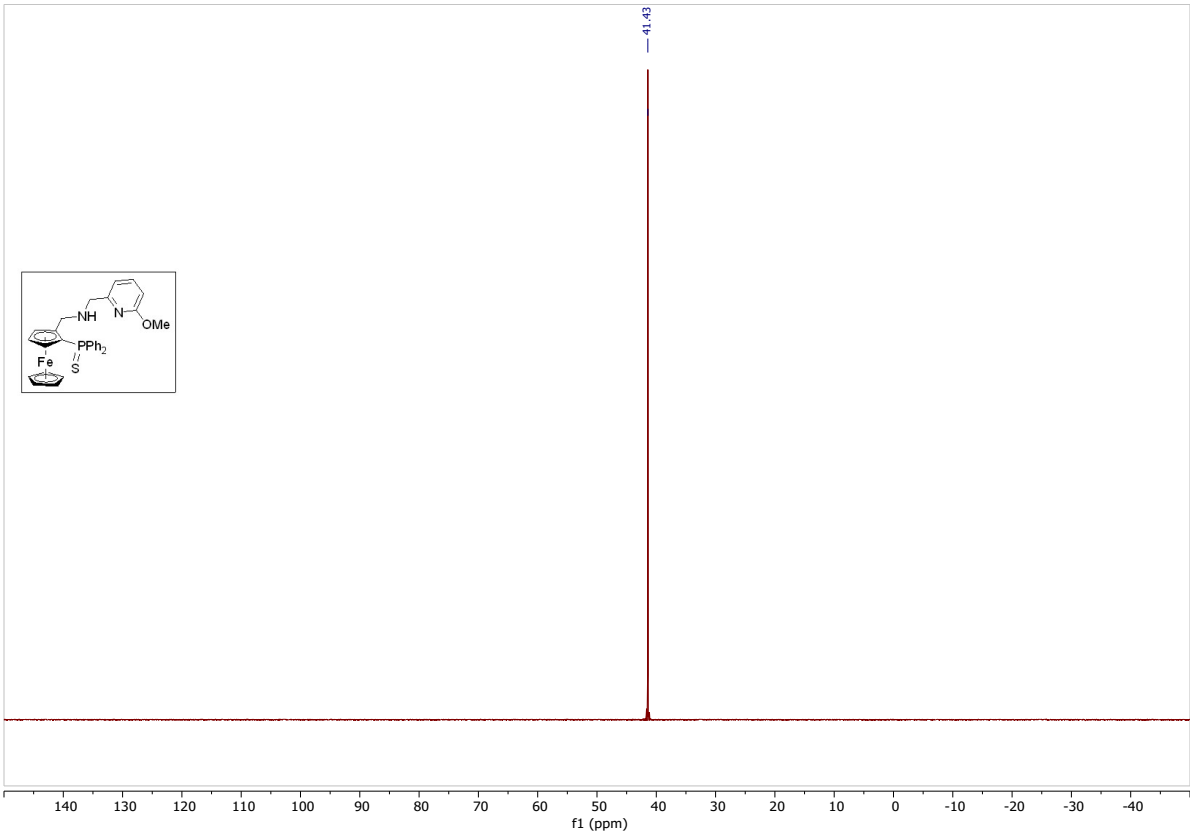


Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum of ligand **3b** (101 MHz, $CDCl_3$)

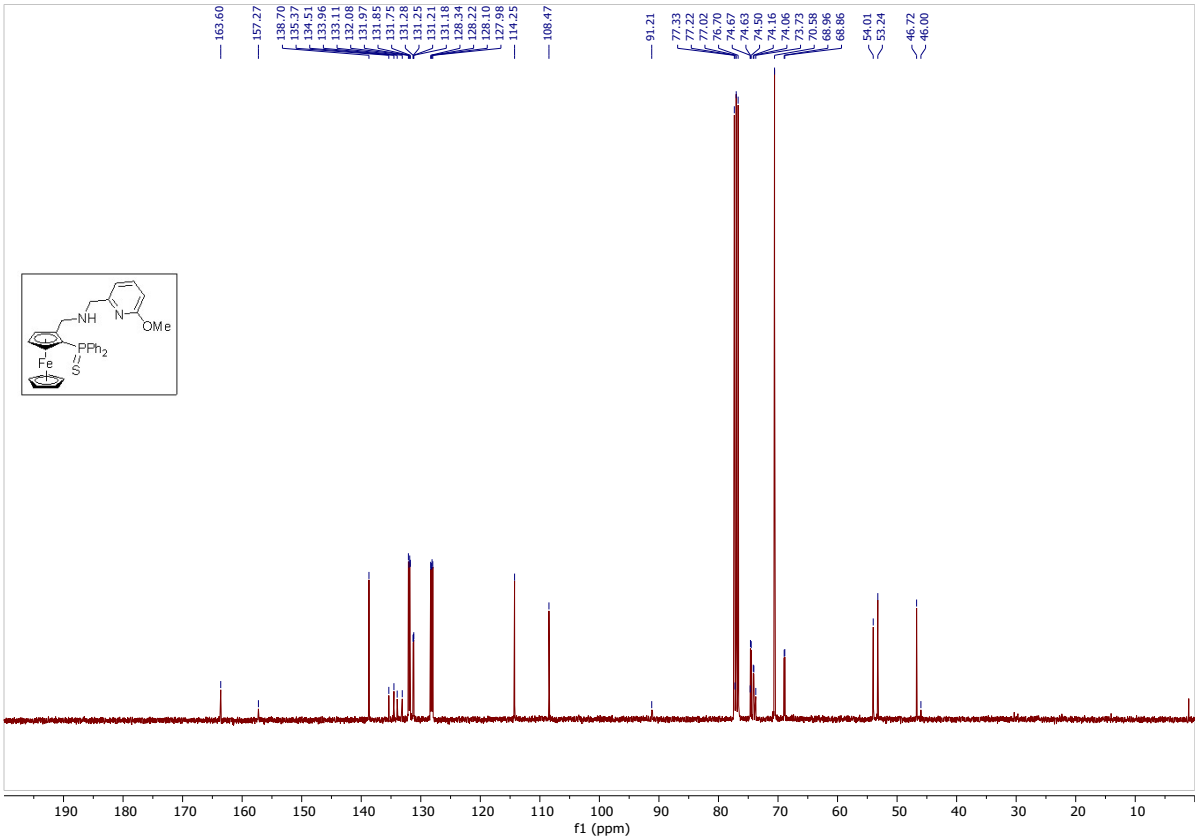


Figure S10. ^{1}H NMR spectrum of ligand **3a-Me** (400 MHz, $CDCl_3$)

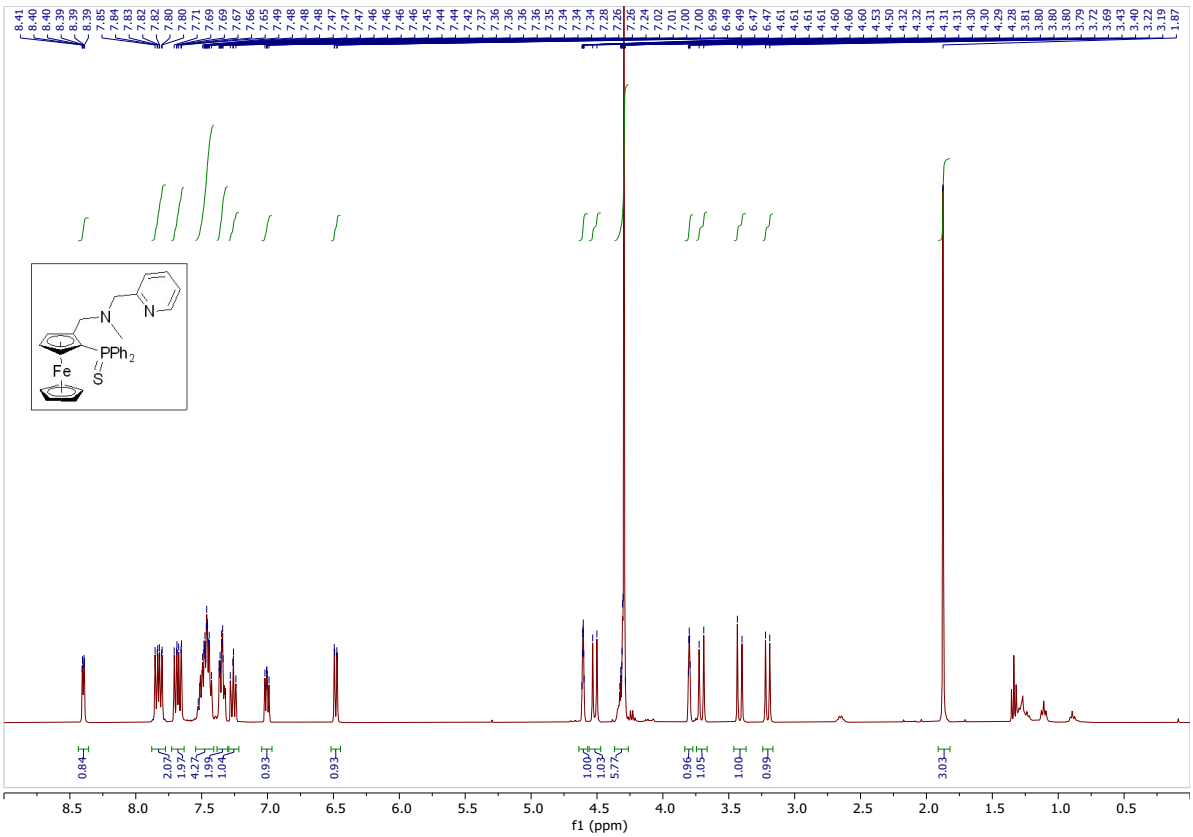


Figure S11. $^{31}P\{^{1}H\}$ NMR spectrum of ligand **3a-Me** (162 MHz, $CDCl_3$)

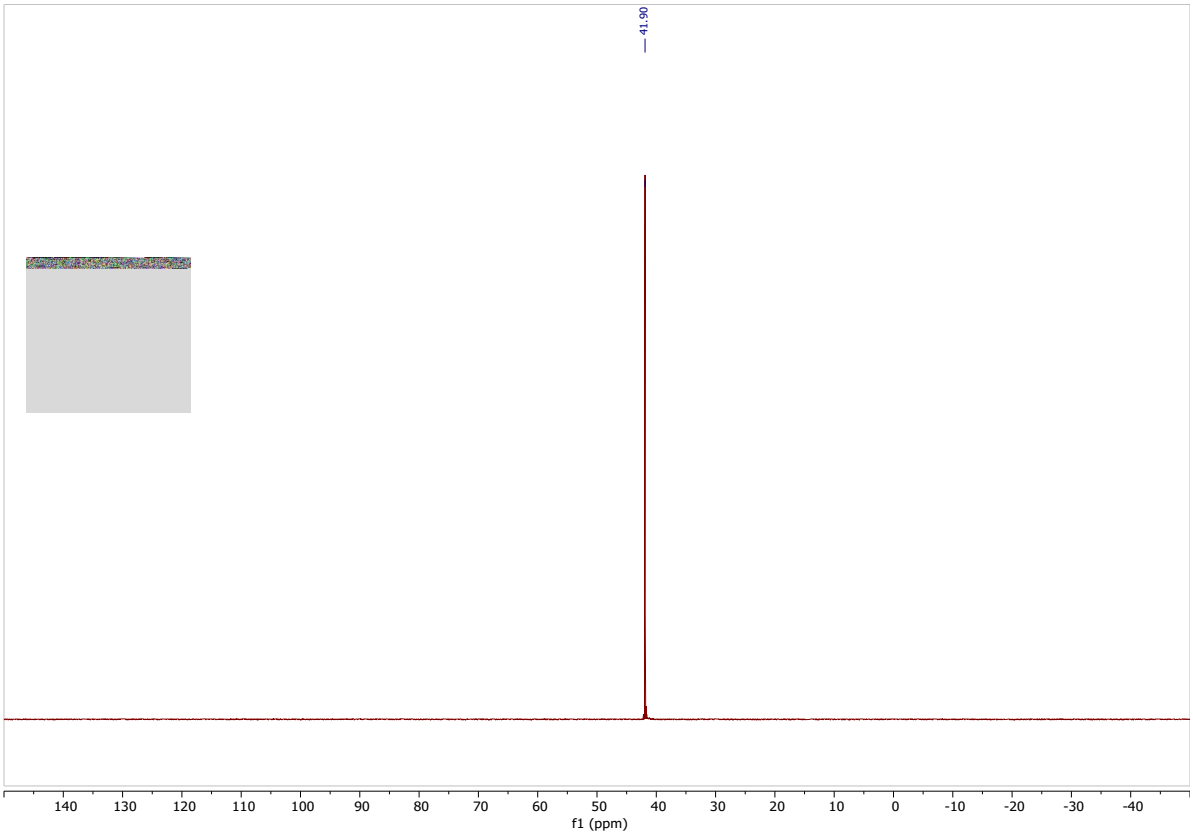


Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum of ligand **3a-Me** (101 MHz, $CDCl_3$)

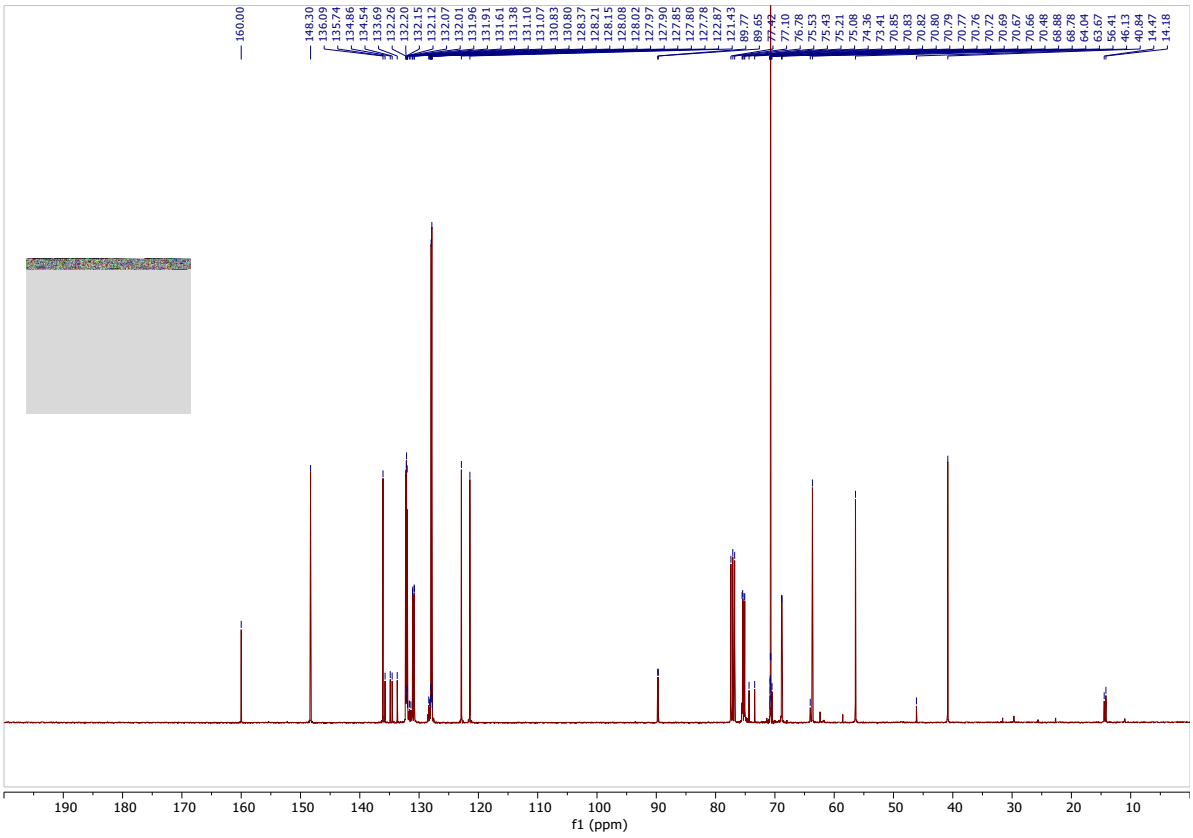


Figure S13. ^{1}H NMR spectrum of ligand **4a** (400 MHz, $CDCl_3$)

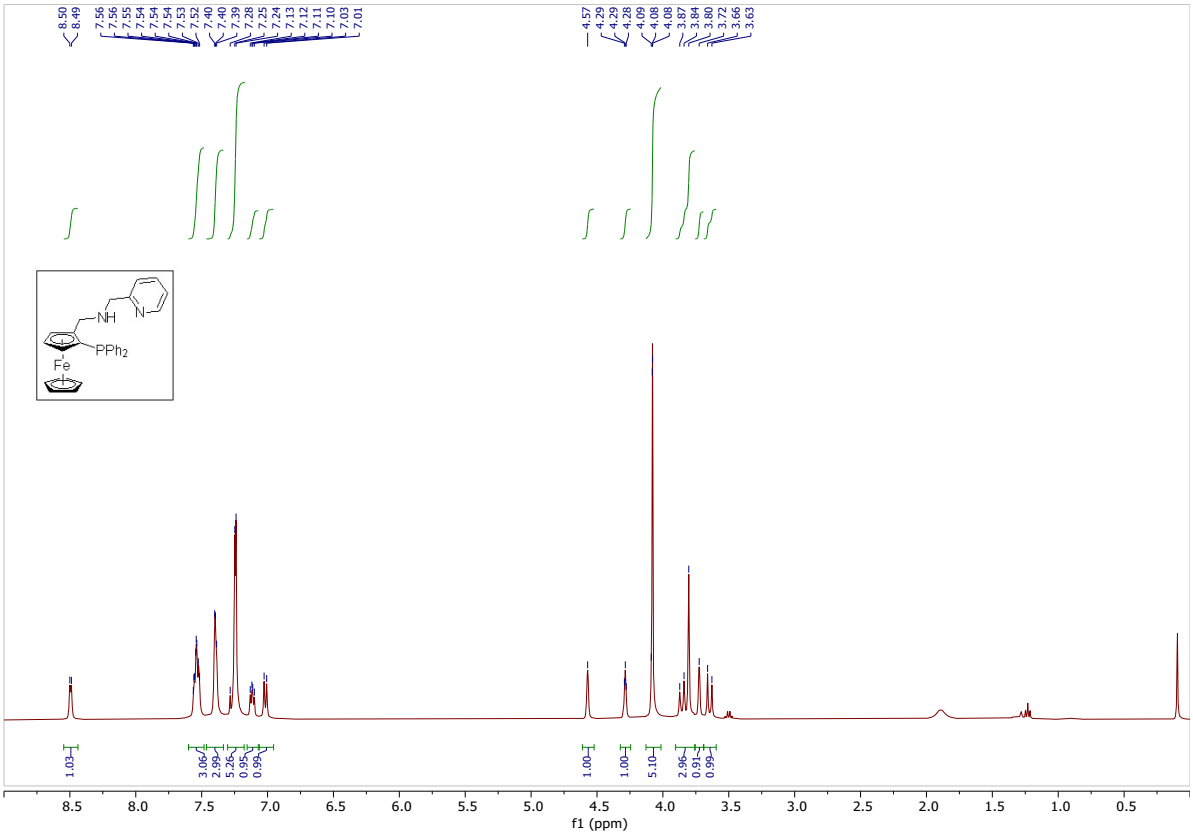


Figure S14. $^{31}P\{^{1}H\}$ NMR spectrum of ligand **4a** (162 MHz, $CDCl_3$)

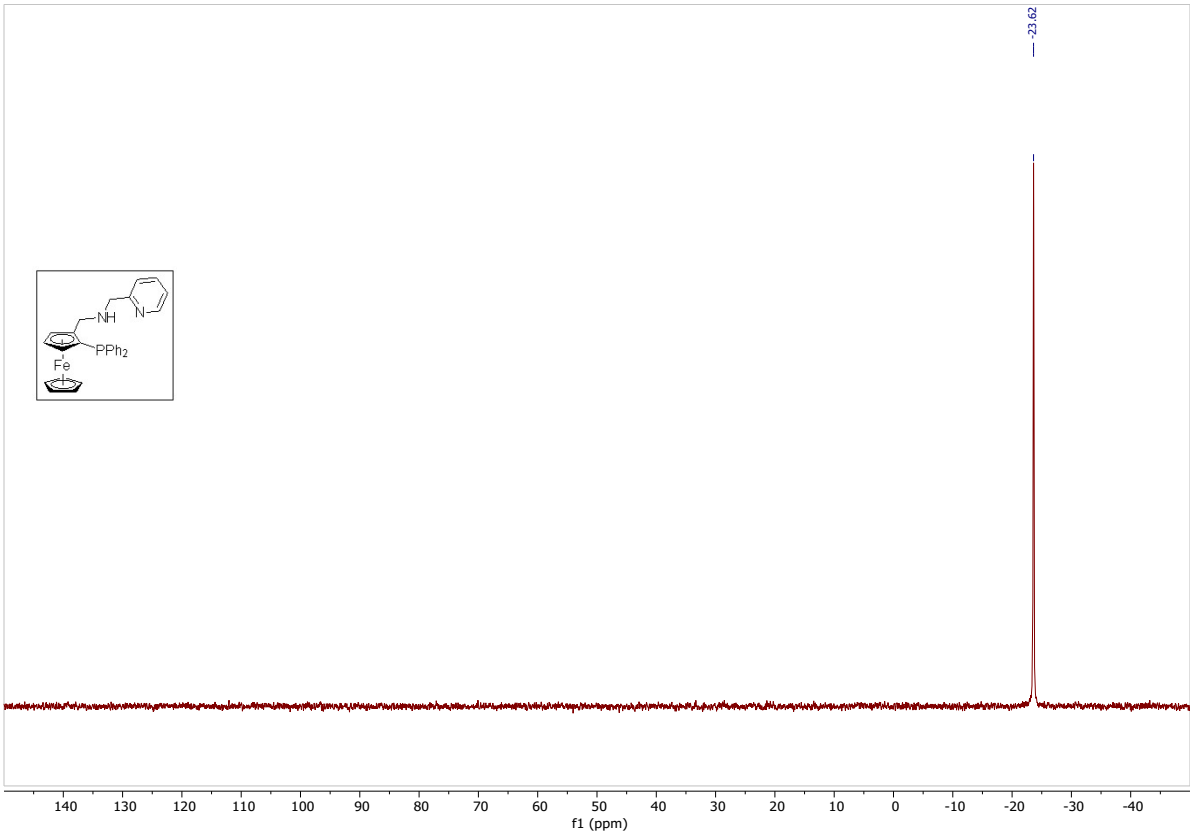


Figure S15. $^{13}C\{^{1}H\}$ NMR spectrum of ligand **4a** (101 MHz, $CDCl_3$)

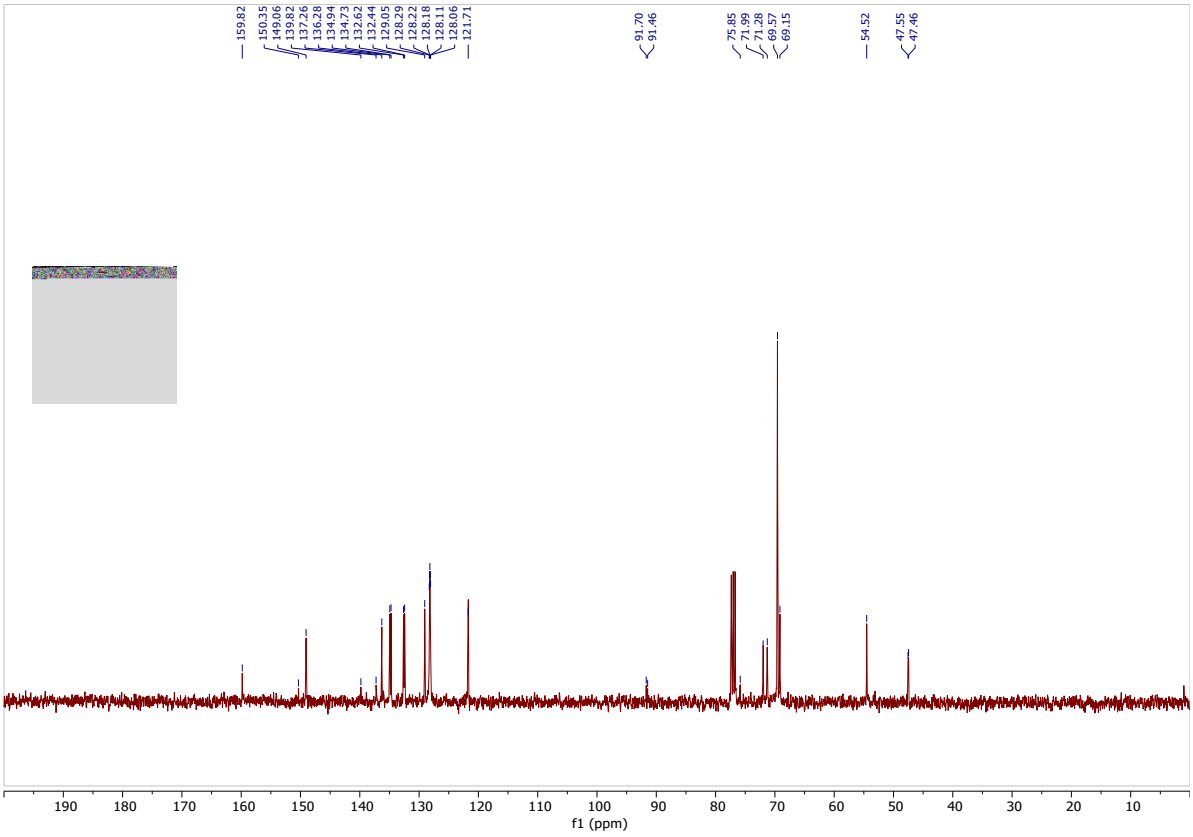


Figure S16. ^{1}H NMR spectrum of ligand **4b** (400 MHz, $CDCl_3$)

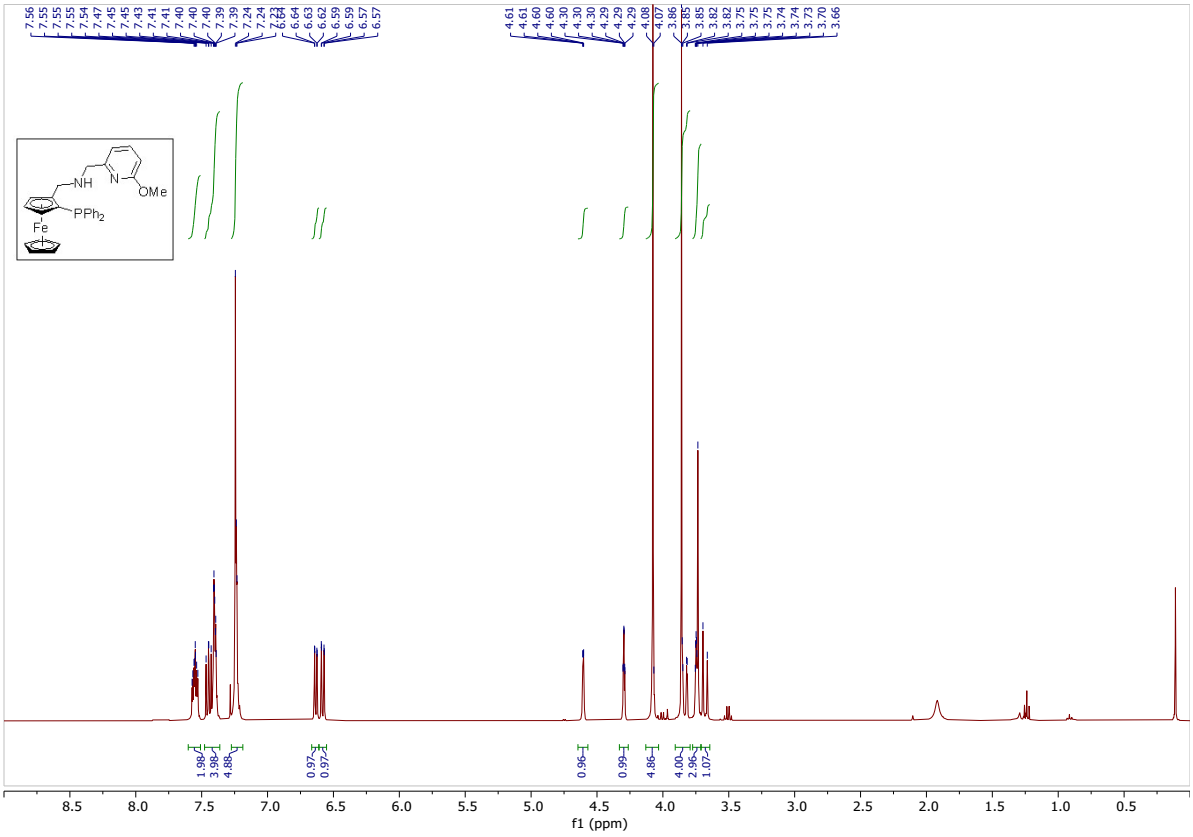


Figure S17. $^{31}P\{^{1}H\}$ NMR spectrum of ligand **4b** (162 MHz, $CDCl_3$)

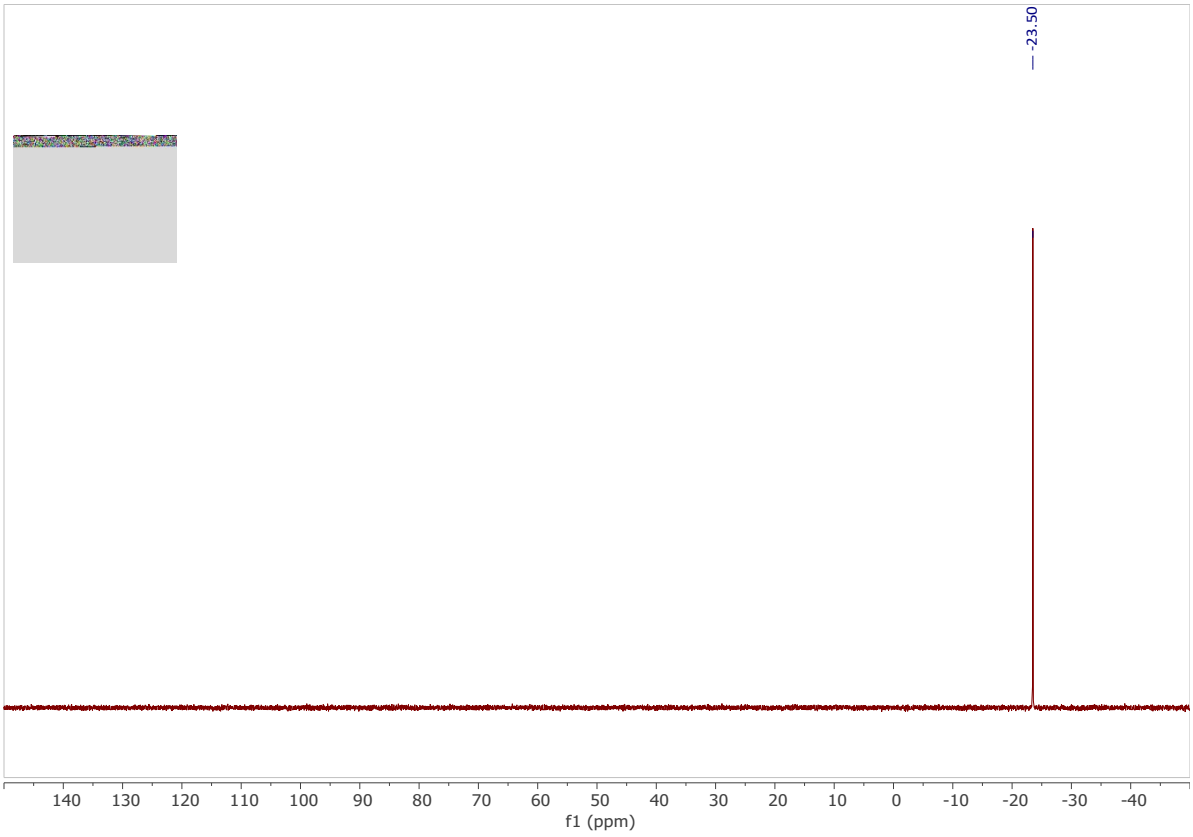


Figure S18. $^{13}C\{^{1}H\}$ (JMOD) NMR spectrum of ligand **4b** (101 MHz, $CDCl_3$)

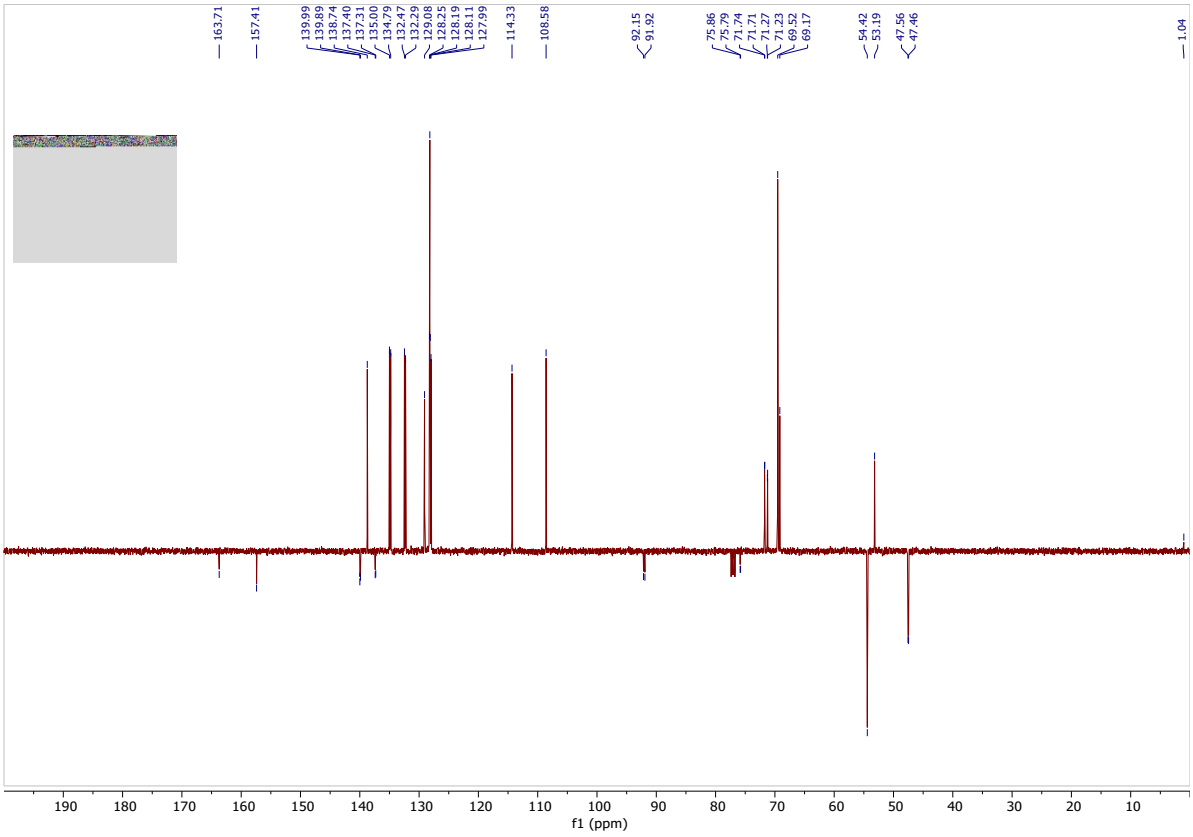


Figure S19. ^{1}H NMR spectrum of ligand **4a-Me** (400 MHz, $CDCl_3$)

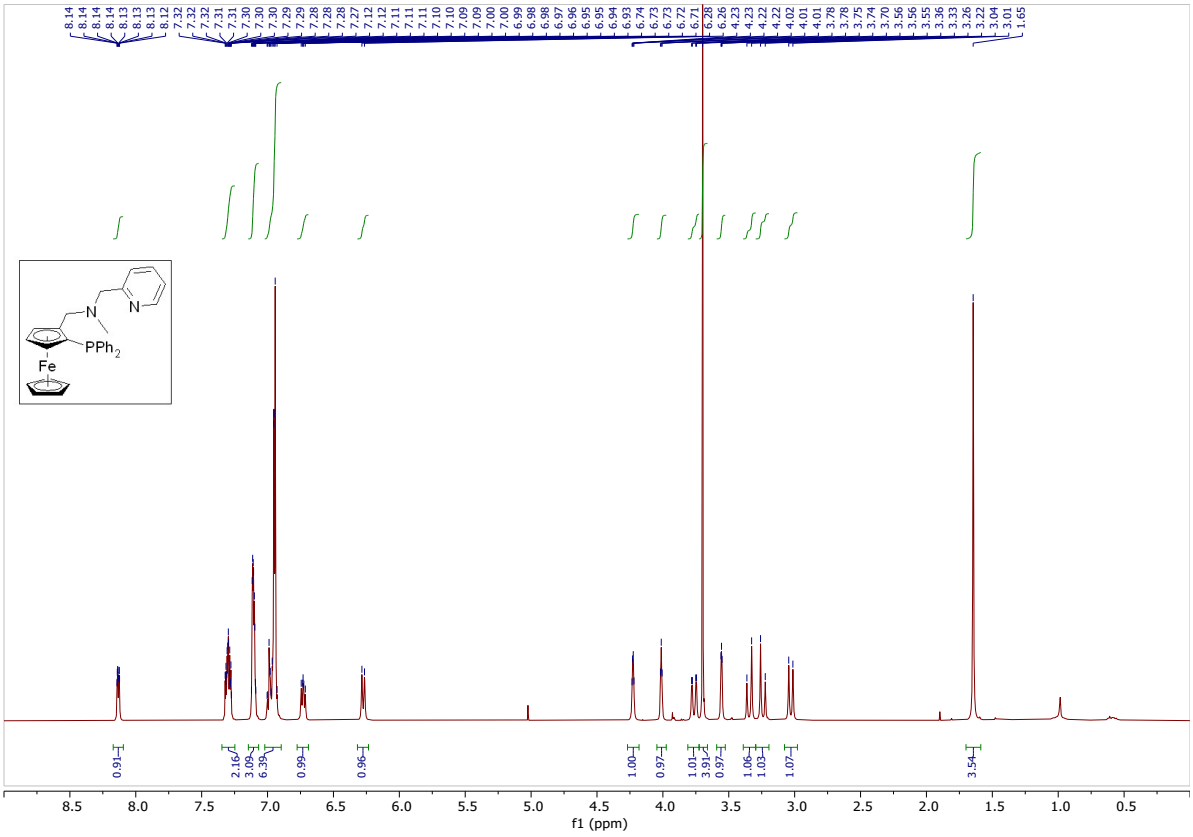


Figure S20. $^{31}P\{^{1}H\}$ NMR spectrum of ligand **4a-Me** (162 MHz, $CDCl_3$)

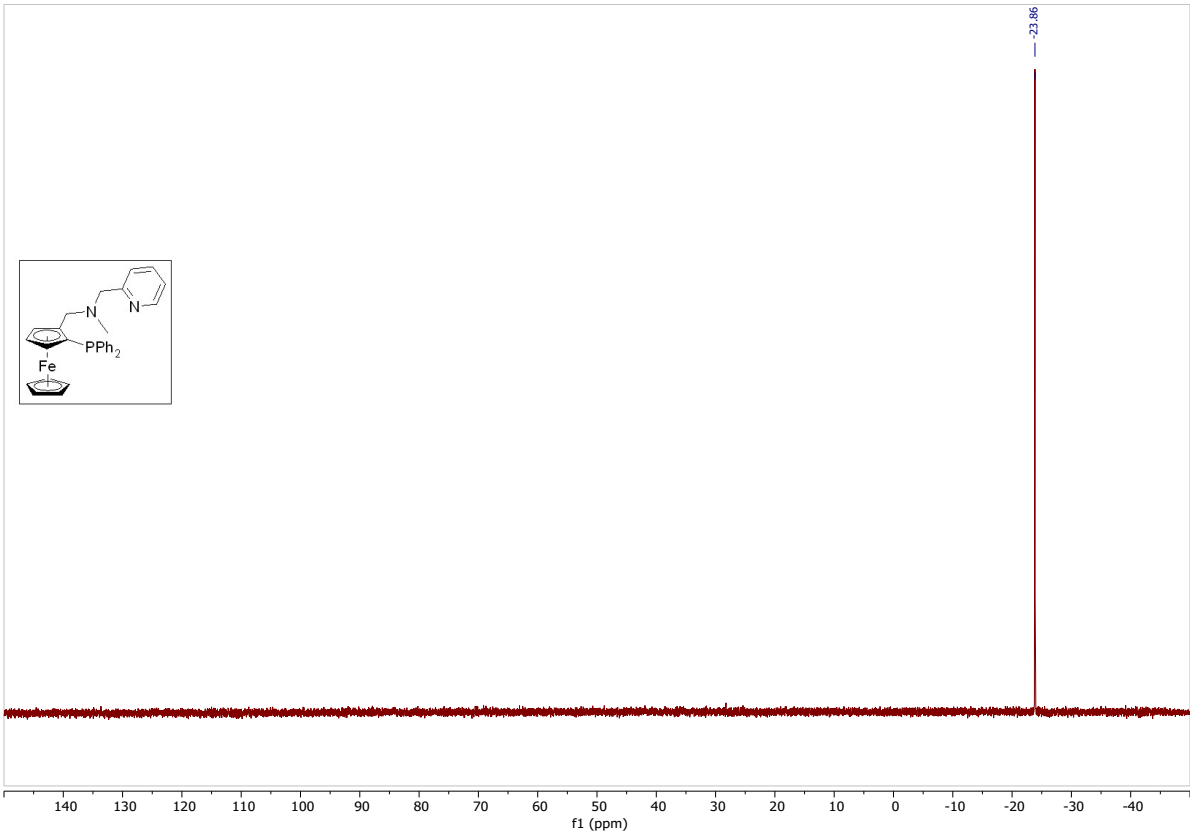


Figure S21. $^{13}C\{^{1}H\}$ NMR spectrum of ligand **4a-Me** (101 MHz, $CDCl_3$)

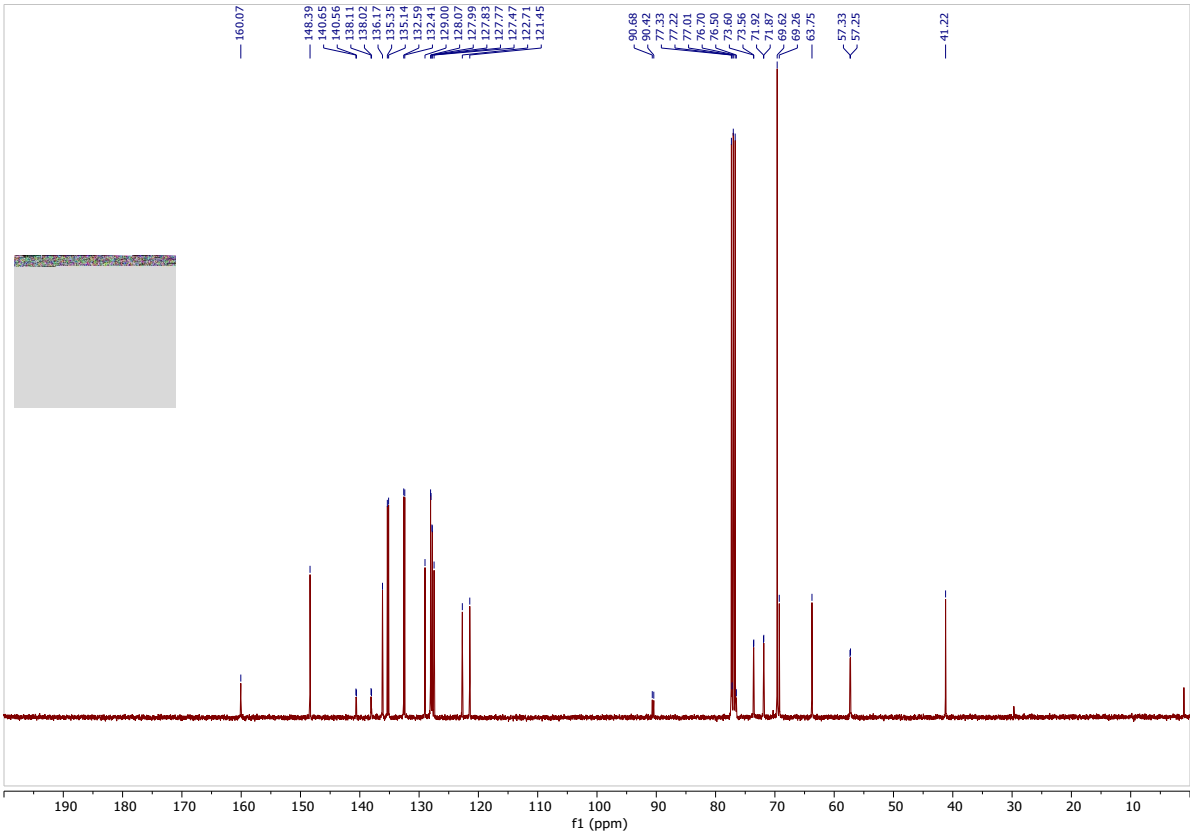


Figure S22. ^{1}H NMR spectrum of complex **5a** (400 MHz, CD_2Cl_2)

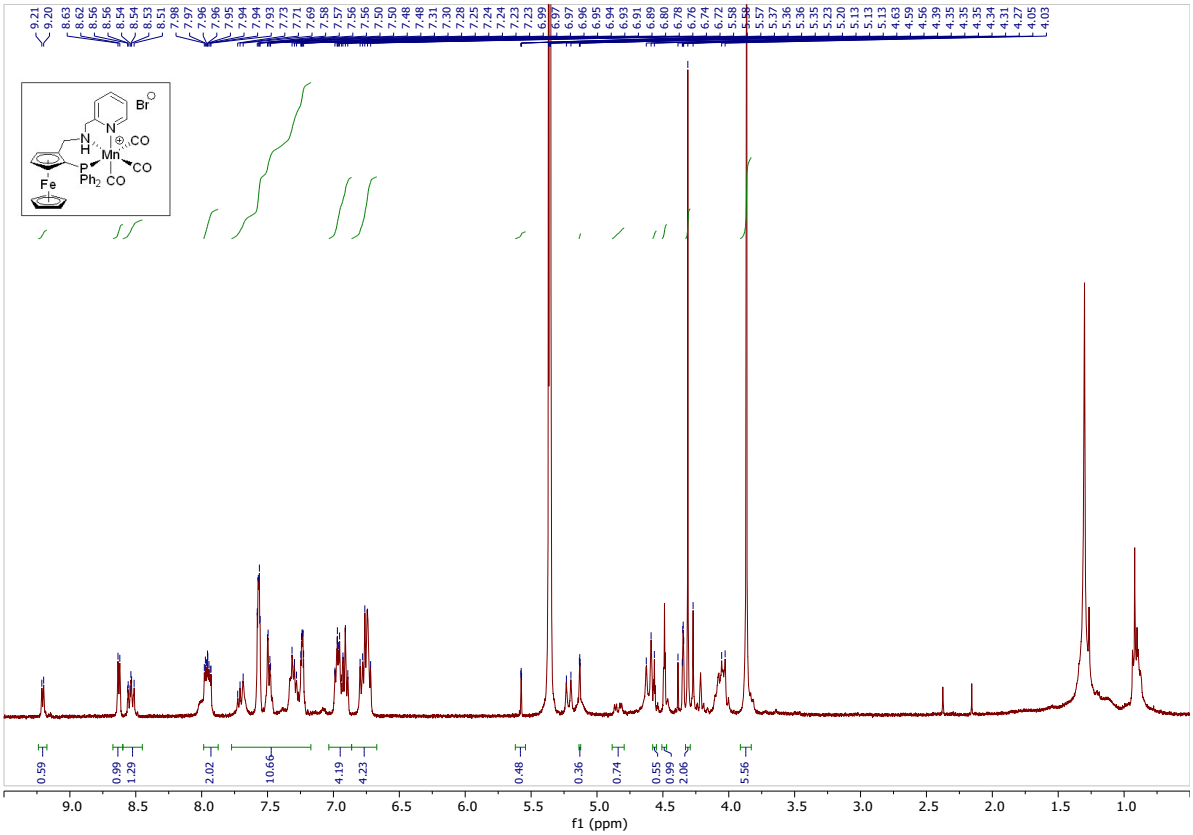


Figure S23. $^{31}P\{^{1}H\}$ NMR spectrum of complex **5a** (162 MHz, CD_2Cl_2)

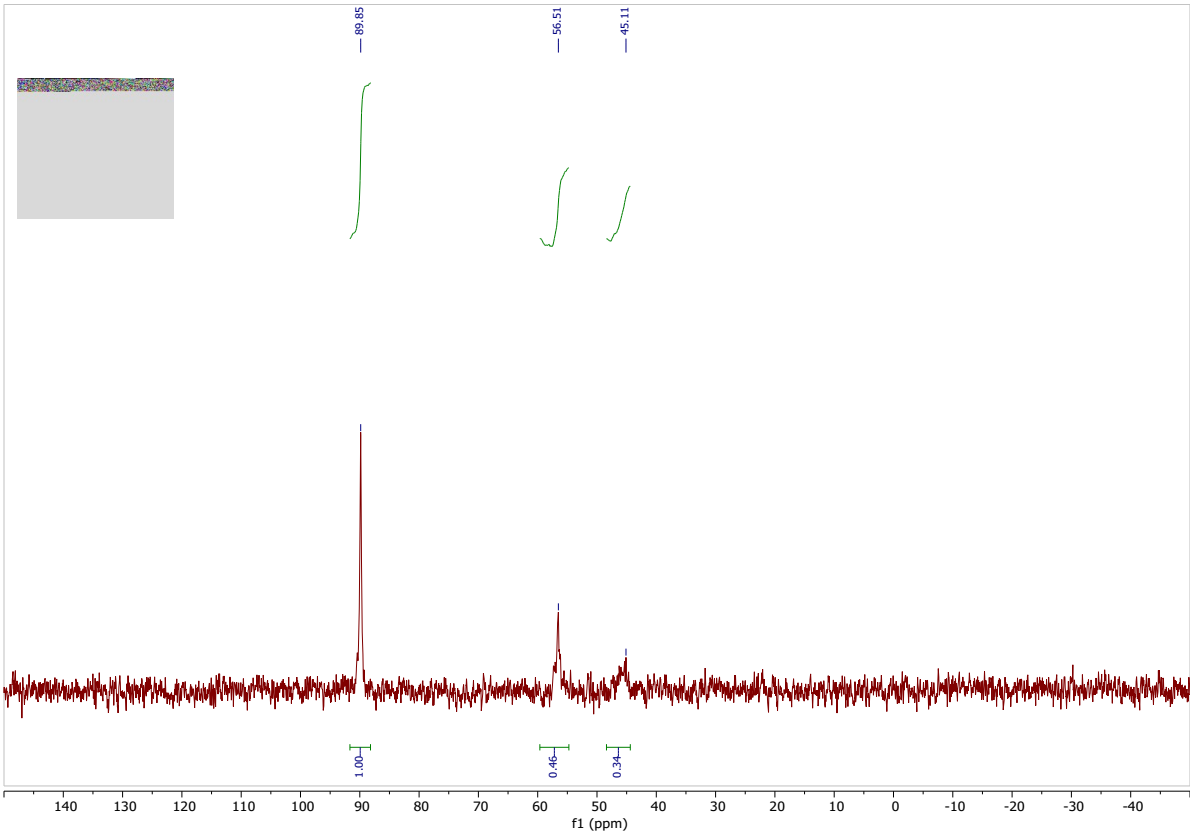


Figure S24. ^{1}H NMR spectrum of complex **5b** (600 MHz, CD_2Cl_2)

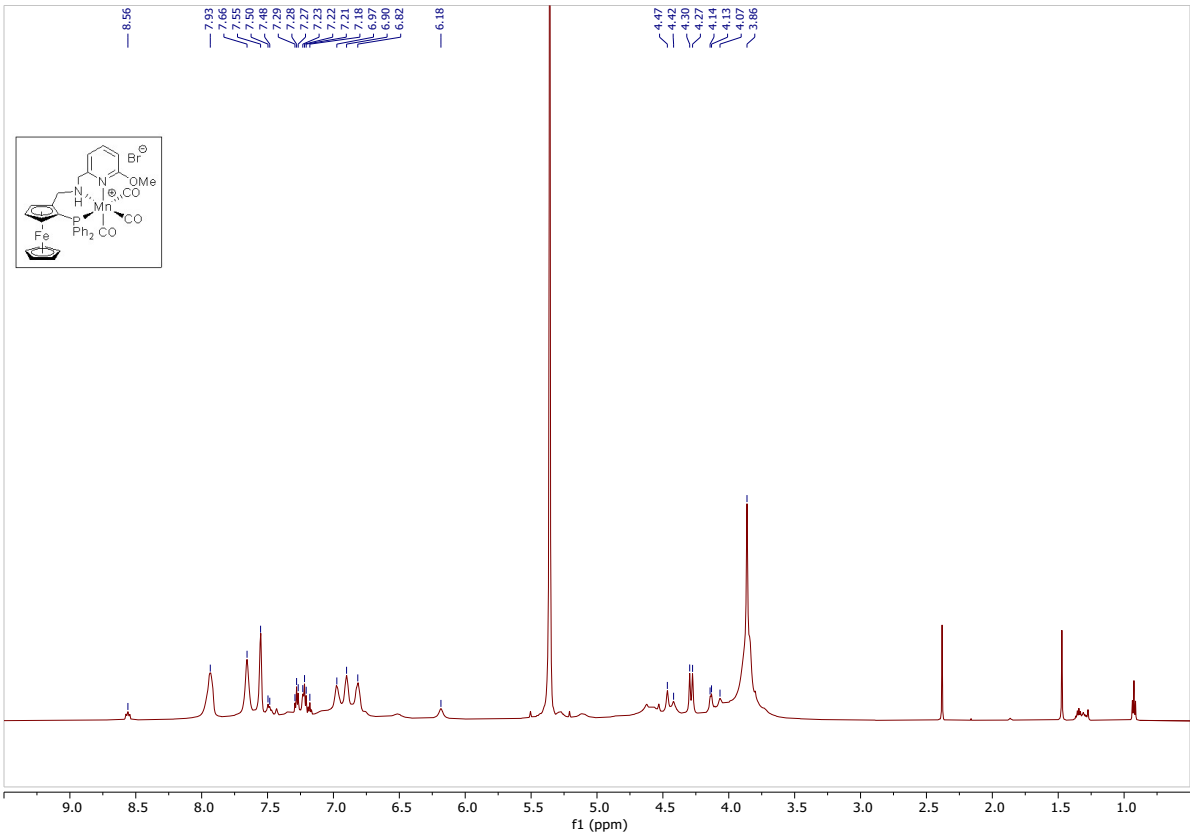


Figure S25. $^{31}P\{^{1}H\}$ NMR spectrum of complex **5b** (243 MHz, CD_2Cl_2)

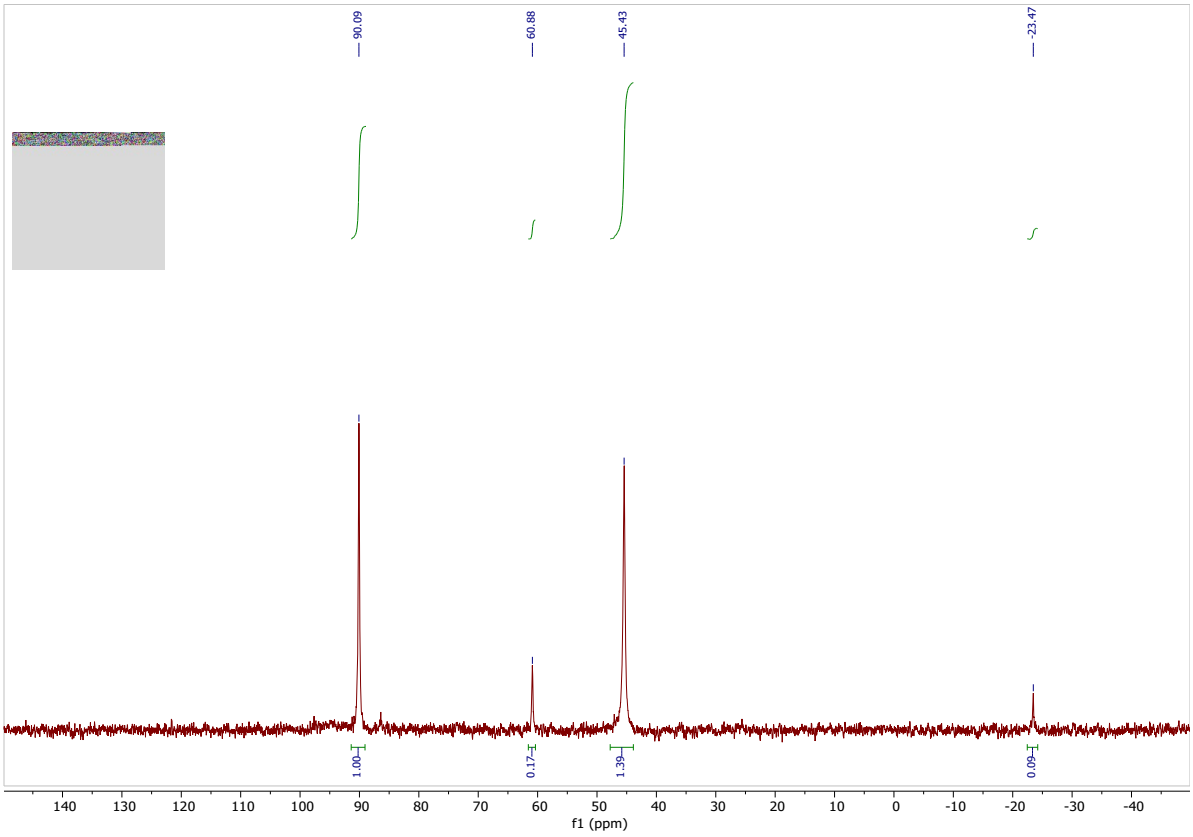


Figure S26. $^{13}C\{^{1}H\}$ NMR spectrum of complex **5b** (151 MHz, CD_2Cl_2)

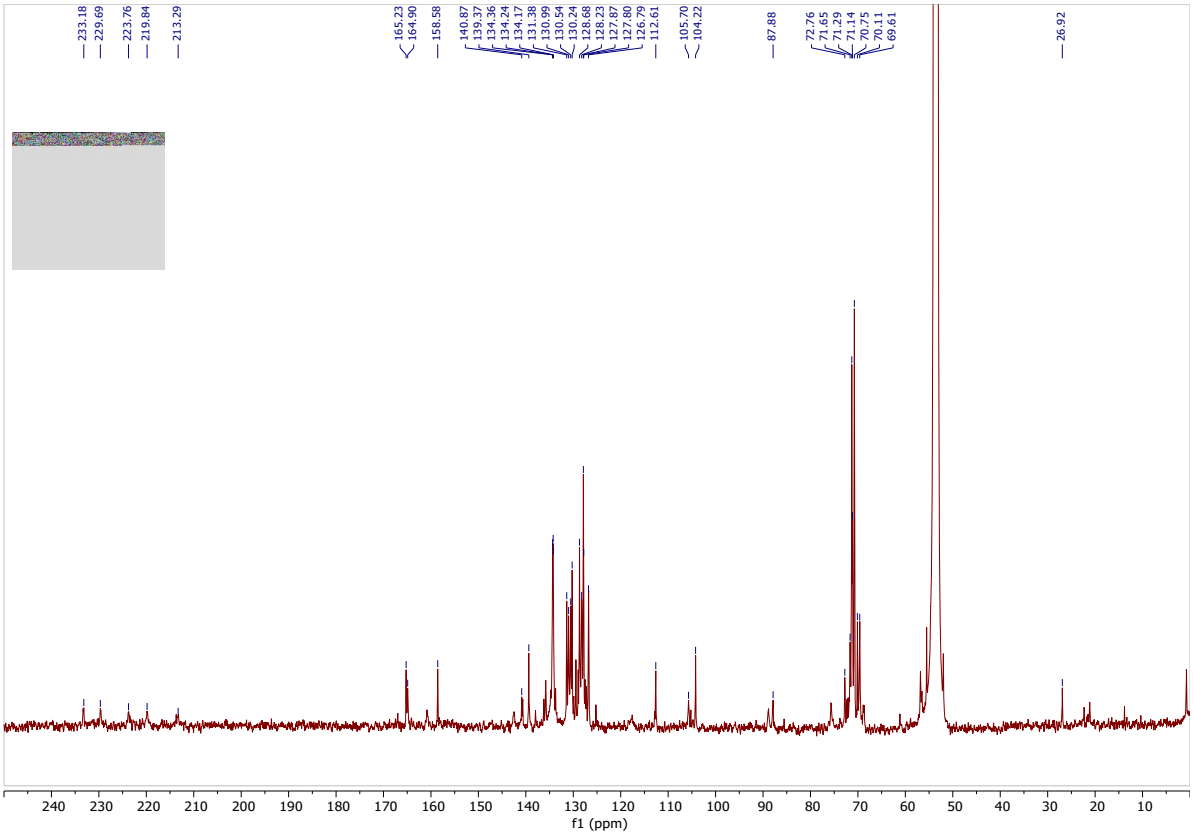


Figure S27. ^{1}H NMR spectrum of complex **5b** with BARF anion (600 MHz, acetone-d_6)

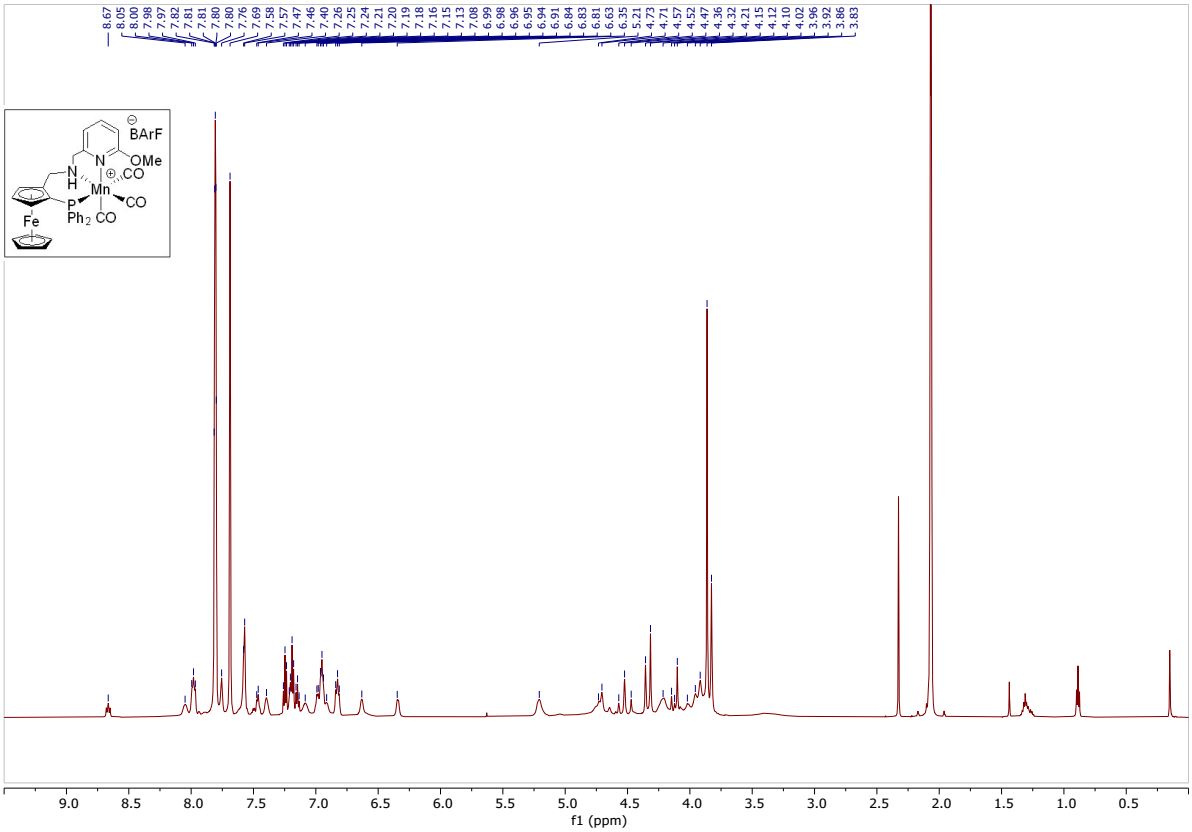


Figure S28. ^{31}P{^{1}H} NMR spectrum of complex **5b** with BARF anion (243 MHz, acetone-d_6)

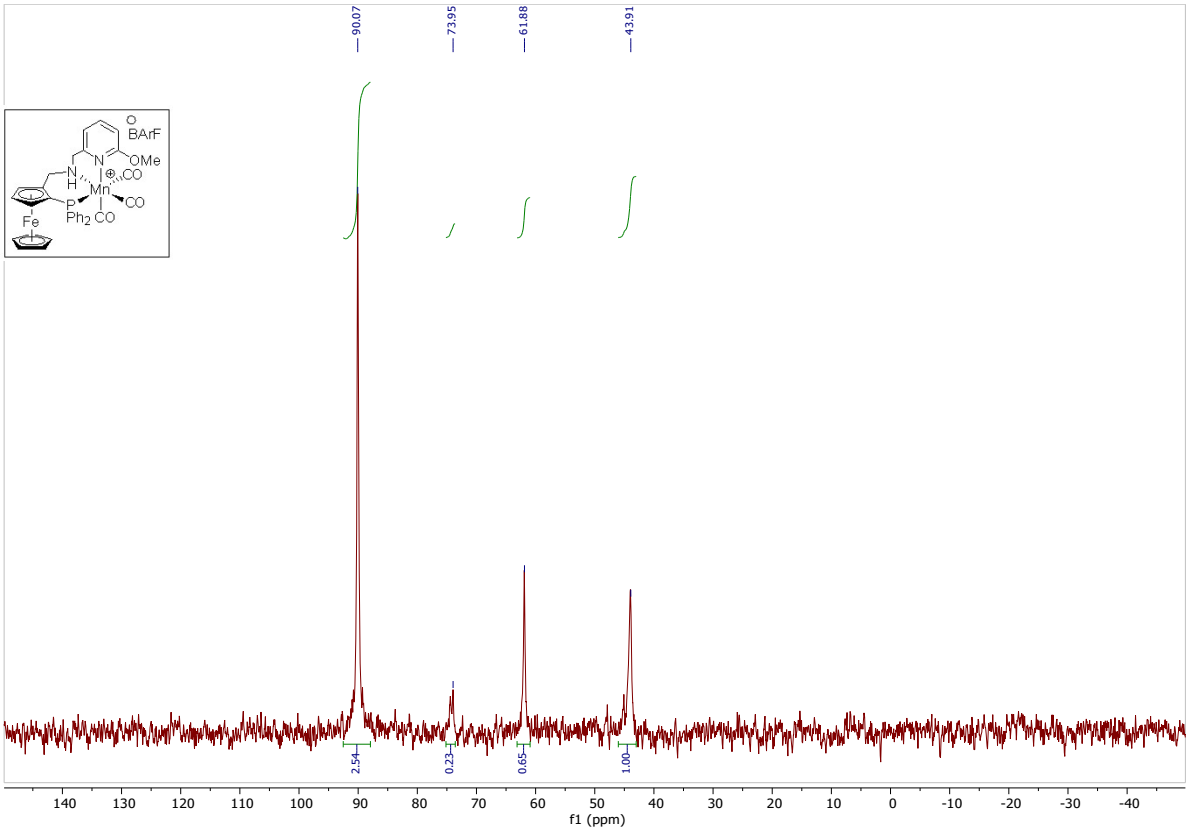


Figure S29. ^{13}C{^{1}H} NMR spectrum of complex **5b** with BARF anion (151 MHz, acetone-d_6)

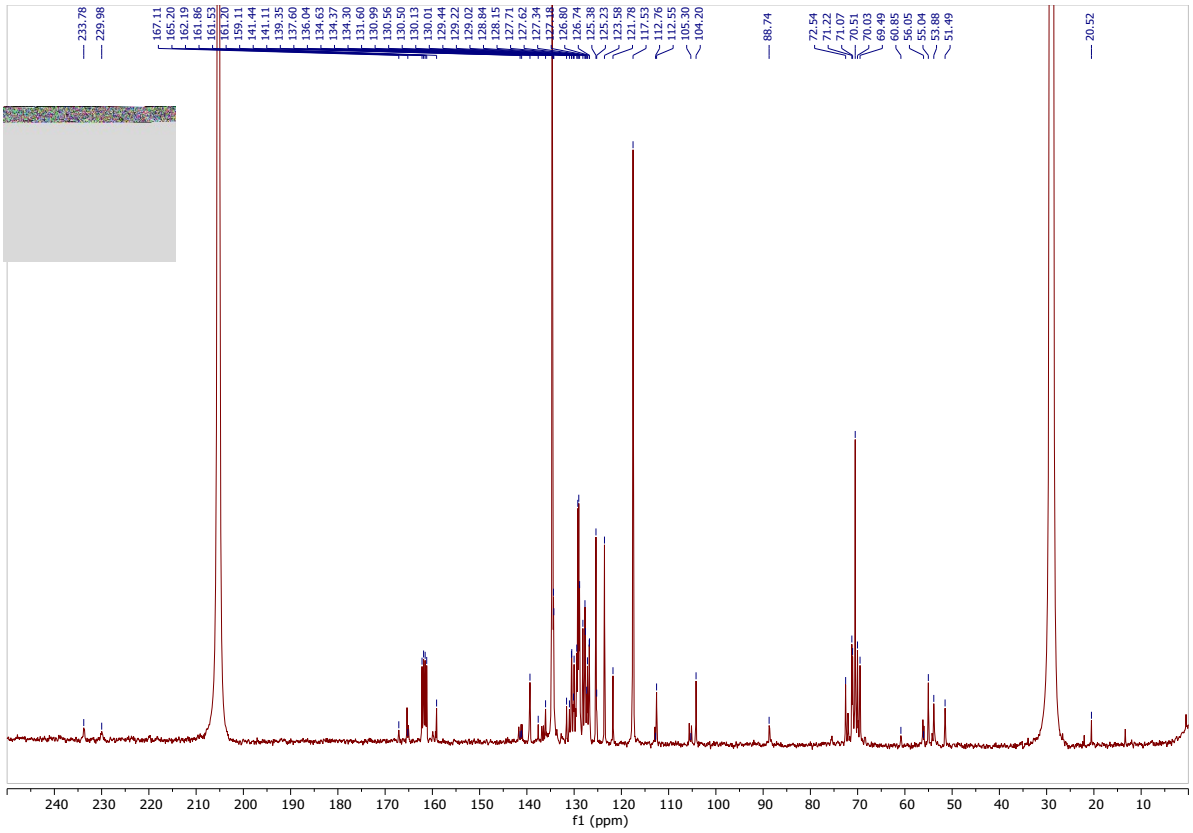


Figure S30. ^{31}P CP-MAS NMR spectrum of complex **5a**

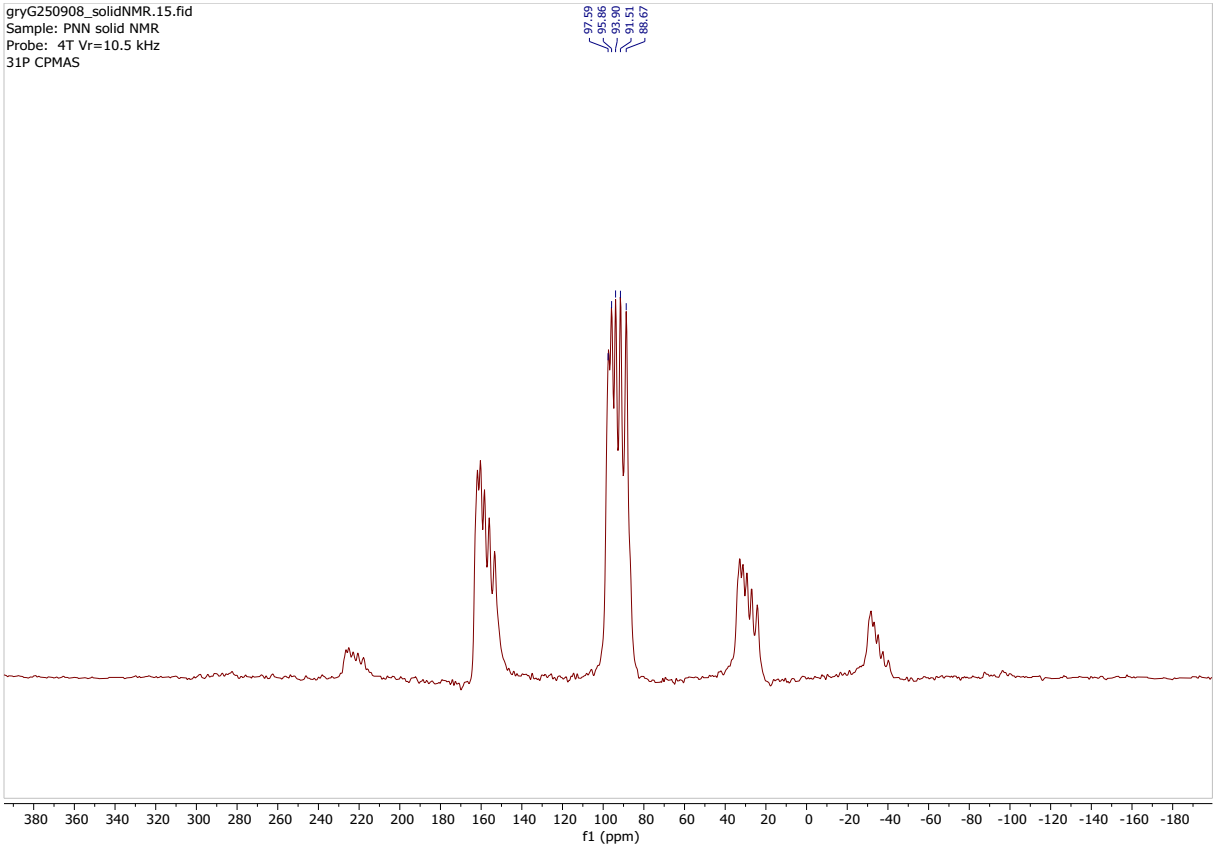
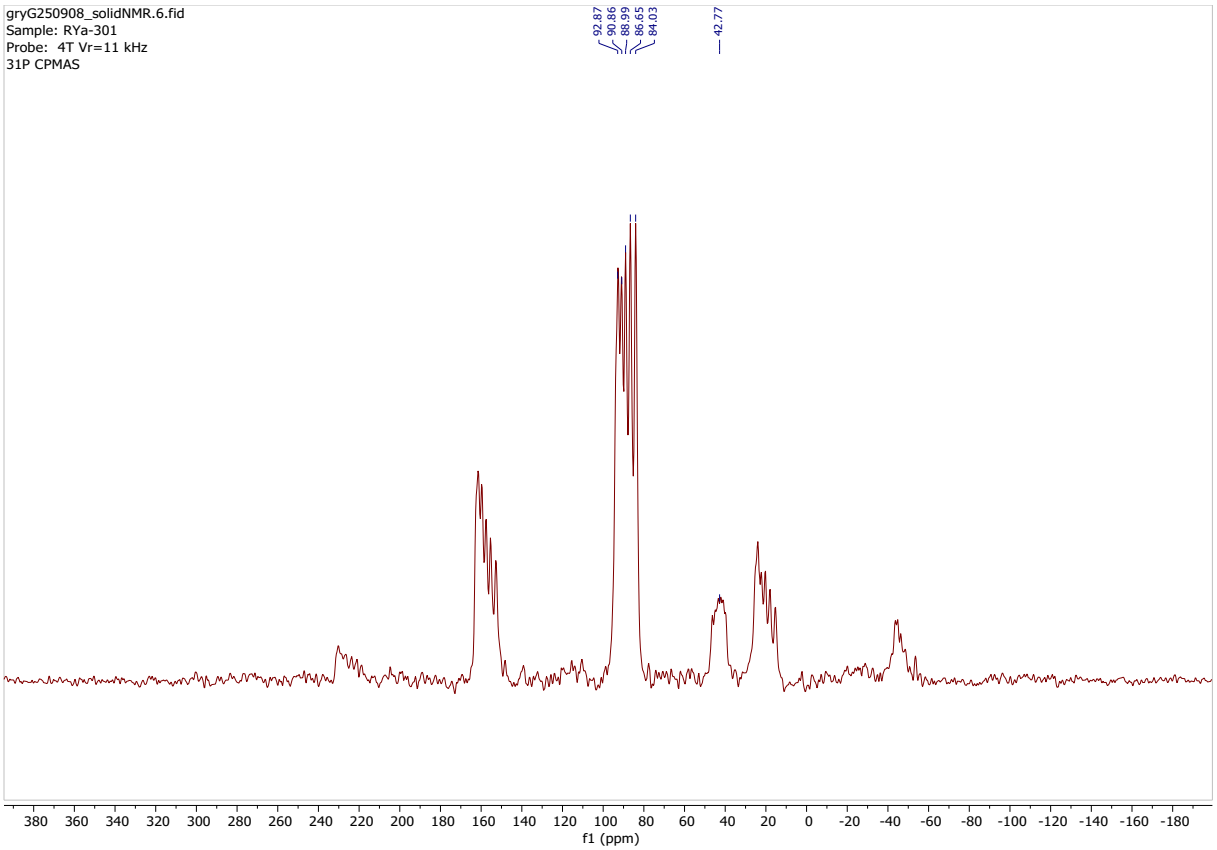


Figure S31. ^{31}P CP-MAS NMR spectrum of complex **5b**


gryG250908_solidNMR.6.fid
Sample: RYa-301
Probe: 4T Vr=11 kHz
31P CPMAS
92.87
90.86
88.99
86.65
84.03
42.77
380 360 340 320 300 280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180
f1 (ppm)

IR spectra

Figure S32. IR spectra of complex **5a** (ATR and DCM solution)

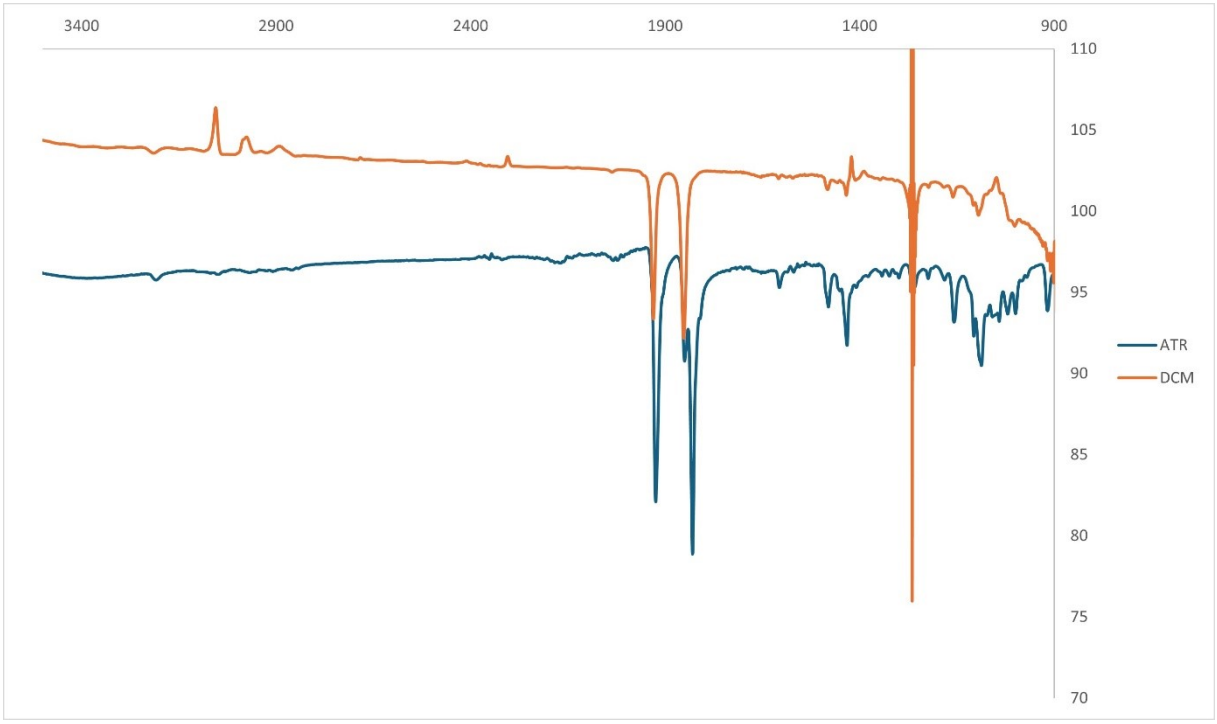
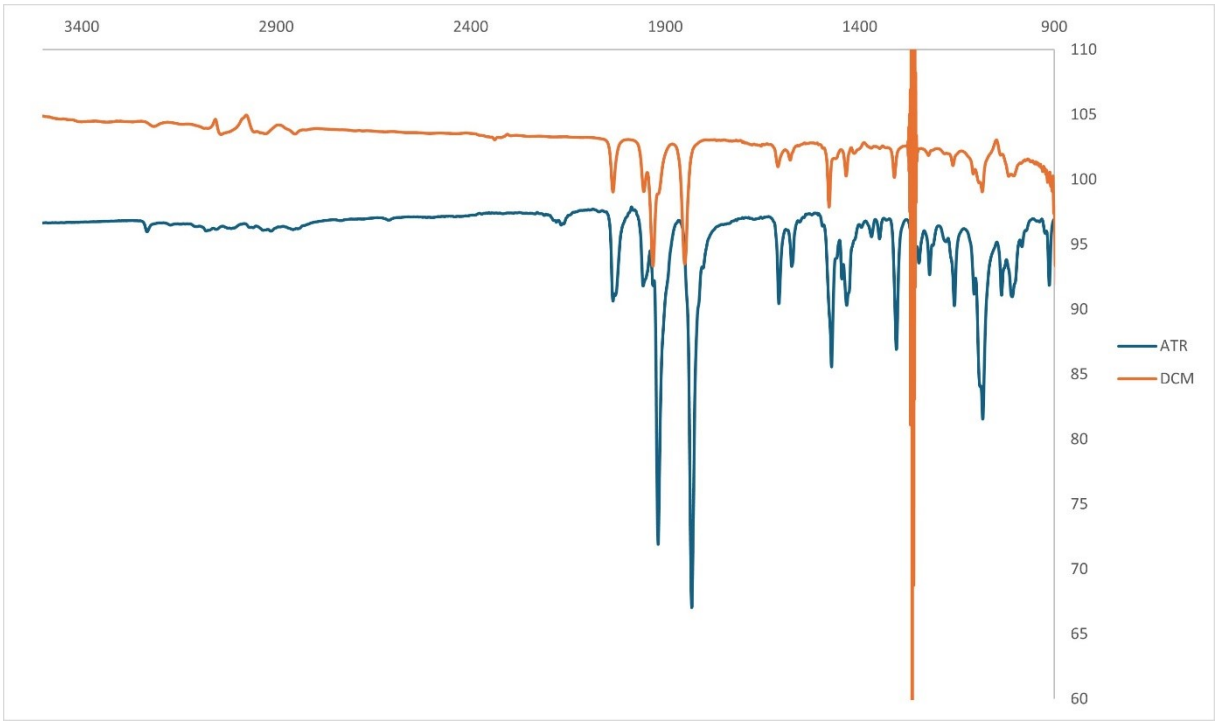


Figure S33. IR spectra of complex **5b** (ATR and DCM solution)



Computational studies

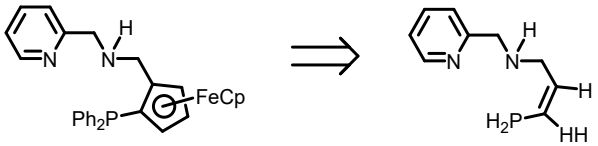
1. Computational details

DFT calculations for the full catalytic cycle and for the relative energies and IR absorption spectra of the $[MnBr(CO)_2(L)]$ and $[Mn(CO)_3(L)]^+Br^-$ stereoisomers were carried out using the Gaussian 16 suite of programs[9] with the M06 functional[10] and an SMD polarizable continuum model[11] to account for solvation effects in ethanol (ε = 24.852). Optimisations were performed using basis set BS1, which includes the 6-31G(d,p) basis set for the main-group atoms,[12, 13] and the scalar relativistic Stuttgart-Dresden (SDD) effective core potential (ECP) and its associated double-ξ basis set,[14] complemented with a set of polarisation functions for the Mn (α = 2.195) and Fe (α = 2.462) atoms.[15] Frequency calculations were carried out with BS1 to obtain thermal corrections and to verify the number of imaginary frequencies. Connections between the transition states and the corresponding minima were checked by displacing the geometry of the transition states along the normal coordinate with negative curvature in both directions and subsequent geometry optimisation. The energies were refined by single-point calculations at the optimized BS1 geometries using the same functional (M06), adding Grimme's D3 correction to account for long-range dispersion effects,[16] and an extended basis set (BS2), which consists of the def2-TZVP basis set for the main group atoms, and the quadruple-ζ def2-QZVP basis set for Mn and Fe.[17, 18] Gibbs energies in ethanol were calculated by adding the thermal and entropic corrections obtained with BS1 to the BS2 energies in solvent. An additional correction of 1.9 kcal/mol was applied to all Gibbs energies to change the standard state from the gas phase (1 atm) to the condensed phase (1 M) at 298.15 K.

The enantiodetermining transition states ($\mathbf{TS_{FG}}$) for both catalysts were recalculated at the same computational level used in a previous publication.[19] This consists of geometry optimizations with the BP86 functional [20, 21] and the def2-SVP basis set [17, 18, 22, 23] with implicit solvation handled with the IEF-PCM. The energies were then refined at the fixed BP96/def2-SVP-optimized geometries using the PBE0 functional [24, 25] with the def2-TZVP basis set and including the D3BJ empirical dispersion correction and implicit solvent model.

2. Relative energies of the $[MnBr(CO)_2(L)]$ and $[Mn(CO)_3(L)]^+Br^-$ stereoisomers: preliminary investigations on a simplified model

For these initial calculations, the full ligand **4a** was simplified as follows:



This allows to run faster calculations on all possible isomers and see whether certain stereochemical possibilities can be neglected. The relevant results are shown in Figure S34.

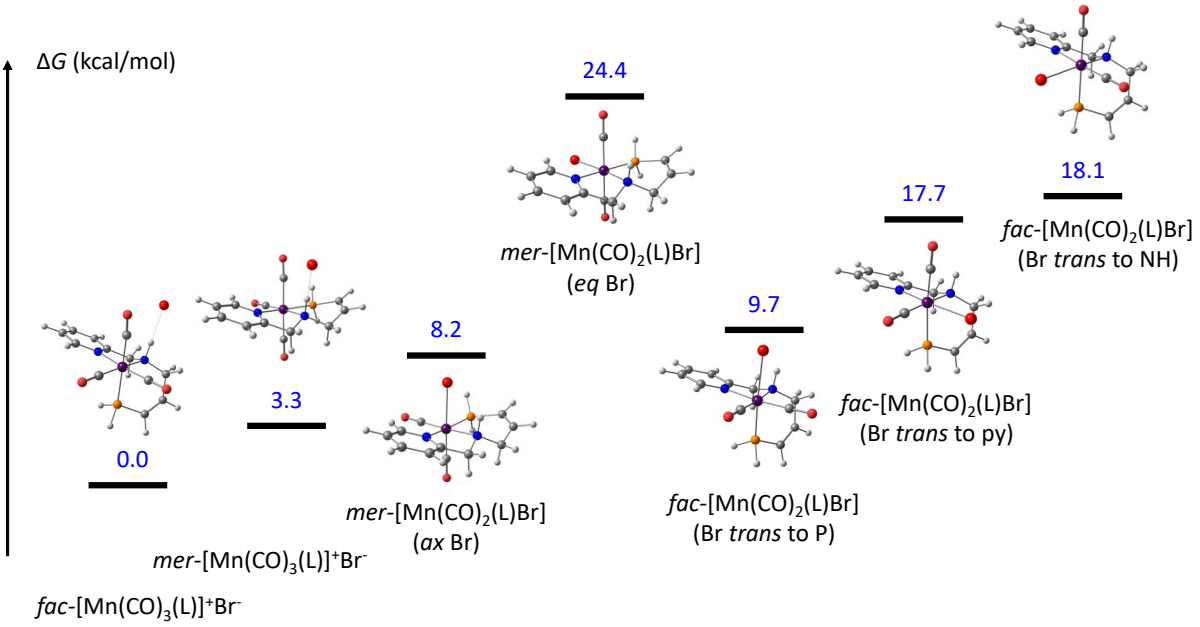


Figure S34. Relative Gibbs energies and views of the optimized geometries of all possible stereoisomers of $[Mn(CO)_3(L)]^+Br^-$ and $[MnBr(CO)_2(L)]$.

For the ionic tricarbonyl derivatives (1st and 2nd structure), the *facial* is slightly more stable than the *meridional*. This is expected because there is no competition between the strong π-acidic carbonyl ligands (only a weak one between the mutually *trans* CO and PH_2 donors). However, this energy difference may be modulated by the different strain of the tridentate P,N,N ligand when occupying *mer* or *fac* positions.

For the dicarbonyl derivatives with L occupying *mer* positions, there are two stereochemical possibilities, with the Br atom in an *axial* or in an *equatorial* position (3rd and 4th structure). The *equatorial* isomer is greatly disfavored, because the two residual CO ligands are *trans* to each other and competing for the metal *d* electrons in π back-bonding.

For the dicarbonyl derivatives with L occupying *fac* positions, there are three possibilities, with Br *trans* to the PH_2, NH and pyridine donor function (5th, 6th and 7th structure). The 5th is favoured because the two CO ligands have stronger σ-donor and weaker (or no) π-accepting ligands *trans* to them. The strongest π-acceptor (after the two CO ligands) is PH_2, which is *trans* to Br, whereas in the other two structures there is π-competition between CO and PH_2.

Note that the relative Gibbs energies are calculated under standard conditions (all concentrations equal to 1 molar in solution including that of CO). Since CO is very little soluble in DCM, the dicarbonyl structures are greatly stabilized relative to the tricarbonyl ones, but it is impossible to estimate by how much.

For the calculations with the full ligand, only the four lower-energy structures were used.

3. Relative energies and IR spectra of the $[Mn(CO)_3(L)]^+Br^-$ and $[MnBr(CO)_2(L)]$ stereoisomers with the full ligand.

The molecules were calculated at the full quantum-mechanical level. The relative Gibbs energies in Figure S35 are given in blue color and the optimized geometry and IR spectrum in the CO stretching region are shown with the calculated frequencies in cm^{-1}. With the full ligand, the dicarbonyl *fac* complex becomes more stable than the dicarbonyl *mer* isomer. The major electronic change is from PH_2 to PPh_2, which might introduce more π-competition in the *mer* structure between the PPh_2 and pyridine donors. The Gibbs energy difference between tricarbonyl *fac* and *mer* has remained approximately the same.

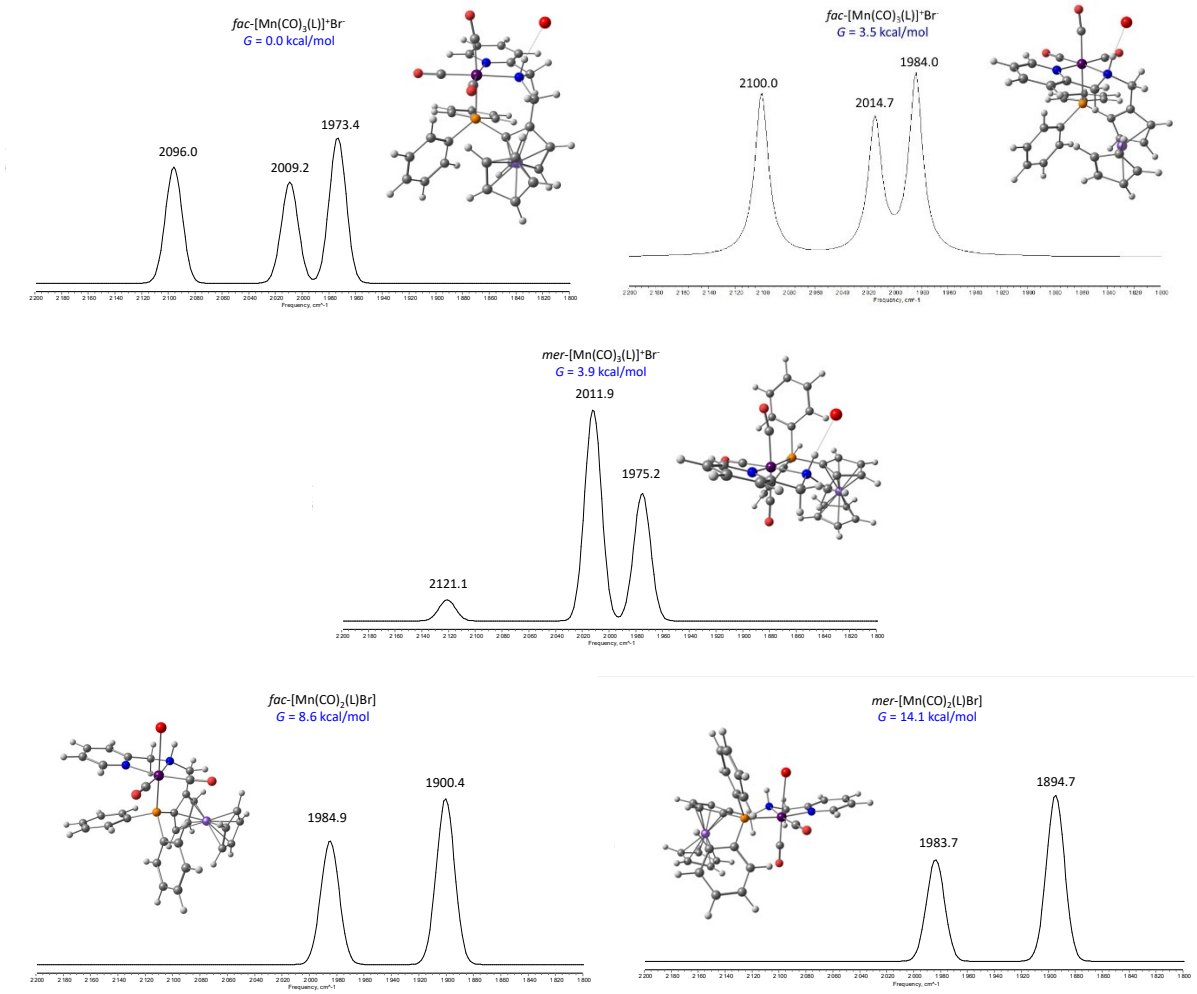


Figure S35. Views of the optimized geometries and of the simulated IR spectra in the CO stretching region of various stereoisomers of $[Mn(CO)_3(L)]^+Br^-$ and $[MnBr(CO)_2(L)]$. An artificial Lorentzian line broadening of 15 cm^{-1} (width at half-height) was applied.

4. Cartesian coordinates (Å), energies (hartrees), and views of all optimized geometries

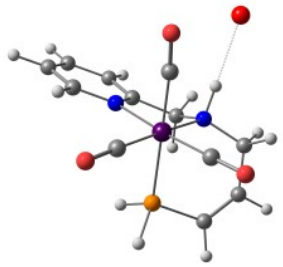
A. Simplified L molecules (Figure S34).

CO
E (BS1) = -113.243514629
E (BS2) = -113.29581323
G_{1M} = -113.306884

8 0.000000000 0.000000000 -0.487385000

6 0.000000000 0.000000000 0.649847000

***fac*-[Mn(CO)$_3$(L)]$^+$Br$^-$**
E (BS1) = -1258.90223273
E (BS2) = -4866.63231426
G_{1M} = -4866.445669



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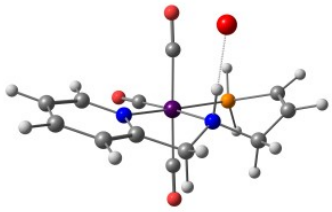
8	-1.975520000	2.738440000	-1.426335000
7	0.320415000	0.856854000	0.833929000
7	-0.144190000	-1.659266000	0.118514000
6	-2.326001000	1.547890000	2.193920000
6	-1.227835000	2.310543000	2.212170000
6	0.062534000	2.154403000	1.477375000
1	0.128522000	2.935109000	0.704273000
6	0.664539000	-0.172737000	1.831882000
1	1.651430000	0.037289000	2.270059000
1	-0.061489000	-0.140980000	2.658216000
6	0.642419000	-1.525075000	1.203238000
6	-0.230660000	-2.863055000	-0.475262000
1	-0.861059000	-2.928815000	-1.359103000
6	0.446843000	-3.973713000	-0.005053000
1	0.341051000	-4.924086000	-0.518941000
6	1.261238000	-3.836558000	1.114563000
6	1.363118000	-2.594334000	1.722259000
1	1.994582000	-2.437179000	2.593018000
6	-2.205614000	-0.717468000	-1.642598000
6	-1.599210000	1.690445000	-1.102065000
6	0.193326000	0.066174000	-1.978919000
8	0.830726000	-0.002400000	-2.938147000
1	1.195717000	0.999981000	0.293095000
1	1.815756000	-4.686544000	1.503596000
1	0.883257000	2.371097000	2.181324000
1	-1.240890000	3.193159000	2.854239000
1	-3.176252000	1.827007000	2.815247000
1	-2.520117000	-0.998788000	2.038506000
1	-3.894705000	0.133406000	0.824186000
35	3.325981000	1.204728000	-0.386901000

***mer*-[Mn(CO)$_3$(L)]$^+$Br$^-$**
E (BS1) = -1258.89443575
E (BS2) = -4866.62606508
G_{1M} = -4866.440447



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8	-2.822093000	1.087625000	2.186456000
7	0.211474000	-0.692113000	1.054241000
7	0.253090000	1.765308000	0.064969000
6	-1.594540000	-3.050173000	0.202144000
6	-0.653392000	-3.032385000	1.148979000
6	-0.180125000	-1.829857000	1.912146000
1	-0.962333000	-1.482752000	2.605783000
6	0.873309000	0.331910000	1.881483000
1	0.206480000	0.588606000	2.720071000
1	1.807558000	-0.056503000	2.313409000
6	1.134705000	1.545712000	1.057326000
6	0.410069000	2.844544000	-0.719898000
1	-0.314560000	2.977418000	-1.520058000
6	1.439271000	3.750735000	-0.534169000
1	1.523866000	4.608875000	-1.193714000
6	2.348883000	3.529985000	0.495067000
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1	2.890681000	2.187191000	2.104276000
6	-2.284305000	1.270005000	-1.172750000
6	-2.140879000	0.806759000	1.297746000
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8	0.014819000	-0.546151000	-2.799177000
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1	3.172172000	4.219270000	0.663531000
1	0.684351000	-2.117695000	2.527401000
1	-2.894802000	-1.908041000	-1.626730000
1	-3.677757000	-1.597528000	0.353293000
1	-1.873931000	-3.988311000	-0.275783000
1	-0.193750000	-3.979078000	1.434141000
35	2.882367000	-1.712075000	-0.572712000

***mer*-[MnBr(CO)$_2$(L)] (*axial* Br)**
E (BS1) = -1145.62534042
E (BS2) = -4753.30840173
G_{1M} = -4753.125734

25	0.337707000	-0.224511000	0.571592000
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8	0.127500000	-2.765160000	2.008685000
8	0.593334000	1.227463000	3.090229000
7	0.383491000	1.543471000	-0.605948000
7	-1.668769000	0.090848000	0.301885000
6	3.365076000	0.763104000	-0.682075000
6	2.827151000	1.944939000	-0.992494000
6	1.510235000	2.495245000	-0.528084000
1	1.585125000	2.829923000	0.518482000
6	-0.875624000	2.260399000	-0.340343000
1	-0.752185000	2.802251000	0.610739000
1	-1.087247000	3.011171000	-1.115035000
6	-2.001744000	1.291421000	-0.206196000
6	-2.635059000	-0.823470000	0.478745000
1	-2.325411000	-1.787101000	0.876874000
6	-3.962973000	-0.573713000	0.172532000
1	-4.707070000	-1.346844000	0.338969000
6	-4.307394000	0.666288000	-0.354249000
6	-3.309005000	1.610502000	-0.551730000
1	-3.527532000	2.589412000	-0.971276000
6	0.208259000	-1.745339000	1.439385000
6	0.469270000	0.656684000	2.072606000
1	0.346668000	1.175850000	-1.561688000
1	-5.338606000	0.891696000	-0.613856000
1	1.269432000	3.387208000	-1.123702000
35	0.257789000	-1.514436000	-1.658610000
1	3.081394000	-1.654200000	-0.064384000
1	4.344565000	0.500878000	-1.082351000
1	3.403446000	2.617718000	-1.629003000
1	3.364953000	-0.310401000	1.579295000

***mer*-[MnBr(CO)$_2$(L)] (*equatorial* Br)**
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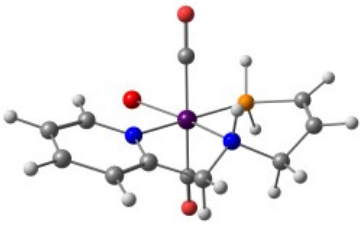
G_{1M} = -4753.099839



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8	-0.777082000	0.165573000	2.943865000
7	-0.233736000	-1.997532000	-0.177625000
7	1.695783000	-0.164599000	-0.039345000
6	-3.271087000	-1.499492000	-0.634592000
6	-2.642960000	-2.655537000	-0.400225000
6	-1.341835000	-2.836795000	0.329283000
1	-1.464967000	-2.595303000	1.396485000
6	1.021917000	-2.401579000	0.482849000
1	0.839544000	-2.380544000	1.568922000
1	1.308923000	-3.429836000	0.219737000
6	2.106101000	-1.432574000	0.150704000
6	2.612524000	0.773828000	-0.318918000
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6	3.966555000	0.489470000	-0.404793000
1	4.669797000	1.285802000	-0.630574000
6	4.391673000	-0.819575000	-0.206013000
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6	-0.430490000	0.448125000	-1.791037000
6	-0.537012000	0.068847000	1.808006000
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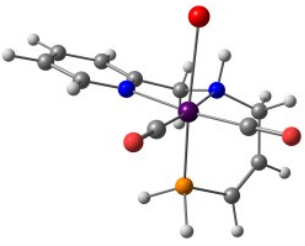
1	5.445619000	-1.077451000	-0.273511000
1	-1.045738000	-3.894142000	0.276766000
35	-0.275318000	2.653269000	0.269277000
1	-3.207738000	0.972959000	-1.036401000
1	-4.227345000	-1.505521000	-1.158139000
1	-3.122925000	-3.578836000	-0.727386000
1	-3.365124000	0.408285000	1.016169000

***fac*-[MnBr(CO)$_2$(L)] (Br *trans* to P)**
E (BS1) = -1145.6234991
E (BS2) = -4753.30622661
G_{1M} = -4753.123370



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8	-3.198511000	-1.448608000	-0.038706000
7	-0.552588000	0.928545000	-1.301746000
7	1.429546000	0.384710000	0.400474000
6	-2.439560000	2.368665000	0.609185000
6	-2.562342000	2.338307000	-0.721801000
6	-1.822434000	1.528485000	-1.739134000
1	-2.476083000	0.716030000	-2.089488000
6	0.516858000	1.936792000	-1.202876000
1	0.814153000	2.303135000	-2.195633000
1	0.124247000	2.806594000	-0.654813000
6	1.691429000	1.383109000	-0.463168000
6	2.445463000	-0.125653000	1.115391000
1	2.201611000	-0.942419000	1.791127000
6	3.745070000	0.341214000	1.010524000
1	4.528000000	-0.106132000	1.615507000
6	4.014971000	1.371369000	0.115678000
6	2.972566000	1.894879000	-0.635354000
1	3.136448000	2.693418000	-1.354868000
6	-0.315134000	-1.447858000	1.744454000
6	-2.125768000	-1.011536000	0.130452000
1	-0.276677000	0.253228000	-2.020036000
1	5.025169000	1.755914000	0.000302000
1	-1.643229000	2.169217000	-2.617303000
35	0.400924000	-2.137527000	-1.264880000
1	-3.312886000	2.990587000	-1.172735000
1	-3.081232000	3.043426000	1.176556000
1	-2.096095000	1.051421000	2.703067000
1	-0.425249000	2.260009000	2.134553000

***fac*-[MnBr(CO)$_2$(L)] (Br *trans* to py)**
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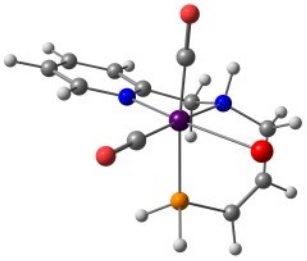
E (BS2) = -4753.29273971
G_{1M} = -4753.110555



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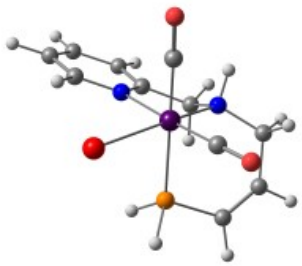
8	-0.394313000	-2.869810000	1.726630000
7	0.022097000	1.296497000	-1.138481000
7	1.828789000	-0.258091000	0.099770000
6	-1.322104000	2.492963000	1.347917000
6	-1.444499000	2.944550000	0.096311000
6	-1.044411000	2.313206000	-1.197890000
1	-1.931403000	1.834876000	-1.636482000
6	1.317523000	1.917999000	-0.809732000
1	1.696248000	2.526174000	-1.643391000
1	1.160443000	2.608530000	0.032355000
6	2.321479000	0.893019000	-0.398274000
6	2.700077000	-1.184873000	0.541187000
1	2.269620000	-2.105139000	0.928760000
6	4.071447000	-1.002714000	0.507290000
1	4.724750000	-1.785975000	0.880013000
6	4.578753000	0.182465000	-0.015623000
6	3.687654000	1.139381000	-0.477484000
1	4.033324000	2.080256000	-0.899057000
6	-0.052082000	-1.612590000	-1.410555000
6	-0.289212000	-1.932494000	1.027739000
1	0.099443000	0.930176000	-2.086132000
1	5.650659000	0.355224000	-0.066154000
1	-0.739617000	3.114288000	-1.889736000
35	-2.720862000	-0.583137000	-0.321876000
1	-1.926205000	3.914920000	-0.040773000
1	-1.697263000	3.110681000	2.164318000
1	-1.550141000	0.433516000	2.752348000
1	0.413541000	1.274146000	2.688794000

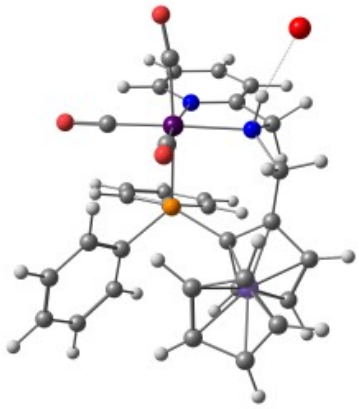
***fac*-[MnBr(CO)$_2$(L)] (Br *trans* to NH)**
E (BS1) = -1145.60922504
E (BS2) = -4753.29239409
G_{1M} = -4753.109994



25	0.481860000	-0.207395000	0.379700000
15	1.085997000	0.654984000	-1.690502000
8	-0.101647000	-1.511049000	2.948407000
8	3.325106000	-0.353746000	1.037575000
7	0.176500000	1.793310000	0.949130000
7	-1.573933000	0.026472000	-0.029785000
6	1.939805000	2.251600000	-1.541481000
6	1.964136000	2.973906000	-0.416149000
6	1.304015000	2.744481000	0.907072000
1	2.059935000	2.395608000	1.624828000
6	-1.011657000	2.348028000	0.269604000
1	-1.427561000	3.197123000	0.829720000
1	-0.699250000	2.743136000	-0.708288000
6	-2.040145000	1.285493000	0.063505000
6	-2.450306000	-0.968133000	-0.237725000
1	-2.020025000	-1.966989000	-0.294466000
6	-3.811284000	-0.748006000	-0.378903000
1	-4.477834000	-1.588558000	-0.548236000
6	-4.291720000	0.553592000	-0.288848000
6	-3.391916000	1.584748000	-0.057846000
1	-3.721908000	2.616846000	0.032105000
6	0.109863000	-0.953609000	1.942528000
6	2.183626000	-0.286919000	0.770724000
1	-0.065830000	1.703829000	1.935061000
1	-5.354178000	0.761779000	-0.387652000
1	0.961132000	3.722670000	1.281184000
35	0.575931000	-2.517105000	-0.697601000
1	2.555728000	3.891826000	-0.422597000
1	2.498417000	2.616628000	-2.403581000
1	2.020963000	-0.078731000	-2.453519000
1	0.144218000	0.912401000	-2.721676000

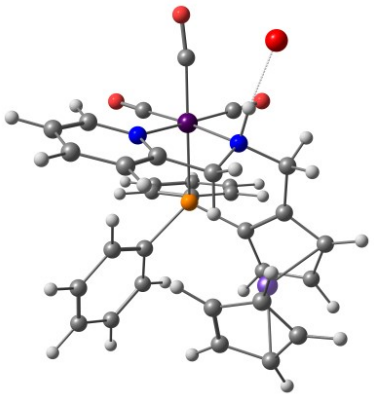
B. Full L molecules (Figure S35).

***fac*-[Mn(CO)$_3$(L)]$^+$Br$^-$ (best diastereoisomer)**
E (BS1) = -2152.88032312
E (BS2) = -6900.66601254
G_{1M} = -6900.215713



26	-2.768919000	-1.436445000	-1.109901000
25	1.238621000	-0.065745000	1.136611000
15	-0.588611000	0.990401000	0.102930000
8	0.964733000	1.846858000	3.355828000
8	-0.380464000	-2.127699000	2.479715000
7	1.457703000	-1.290958000	-0.562950000
7	2.541143000	1.090772000	0.007610000
6	-1.306245000	-0.027718000	-1.206881000
6	-0.799438000	-1.306403000	-1.638635000
6	-1.582928000	-1.719861000	-2.754175000
1	-1.465983000	-2.662899000	-3.279530000
6	-2.569018000	-0.725901000	-3.015038000
1	-3.341241000	-0.778246000	-3.774874000
6	-2.403287000	0.318884000	-2.067289000
1	-3.007018000	1.217653000	-1.993471000
6	-3.286915000	-1.813441000	0.838320000
1	-2.773254000	-1.425240000	1.710866000
6	-2.981622000	-3.027334000	0.160310000
1	-2.189146000	-3.721678000	0.420731000
6	-3.868736000	-3.145256000	-0.949328000
1	-3.865285000	-3.941431000	-1.686008000
6	-4.720257000	-2.001737000	-0.956827000
1	-5.476638000	-1.778084000	-1.701396000
6	-4.358374000	-1.174704000	0.146917000
1	-4.797378000	-0.214144000	0.397836000
6	-0.063412000	2.531549000	-0.731643000
6	0.134121000	3.680724000	0.044038000
1	-0.120565000	3.674982000	1.104173000
6	0.655353000	4.834044000	-0.530829000
1	0.796932000	5.724077000	0.078372000
6	1.002841000	4.845544000	-1.880040000
1	1.416828000	5.745946000	-2.328515000
6	0.816717000	3.704149000	-2.654020000
1	1.082900000	3.709658000	-3.708904000
6	0.281730000	2.550579000	-2.084964000
1	0.136540000	1.663727000	-2.701888000
6	-2.010819000	1.546301000	1.118958000
6	-2.221761000	1.034229000	2.401568000
1	-1.520724000	0.325093000	2.837215000
6	-3.339539000	1.414280000	3.140104000
1	-3.489969000	1.005593000	4.136667000
6	-4.254288000	2.315628000	2.605809000
1	-5.126454000	2.614238000	3.183116000
6	-4.045868000	2.843573000	1.333197000
1	-4.751566000	3.557687000	0.914691000
6	-2.929774000	2.465706000	0.595312000
1	-2.769378000	2.899275000	-0.390802000
6	0.329529000	-2.105183000	-1.060628000
1	-0.003935000	-2.737763000	-0.229922000
6	2.132543000	-0.598331000	-1.672464000
1	2.800915000	-1.290896000	-2.206377000
1	1.379090000	-0.265354000	-2.402364000
6	2.875981000	0.604389000	-1.201781000
6	3.132325000	2.222021000	0.433814000
1	2.848728000	2.581281000	1.420273000
6	4.057881000	2.912892000	-0.327371000
1	4.497932000	3.825898000	0.061858000
6	4.407039000	2.408221000	-1.576372000
6	3.812976000	1.235174000	-2.013519000
1	4.054493000	0.800787000	-2.980471000
6	1.068040000	1.091658000	2.479134000
6	0.220399000	-1.286686000	1.950609000
6	2.720623000	-0.719762000	1.979727000
8	3.634558000	-0.988659000	2.630920000
1	2.130382000	-2.000494000	-0.214900000
1	5.136967000	2.921160000	-2.197294000
1	0.705036000	-2.790422000	-1.837460000
35	3.439711000	-3.783180000	0.199605000

***fac*-[Mn(CO)$_3$(L)]$^+$Br$^-$ (second diastereoisomer)**
E (BS1) = -2152.87134063
E (BS2) = -6900.65772182
G_{1M} = -6900.210088



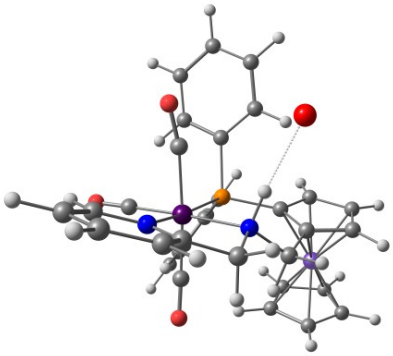
26	-1.798514000	-2.420128000	-0.939461000
25	1.330325000	1.373797000	-0.060784000
15	-1.007083000	0.900103000	-0.003895000
8	0.787444000	4.033330000	1.081544000
8	0.972578000	2.351921000	-2.816060000
7	1.690022000	-0.595242000	-0.696368000
7	1.815030000	0.476874000	1.744057000
6	-1.400338000	-0.418013000	-1.184736000
6	-0.442624000	-1.196073000	-1.922314000
6	-1.170961000	-2.009877000	-2.839005000
1	-0.728286000	-2.738172000	-3.511824000
6	-2.559901000	-1.729852000	-2.696263000
1	-3.366546000	-2.219699000	-3.231010000
6	-2.709601000	-0.764997000	-1.665083000
1	-3.646846000	-0.361830000	-1.294966000
6	-1.489328000	-3.108850000	0.979340000
1	-0.989074000	-2.572716000	1.780789000
6	-0.870538000	-3.976892000	0.033196000
1	0.187730000	-4.209374000	-0.028056000
6	-1.882094000	-4.455587000	-0.847274000
1	-1.728064000	-5.104690000	-1.702484000
6	-3.124281000	-3.883646000	-0.444398000
1	-4.077262000	-4.019415000	-0.944587000
6	-2.881387000	-3.046252000	0.682670000
1	-3.617542000	-2.441212000	1.202594000
6	-1.900432000	2.349674000	-0.692720000
6	-2.224017000	3.419914000	0.149954000
1	-2.019732000	3.355984000	1.218567000
6	-2.814464000	4.568069000	-0.366052000
1	-3.067707000	5.389430000	0.300614000
6	-3.081654000	4.664172000	-1.729614000
1	-3.545032000	5.562050000	-2.132432000
6	-2.754913000	3.608334000	-2.574738000
1	-2.961207000	3.676519000	-3.640624000
6	-2.165815000	2.456005000	-2.061155000
1	-1.912435000	1.639489000	-2.735711000
6	-1.992453000	0.504812000	1.494857000
6	-1.379265000	-0.007376000	2.640991000
1	-0.301799000	-0.138190000	2.674688000
6	-2.141952000	-0.372307000	3.748358000
1	-1.648043000	-0.768700000	4.632862000
6	-3.524539000	-0.226377000	3.721490000
1	-4.120155000	-0.508336000	4.586859000
6	-4.145107000	0.289885000	2.585167000
1	-5.225520000	0.413558000	2.560413000
6	-3.385807000	0.655911000	1.479704000
1	-3.883364000	1.069696000	0.603995000
6	1.052744000	-1.144843000	-1.907484000
1	1.442819000	-2.160718000	-2.087417000
6	1.580495000	-1.526793000	0.434584000
1	0.536489000	-1.856653000	0.505473000
1	2.197836000	-2.421041000	0.258370000
6	1.957974000	-0.861621000	1.709635000
6	2.083989000	1.128652000	2.890421000
1	1.977740000	2.210860000	2.876256000
6	2.469035000	0.472180000	4.045538000
1	2.666388000	1.043534000	4.947270000
6	2.602211000	-0.913076000	4.016047000
6	2.350276000	-1.586283000	2.830253000
1	2.451182000	-2.666331000	2.755568000
6	0.982011000	2.980683000	0.633660000
6	1.077158000	1.970207000	-1.726087000
6	3.073635000	1.886485000	-0.170759000
8	4.123866000	2.364554000	-0.186787000
1	2.701217000	-0.581841000	-0.929404000
1	2.906503000	-1.459164000	4.905188000
1	1.399162000	-0.530795000	-2.751450000
35	4.864178000	-1.144367000	-1.264801000

***mer*-[Mn(CO)$_3$(L)]$^+$Br$^-$**

E (BS1) = -2152.87027356

E (BS2) = -6900.65635061

G_{1M} = -6900.209477



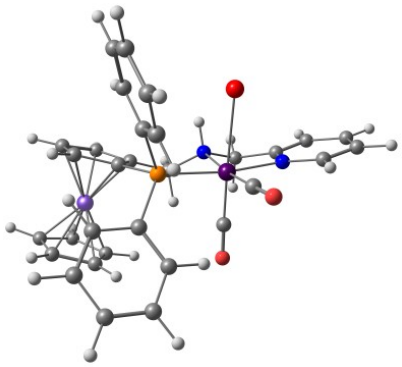
26	2.814376000	-1.828763000	0.273121000
25	-1.256000000	0.503212000	-1.013127000
15	0.670429000	0.925479000	0.155312000
8	-1.122341000	3.179190000	-2.216128000
8	0.053004000	-0.659721000	-3.428941000
7	-1.417716000	-1.471749000	-0.256273000
7	-3.127627000	0.001930000	-1.741814000
6	1.368319000	-0.558767000	0.915813000
6	0.832844000	-1.884780000	0.764452000
6	1.574041000	-2.747819000	1.621472000
1	1.429780000	-3.821231000	1.698804000
6	2.561299000	-1.977652000	2.299557000
1	3.305194000	-2.360278000	2.989880000
6	2.439132000	-0.629106000	1.870449000
1	3.052467000	0.204393000	2.196788000
6	3.196109000	-1.526297000	-1.711654000
1	2.560907000	-0.956047000	-2.383038000
6	3.082552000	-2.918673000	-1.435228000
1	2.342399000	-3.593911000	-1.852343000
6	4.071964000	-3.257876000	-0.466843000
1	4.215809000	-4.235218000	-0.018865000
6	4.798881000	-2.074622000	-0.146541000
1	5.592284000	-1.995342000	0.588902000
6	4.257229000	-1.002261000	-0.912735000
1	4.570755000	0.036084000	-0.866725000
6	0.297473000	1.994176000	1.597775000
6	0.168854000	3.375872000	1.413065000
1	0.413209000	3.824603000	0.449756000
6	-0.275964000	4.182685000	2.454316000
1	-0.368569000	5.256064000	2.303451000
6	-0.603664000	3.617195000	3.685102000
1	-0.953676000	4.248919000	4.498599000
6	-0.486877000	2.243017000	3.870183000
1	-0.748451000	1.795062000	4.826756000
6	-0.040367000	1.431084000	2.831007000
1	0.014955000	0.352986000	2.979133000
6	2.081262000	1.793609000	-0.634422000
6	2.195258000	1.871177000	-2.024192000
1	1.426475000	1.450466000	-2.668371000

6	3.300231000	2.484977000	-2.610037000
1	3.374670000	2.537652000	-3.693812000
6	4.298250000	3.032793000	-1.811431000
1	5.158962000	3.515707000	-2.268716000
6	4.188079000	2.971448000	-0.423273000
1	4.959954000	3.407917000	0.206730000
6	3.085774000	2.359816000	0.162031000
1	3.003808000	2.332916000	1.247818000
6	-0.229157000	-2.347492000	-0.180493000
1	0.167082000	-2.446831000	-1.200291000
6	-2.442819000	-2.187504000	-1.038966000
1	-1.951575000	-2.633155000	-1.918754000
1	-2.868456000	-3.015383000	-0.453792000
6	-3.508743000	-1.269083000	-1.523194000
6	-4.018862000	0.870368000	-2.250816000
1	-3.676086000	1.891701000	-2.400890000
6	-5.314981000	0.502206000	-2.566251000
1	-5.996594000	1.239936000	-2.978259000
6	-5.715092000	-0.809172000	-2.330569000
6	-4.799256000	-1.705165000	-1.799218000
1	-5.066984000	-2.738671000	-1.594704000
6	-1.178322000	2.119673000	-1.734628000
6	-0.423387000	-0.204469000	-2.478620000
6	-2.251810000	1.250510000	0.389199000
8	-2.937344000	1.829042000	1.107486000
1	-1.796432000	-1.392858000	0.707601000
1	-6.730253000	-1.126883000	-2.553668000
1	-0.548827000	-3.354745000	0.132968000
35	-2.911191000	-1.595345000	2.669652000

***fac*-[MnBr(CO)$_2$(L)] (Br *trans* to P)**
E (BS1) = -2039.60235249
E (BS2) = -6787.3404918
G_{1M} = -6786.895148

26	-3.115349000	-0.511152000	-1.165559000
25	1.203621000	-0.956983000	0.711177000
15	-0.166793000	0.750663000	0.234413000
8	1.848949000	0.106093000	3.359786000
8	-0.851270000	-2.676729000	1.891792000
7	0.954636000	-1.749601000	-1.242602000
7	2.796230000	-0.064791000	-0.284883000
6	-1.281482000	0.375789000	-1.152653000
6	-1.249797000	-0.835101000	-1.936481000
6	-2.201614000	-0.691251000	-2.987415000
1	-2.432812000	-1.453720000	-3.725297000
6	-2.828016000	0.582045000	-2.865893000
1	-3.626722000	0.962734000	-3.493449000
6	-2.264662000	1.241874000	-1.740428000
1	-2.541506000	2.225239000	-1.374350000
6	-3.585581000	-1.197911000	0.708150000
1	-2.908303000	-1.214663000	1.555009000
6	-3.738018000	-2.234584000	-0.255823000
1	-3.195105000	-3.174347000	-0.272151000
6	-4.693575000	-1.800528000	-1.220789000
1	-5.001956000	-2.348882000	-2.104488000
6	-5.128980000	-0.493475000	-0.852735000
1	-5.824981000	0.124799000	-1.409543000
6	-4.440768000	-0.118068000	0.338319000
1	-4.526427000	0.833769000	0.853092000
6	0.748302000	2.239640000	-0.330222000
6	1.420938000	3.004705000	0.630840000
1	1.309384000	2.767827000	1.690089000
6	2.235941000	4.062837000	0.245718000
1	2.748152000	4.653318000	1.002558000
6	2.399312000	4.362419000	-1.105670000
1	3.038883000	5.188945000	-1.407693000
6	1.740892000	3.602017000	-2.067026000
1	1.862080000	3.833026000	-3.123449000
6	0.918081000	2.544850000	-1.682377000
1	0.406208000	1.957597000	-2.444966000
6	-1.271652000	1.466877000	1.520378000
6	-1.558246000	0.760609000	2.691335000
1	-1.102286000	-0.210570000	2.872002000
6	-2.436258000	1.283111000	3.638336000
1	-2.649208000	0.719132000	4.543790000
6	-3.032331000	2.522251000	3.428179000
1	-3.716027000	2.931886000	4.168541000
6	-2.741568000	3.243201000	2.271661000
1	-3.193729000	4.218938000	2.107161000
6	-1.864160000	2.721963000	1.327069000
1	-1.629409000	3.306020000	0.438158000
6	-0.400267000	-2.056880000	-1.736767000
1	-0.854237000	-2.748101000	-1.017113000
6	1.745176000	-1.014437000	-2.241388000
1	2.089137000	-1.676837000	-3.048414000
1	1.094490000	-0.262107000	-2.712593000
6	2.892382000	-0.301105000	-1.605228000
6	3.776306000	0.636576000	0.308717000
1	3.679193000	0.799935000	1.379867000
6	4.866899000	1.138309000	-0.381124000
1	5.624519000	1.706555000	0.150318000
6	4.966291000	0.888790000	-1.746262000
6	3.967348000	0.151202000	-2.363394000
1	4.001960000	-0.074418000	-3.426666000
6	1.584844000	-0.311209000	2.296457000
6	-0.062882000	-1.952460000	1.414900000
1	1.422799000	-2.643677000	-1.072772000
1	5.812917000	1.259591000	-2.318625000
1	-0.334770000	-2.592826000	-2.696913000
35	2.820673000	-2.937174000	1.065321000

***mer*-[MnBr(CO)$_2$(L)] (*axial* Br)**
E (BS1) = -2039.59341977
E (BS2) = -6787.33112747
G_{1M} = -6786.886288



26	-2.957813000	-1.507183000	-0.787281000
25	1.585602000	-0.156889000	0.538084000
15	-0.429212000	0.823292000	0.069437000
8	2.198989000	2.036055000	2.378960000
8	0.488337000	-1.918252000	2.592280000
7	1.346539000	-1.722077000	-0.889113000

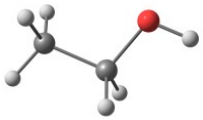
7	3.442062000	-1.044262000	0.672519000
6	-1.433242000	-0.182399000	-1.075145000
6	-1.056750000	-1.497901000	-1.529547000
6	-1.981236000	-1.893429000	-2.540142000
1	-1.977385000	-2.855050000	-3.044483000
6	-2.930144000	-0.848456000	-2.720507000
1	-3.781663000	-0.866404000	-3.392069000
6	-2.597891000	0.203463000	-1.824659000
1	-3.133708000	1.142051000	-1.731051000
6	-3.376567000	-1.641673000	1.214226000
1	-2.844103000	-1.108502000	1.995990000
6	-3.031376000	-2.919930000	0.689173000
1	-2.191934000	-3.531652000	1.004096000
6	-3.953113000	-3.232550000	-0.352530000
1	-3.935641000	-4.121129000	-0.974437000
6	-4.867587000	-2.145062000	-0.471849000
1	-5.666859000	-2.062425000	-1.200563000
6	-4.510234000	-1.160141000	0.495441000
1	-4.993546000	-0.199010000	0.635925000
6	-0.352507000	2.448587000	-0.787932000
6	-0.127446000	3.600715000	-0.028246000
1	-0.081105000	3.538746000	1.059144000
6	0.031623000	4.835761000	-0.648486000
1	0.201526000	5.725029000	-0.044830000
6	-0.036125000	4.933519000	-2.036283000
1	0.080213000	5.900236000	-2.521914000
6	-0.257252000	3.790089000	-2.799053000
1	-0.310705000	3.859056000	-3.883790000
6	-0.405418000	2.553116000	-2.179234000
1	-0.553480000	1.663153000	-2.788794000
6	-1.548047000	1.255998000	1.473836000
6	-1.189846000	0.992349000	2.797842000
1	-0.227823000	0.545069000	3.031022000
6	-2.055500000	1.301982000	3.846153000
1	-1.757587000	1.086107000	4.869898000
6	-3.289100000	1.885615000	3.583998000
1	-3.966775000	2.123918000	4.400893000
6	-3.646497000	2.180646000	2.269315000
1	-4.601447000	2.656416000	2.055265000
6	-2.780478000	1.876154000	1.226345000
1	-3.070038000	2.134566000	0.209401000
6	0.032069000	-2.381592000	-1.012320000
1	-0.213273000	-2.768849000	-0.014989000
6	2.357031000	-2.757807000	-0.609435000
1	1.927215000	-3.437608000	0.143265000
1	2.570106000	-3.365135000	-1.499969000
6	3.603634000	-2.171099000	-0.041468000
6	4.516440000	-0.502501000	1.266658000
1	4.353148000	0.415250000	1.826411000
6	5.781792000	-1.058803000	1.175525000
1	6.616347000	-0.579463000	1.678441000
6	5.951300000	-2.216999000	0.424581000
6	4.844011000	-2.779092000	-0.194981000
1	4.925936000	-3.681261000	-0.796271000
6	1.941868000	1.157345000	1.648045000
6	0.906195000	-1.180375000	1.780104000
1	1.582020000	-1.269934000	-1.777251000
1	6.932727000	-2.672640000	0.320318000
1	0.113303000	-3.254454000	-1.679499000
35	2.727124000	1.128352000	-1.382710000

C. Catalytic cycles: small molecules

H_2
E (BS1) = -1.16926221763
E (BS2) = -1.17038669646
G_{1M} = -1.168753

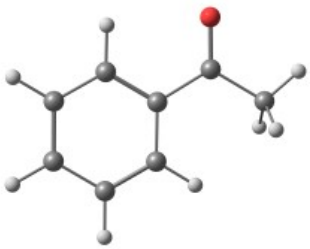
1	0.000000000	0.000000000	0.371361000
1	0.000000000	0.000000000	-0.371361000

EtOH
E (BS1) = -154.94651153
E (BS2) = -155.008387989
G_{1M} = -154.951037



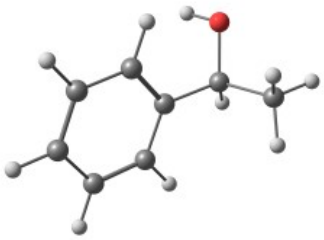
6	0.085348000	0.543034000	-0.000037000
1	0.140030000	1.198280000	0.885354000
6	-1.214494000	-0.219555000	0.000092000
1	-1.287646000	-0.858895000	-0.887786000
1	-2.067405000	0.467599000	0.000055000
1	-1.287687000	-0.859179000	0.887747000
8	1.145215000	-0.397368000	-0.000143000
1	1.976187000	0.092023000	0.000912000
1	0.139680000	1.198245000	-0.885465000

PhCOMe
E (BS1) = -384.629365128
E (BS2) = -384.768692114
G_{1M} = -384.660769



6	-0.270513000	1.679678000	0.000000000
8	0.653588000	2.484722000	0.000000000
6	-1.694971000	2.146898000	0.000000000
1	-1.718477000	3.239104000	0.000000000
1	-2.227767000	1.771618000	0.881943000
1	-2.227767000	1.771618000	-0.881943000
6	0.000000000	0.216527000	0.000000000
6	1.330330000	-0.218842000	0.000000000
6	-1.030074000	-0.730334000	0.000000000
6	1.626909000	-1.574025000	0.000000000
6	-0.732449000	-2.088242000	0.000000000
6	0.594261000	-2.510770000	0.000000000
1	2.124129000	0.524726000	0.000000000
1	-2.070370000	-0.412664000	0.000000000
1	2.663164000	-1.904417000	0.000000000
1	-1.537807000	-2.819169000	0.000000000
1	0.825234000	-3.573936000	0.000000000

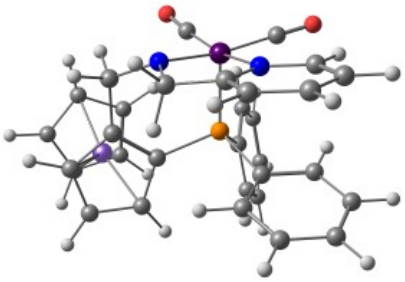
PhCH(OH)Me
E (BS1) = -385.827402383
E (BS2) = -385.966965111
G_{1M} = -385.836396



6	1.653671000	-0.284696000	-0.293810000
1	1.851567000	-1.082254000	-1.032430000
6	2.256821000	-0.692799000	1.035887000
1	1.821894000	-1.635133000	1.386678000
1	3.341412000	-0.820865000	0.942603000
1	2.059161000	0.081597000	1.788475000
6	0.156093000	-0.115712000	-0.177188000
6	-0.401902000	1.111877000	0.181722000
6	-0.685933000	-1.210899000	-0.376870000
6	-1.779514000	1.242027000	0.335489000
6	-2.062556000	-1.084402000	-0.219690000
6	-2.613452000	0.144854000	0.135871000
1	0.253279000	1.968110000	0.334071000
1	-0.253403000	-2.171002000	-0.661431000
1	-2.204079000	2.205326000	0.612126000
1	-2.708382000	-1.945218000	-0.382021000
1	-3.690213000	0.247751000	0.254145000
8	2.306972000	0.911869000	-0.680677000
1	1.933619000	1.195230000	-1.525274000

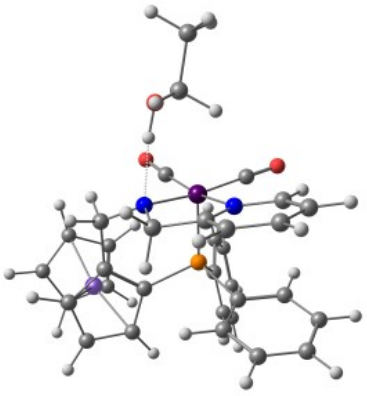
D. Catalytic cycles: catalyst 5a

[Mn(CO)$_2$(L^{-H})] (A)
E (BS1) = -2025.5593187
E (BS2) = -4212.54143687
G_{1M} = -4212.107349



26	-2.853037000	-1.060280000	-0.654378000
25	1.075060000	-0.407293000	1.685820000
15	0.191343000	0.546221000	-0.067508000
8	1.870729000	2.100177000	3.020957000
8	-1.374726000	-0.393060000	3.280726000
7	0.865154000	-2.173777000	1.034074000
7	2.977245000	-0.719724000	0.923514000
6	-0.872406000	-0.656752000	-0.922910000
6	-1.043607000	-2.033775000	-0.529549000
6	-1.882455000	-2.651869000	-1.500447000
1	-2.225424000	-3.681737000	-1.461863000
6	-2.230688000	-1.686729000	-2.490818000
1	-2.889753000	-1.848315000	-3.337455000
6	-1.611202000	-0.456274000	-2.138958000
1	-1.697954000	0.478217000	-2.684139000
6	-3.582983000	-0.001048000	0.944021000
1	-2.981668000	0.585873000	1.629333000
6	-3.887273000	-1.385288000	1.081435000
1	-3.558388000	-2.032101000	1.888517000
6	-4.661954000	-1.778529000	-0.049337000
1	-5.022279000	-2.780056000	-0.258809000
6	-4.832049000	-0.636143000	-0.886096000
1	-5.342301000	-0.619771000	-1.843267000
6	-4.161350000	0.463358000	-0.273423000
1	-4.074081000	1.467222000	-0.677584000
6	1.485448000	0.964630000	-1.296781000
6	2.249877000	2.117891000	-1.079866000
1	1.995745000	2.792274000	-0.260470000
6	3.336760000	2.406316000	-1.896174000
1	3.919416000	3.308573000	-1.722355000
6	3.681851000	1.537971000	-2.930827000
1	4.534619000	1.761250000	-3.568336000
6	2.933262000	0.385043000	-3.146317000
1	3.197700000	-0.294443000	-3.954019000
6	1.837178000	0.097676000	-2.334291000
1	1.255736000	-0.807245000	-2.512095000
6	-0.789750000	2.096593000	0.005715000
6	-1.271351000	2.569027000	1.228952000
1	-1.045579000	2.033315000	2.149118000
6	-2.051935000	3.721340000	1.284718000
1	-2.420696000	4.076443000	2.244486000
6	-2.351599000	4.417528000	0.118115000
1	-2.958413000	5.319355000	0.161376000
6	-1.862241000	3.964138000	-1.105472000
1	-2.081754000	4.512213000	-2.019232000
6	-1.082212000	2.814264000	-1.161443000
1	-0.687309000	2.482874000	-2.121070000
6	-0.434132000	-2.714756000	0.679958000
1	-1.106521000	-2.624874000	1.543023000
6	1.886239000	-2.695377000	0.155212000
1	2.106490000	-3.760047000	0.355841000
1	1.568818000	-2.664964000	-0.909469000
6	3.124458000	-1.885453000	0.264927000
6	4.037989000	0.109413000	1.000336000
1	3.886157000	1.046153000	1.531741000
6	5.264311000	-0.191894000	0.440596000
1	6.084236000	0.514709000	0.528970000
6	5.418357000	-1.407112000	-0.226213000
6	4.334991000	-2.264658000	-0.310329000
1	4.402793000	-3.220192000	-0.825441000
6	1.553338000	1.095954000	2.495859000
6	-0.417761000	-0.385633000	2.597063000
1	6.371813000	-1.675321000	-0.674648000
1	-0.366614000	-3.794657000	0.456283000

[Mn(CO)$_2$(L^{-H})]···EtOH (B)
E (BS1) = -2180.52297884
E (BS2) = -4367.56374499
G_{1M} = -4367.057296



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25	1.167508000	-0.575213000	0.974008000
15	-0.307719000	0.811843000	0.154574000
8	1.660886000	0.978215000	3.428942000
8	-0.776839000	-2.196897000	2.436834000
7	1.181514000	-1.706074000	-0.588628000
7	2.846005000	0.167617000	0.011340000

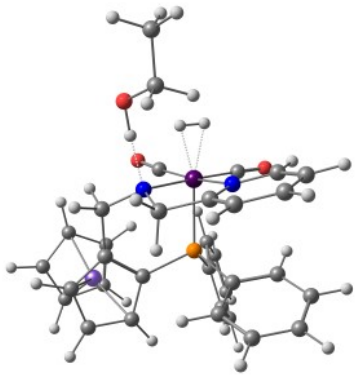
6	-1.262645000	-0.009981000	-1.156620000
6	-1.035738000	-1.354820000	-1.624910000
6	-1.921058000	-1.579227000	-2.717620000
1	-2.014073000	-2.514601000	-3.261833000
6	-2.690121000	-0.398817000	-2.937830000
1	-3.476181000	-0.276038000	-3.675622000
6	-2.288693000	0.570399000	-1.978210000
1	-2.699236000	1.569576000	-1.871873000
6	-3.539942000	-1.334919000	0.916602000
1	-2.939673000	-1.049825000	1.772875000
6	-3.492301000	-2.591791000	0.249443000
1	-2.850293000	-3.426890000	0.510988000
6	-4.403363000	-2.541367000	-0.846435000
1	-4.572978000	-3.329811000	-1.571926000
6	-5.010919000	-1.250997000	-0.855691000
1	-5.720746000	-0.887990000	-1.591362000
6	-4.473846000	-0.502364000	0.233076000
1	-4.705629000	0.529573000	0.477654000
6	0.541937000	2.192272000	-0.700735000
6	1.078129000	3.226402000	0.076878000
1	0.877112000	3.261998000	1.148758000
6	1.873947000	4.204852000	-0.506630000
1	2.280868000	5.006932000	0.105615000
6	2.155283000	4.153479000	-1.871123000
1	2.783406000	4.915750000	-2.327052000
6	1.628514000	3.127368000	-2.649197000
1	1.840473000	3.086933000	-3.715697000
6	0.820439000	2.151382000	-2.068897000
1	0.410954000	1.352537000	-2.687241000
6	-1.552271000	1.685246000	1.182192000
6	-1.836330000	1.247879000	2.478397000
1	-1.295814000	0.403800000	2.903020000
6	-2.819920000	1.877964000	3.237278000
1	-3.031442000	1.525541000	4.244391000
6	-3.523668000	2.956115000	2.710218000
1	-4.290341000	3.449430000	3.303682000
6	-3.236540000	3.410453000	1.424474000
1	-3.774370000	4.261465000	1.012239000
6	-2.254106000	2.782458000	0.666650000
1	-2.025227000	3.158675000	-0.329743000
6	-0.026566000	-2.342902000	-1.078834000
1	-0.469131000	-2.930812000	-0.263554000
6	2.027336000	-1.297741000	-1.688363000
1	2.494889000	-2.161294000	-2.198468000
1	1.454274000	-0.771760000	-2.481957000
6	3.075699000	-0.363475000	-1.205618000
6	3.730666000	1.061511000	0.497222000
6	4.862710000	1.445251000	-0.196261000
6	5.105609000	0.882407000	-1.448711000
6	4.201757000	-0.035151000	-1.956226000
6	1.469559000	0.351526000	2.452689000
6	-0.033851000	-1.518232000	1.830933000
1	2.303624000	-2.792226000	0.497506000
8	2.901650000	-3.253879000	1.130284000
6	4.244215000	-3.014868000	0.745714000
1	4.476354000	-1.934329000	0.786542000
1	4.414602000	-3.340351000	-0.295075000
1	4.347366000	-0.500750000	-2.928254000
1	5.542733000	2.169575000	0.242045000
6	5.157425000	-3.768070000	1.679378000
1	6.207612000	-3.607801000	1.411399000
1	5.012834000	-3.432599000	2.713590000
1	4.952044000	-4.844541000	1.638386000
1	5.990761000	1.158399000	-2.016565000
1	0.205627000	-3.063206000	-1.884411000
1	3.513756000	1.477844000	1.478338000

[Mn(CO)$_2$(L^{-H})(η-H$_2$)]···EtOH (C)

E (BS1) = -2181.69159053

E (BS2) = -4368.73781976

G_{1M} = -4368.213325



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25	1.147705000	-0.483398000	1.279973000
15	-0.290257000	0.819501000	0.104552000
8	1.173981000	1.442961000	3.505129000
8	-0.928172000	-2.073222000	2.603960000
7	1.272328000	-1.699670000	-0.375230000
7	2.816756000	0.303751000	0.329529000
6	-1.224197000	-0.109657000	-1.138144000
6	-0.944380000	-1.469340000	-1.515151000
6	-1.808557000	-1.792649000	-2.600285000
1	-1.863758000	-2.762924000	-3.085573000
6	-2.613613000	-0.654919000	-2.904865000
1	-3.394168000	-0.606985000	-3.657059000
6	-2.259816000	0.385799000	-2.002590000
1	-2.702814000	1.376096000	-1.960470000
6	-3.547495000	-1.333141000	0.973757000
1	-3.005298000	-0.943278000	1.827520000
6	-3.407114000	-2.639931000	0.424439000
1	-2.739092000	-3.414625000	0.786671000
6	-4.269275000	-2.733578000	-0.707484000
1	-4.367172000	-3.590184000	-1.365828000
6	-4.938651000	-1.483074000	-0.857254000
1	-5.630044000	-1.223614000	-1.651954000
6	-4.488999000	-0.614709000	0.181023000
1	-4.781020000	0.421179000	0.322200000
6	0.572787000	2.113304000	-0.875692000
6	1.240499000	3.124705000	-0.174134000
1	1.174568000	3.165504000	0.914514000
6	1.991896000	4.076325000	-0.852872000
1	2.506606000	4.856586000	-0.295922000
6	2.088708000	4.026967000	-2.242633000
1	2.680397000	4.769230000	-2.774138000
6	1.421498000	3.031063000	-2.947973000
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6	-3.621324000	3.249470000	2.233556000
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6	5.043205000	1.167034000	-1.093282000

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1	2.296497000	-2.919121000	0.146296000
8	2.929180000	-3.615001000	0.518019000
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1	4.519651000	-3.113414000	-0.728975000
1	4.383006000	-2.138828000	0.744132000
1	4.297352000	-0.124630000	-2.658468000
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1	5.091738000	-5.123381000	0.665038000
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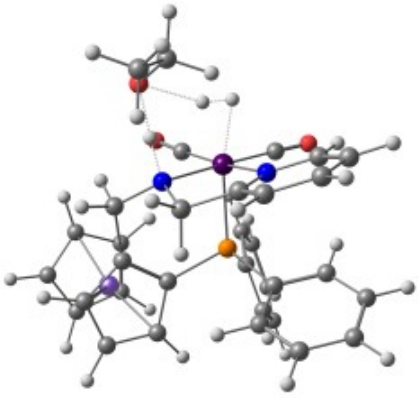

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1	-5.562255000	-1.195172000	-1.768792000
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6	-2.014619000	1.694804000	2.084917000
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6	3.740984000	1.137171000	0.869680000
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6	5.241911000	0.726545000	-0.941318000
6	4.324859000	-0.185492000	-1.440183000
6	1.149397000	0.922189000	2.601507000
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1	2.303575000	-0.989698000	2.462192000
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$[MnH(CO)_2(L)]\cdots EtOH$ (D)
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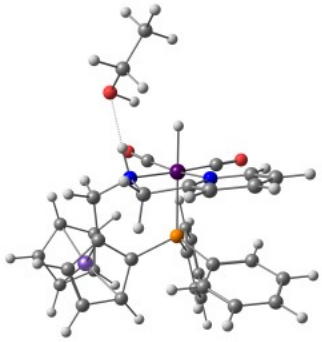

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6	-1.832143000	-1.293902000	-2.867669000
1	-1.911204000	-2.180803000	-3.489543000
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1	0.901167000	3.211908000	1.413603000
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6	4.725561000	1.805873000	-0.151474000
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[MnH(CO)$_2$(L)] (E)

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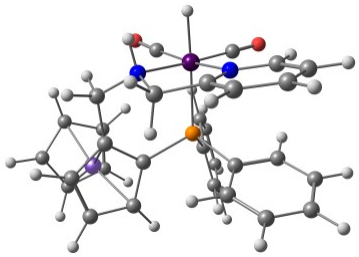

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[MnH(CO)$_2$(L)]···PhCOMe (F-*re*)

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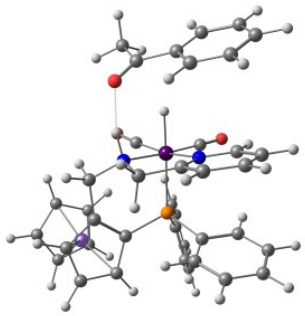
E (BS2) = -4598.52819479

G_{1M} = -4597.948754



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6	-3.133639000	2.375119000	1.307194000
1	-3.071371000	2.977002000	0.401039000
6	-0.484513000	-1.983010000	-1.624100000
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6	1.317679000	-0.436054000	-2.171715000
1	1.833806000	-1.005516000	-2.959830000
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6	2.232628000	0.577543000	-1.564555000
6	2.887035000	1.727582000	0.325404000
6	3.760668000	2.520818000	-0.398978000
1	4.345604000	3.280174000	0.111923000
6	3.865796000	2.320446000	-1.772199000
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1	3.145469000	1.125248000	-3.426010000
6	1.013423000	0.286663000	2.352780000
6	-0.089866000	-1.762439000	1.523953000
1	1.429348000	-2.082122000	-1.014720000
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6	3.689317000	-2.923084000	-0.002309000
6	4.745005000	-1.919023000	0.290605000
6	3.292137000	-3.908549000	1.054460000
6	5.262111000	-1.732282000	1.577762000
6	5.215254000	-1.121492000	-0.759460000
6	6.222298000	-0.754346000	1.810249000
6	6.180722000	-0.151315000	-0.527747000
1	4.811420000	-1.277256000	-1.758032000
6	6.681175000	0.037141000	0.759607000
1	6.615057000	-0.610159000	2.814107000
1	6.544944000	0.461204000	-1.350090000
8	3.184379000	-2.976285000	-1.124928000
1	4.541996000	2.923838000	-2.372856000
1	7.434004000	0.800667000	0.943764000
1	4.909840000	-2.343151000	2.406087000
1	3.068482000	-3.426497000	2.011315000
1	2.413723000	-4.464967000	0.714805000
1	4.117812000	-4.612386000	1.226250000
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[MnH(CO)$_2$(L)]···PhCOMe (F-*si*)

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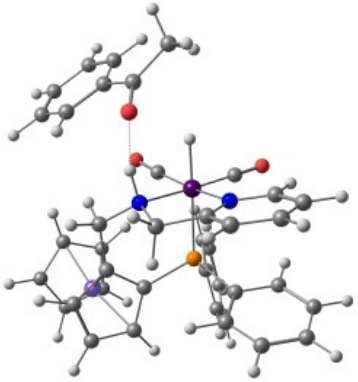
E (BS2) = -4598.52849042

G_{1M} = -4597.949251



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7	1.475250000	0.275192000	-1.187666000
7	1.115847000	2.643107000	-0.003789000
6	-1.564085000	-0.423556000	-1.171905000
6	-0.524348000	-0.993375000	-1.993835000
6	-1.155749000	-1.646436000	-3.092987000
1	-0.636660000	-2.200376000	-3.869765000

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1	-1.297129000	-4.961919000	-2.428907000
6	-2.901947000	-4.143185000	-1.094951000
1	-3.808867000	-4.360996000	-1.648929000
6	-2.822948000	-3.436609000	0.141181000
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1	1.701564000	3.923142000	-3.061560000
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6	4.163553000	-1.989600000	-0.784390000
6	4.635916000	-2.935503000	1.790467000
6	3.896922000	-3.317143000	-0.477099000
1	3.998053000	-1.609469000	-1.791077000
6	4.127677000	-3.789497000	0.813785000
1	4.816915000	-3.305272000	2.797014000
1	3.513936000	-3.986815000	-1.244562000
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1	3.916162000	-4.828269000	1.058154000
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1	5.299060000	-0.947973000	2.254245000
1	5.165124000	1.312070000	1.690299000
1	6.663389000	0.689915000	0.991591000
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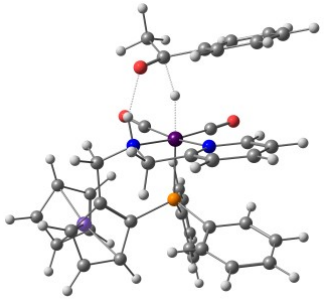
E (BS2) = -4598.52040879

G_{1M} = -4597.938209



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7	0.613049000	-1.361130000	-1.404933000
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6	-2.003942000	0.278946000	-1.071643000
6	-1.786124000	-0.882575000	-1.900055000
6	-2.831113000	-0.918186000	-2.869258000
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6	-4.922774000	-2.531044000	-0.962809000
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1	-6.405131000	-0.850371000	-0.948033000
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1	0.331608000	3.039097000	1.662798000
6	0.874944000	4.526777000	0.208636000
1	1.343752000	5.174980000	0.946287000
6	0.858241000	4.893384000	-1.136195000
1	1.312950000	5.829770000	-1.452337000
6	0.257504000	4.057722000	-2.072492000
1	0.238764000	4.339596000	-3.123386000
6	-0.328503000	2.858882000	-1.669591000
1	-0.798046000	2.213682000	-2.412531000
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1	-0.936584000	-2.704297000	-1.103781000
6	1.165455000	-0.446854000	-2.413949000
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6	5.719188000	-0.676309000	2.040121000
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1	6.870622000	-0.153010000	-1.113765000
8	2.937817000	-2.930584000	-1.160143000
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1	4.007177000	-1.860022000	2.559499000
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1	3.521035000	-4.609188000	1.021505000
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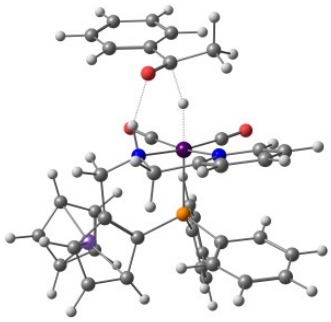

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7	1.134656000	-0.165298000	-1.676002000
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6	-1.878401000	0.220400000	-1.026100000
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6	-2.309535000	-0.735575000	-3.087733000
1	-2.185305000	-1.301903000	-4.006141000
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1	-1.583456000	2.730200000	-1.811848000
6	-2.061362000	0.475912000	1.849811000
6	-1.712553000	-0.512487000	2.773793000
1	-0.775616000	-1.055352000	2.661685000
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1	0.206344000	1.459846000	-2.629667000
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1	2.046732000	-0.627114000	-1.804655000
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1	3.897203000	-5.712199000	1.520451000
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1	2.416819000	2.723659000	1.594102000
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$[Mn(CO)_2(L)]^+\cdots PhCH(Me)O^-$ (G-*S*)
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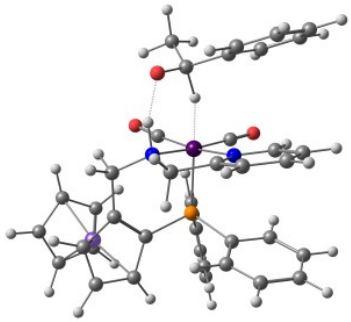
E (BS2) = -4598.53203696
G_{1M} = -4597.947131



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6	-3.636979000	0.104672000	-2.712905000
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$[Mn(CO)_2(L)]^+\cdots PhCH(Me)O^-$ (G-*R*)

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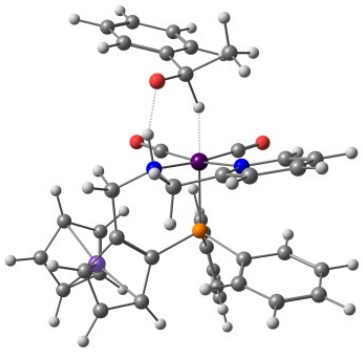
E (BS2) = -4598.52894224

G_{1M} = -4597.943518



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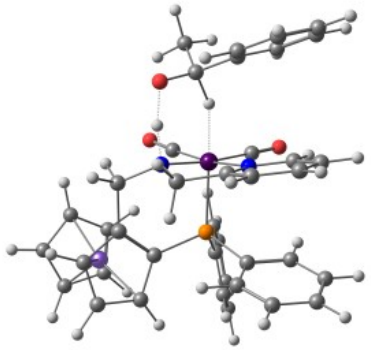
E (BS2) = -4598.53203696

G_{1M} = -4597.947131



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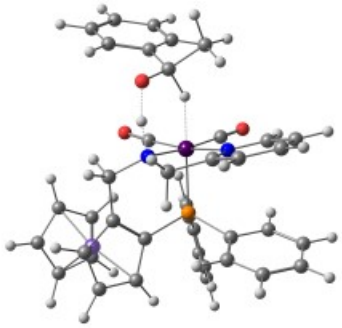
E (BS2) = -4598.53203696
G_{1M} = -4597.947131



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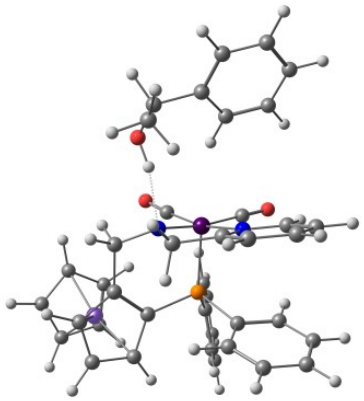
1	5.145751000	0.136654000	0.703209000
1	5.833009000	-0.435299000	-0.837122000
1	2.634165000	2.538547000	1.613096000
1	0.223039000	-0.967144000	-3.428403000

$[Mn(CO)_2(L^{-H})]$···HOCHPhMe (H-*S*)
E (BS1) = -2411.40805807
E (BS2) = -4598.53051332
G_{1M} = -4597.947790



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8	1.331580000	1.235741000	3.159654000
8	-0.335457000	-2.364981000	2.071836000
7	0.867639000	-1.039212000	-1.102723000
7	2.076898000	1.145361000	-0.458505000
6	-1.991826000	-0.028077000	-1.071143000
6	-1.514889000	-1.200344000	-1.762577000
6	-2.496126000	-1.548591000	-2.734073000
1	-2.443142000	-2.411750000	-3.391245000
6	-3.569860000	-0.612932000	-2.661015000
1	-4.481466000	-0.638678000	-3.248851000
6	-3.264093000	0.325385000	-1.637594000
1	-3.890905000	1.154523000	-1.324671000
6	-3.439699000	-2.129409000	1.097589000
1	-2.792604000	-1.773237000	1.890984000
6	-3.187124000	-3.251408000	0.258127000
1	-2.313749000	-3.894434000	0.300539000
6	-4.260722000	-3.351205000	-0.675209000
1	-4.346601000	-4.080740000	-1.473456000
6	-5.174354000	-2.288114000	-0.412025000
1	-6.073682000	-2.068332000	-0.977512000
6	-4.664518000	-1.528863000	0.682427000
1	-5.108498000	-0.631834000	1.102902000
6	-0.749997000	2.522663000	-0.567725000
6	-0.333847000	3.571534000	0.261939000
1	-0.313556000	3.433526000	1.344240000
6	0.063163000	4.785726000	-0.284999000
1	0.379850000	5.595785000	0.368650000
6	0.062488000	4.961606000	-1.668121000
1	0.379129000	5.909990000	-2.096805000
6	-0.347599000	3.923549000	-2.498634000
1	-0.356307000	4.058924000	-3.578237000
6	-0.756170000	2.708238000	-1.952099000
1	-1.078896000	1.902173000	-2.610764000
6	-2.288446000	1.283613000	1.499141000
6	-2.222601000	0.666888000	2.750893000
1	-1.419226000	-0.032430000	2.975584000
6	-3.187426000	0.930972000	3.720303000
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6	-4.222668000	1.820134000	3.449830000
1	-4.974772000	2.027972000	4.207729000
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1	-5.087832000	3.159272000	1.997914000
6	-3.324489000	2.190719000	1.242266000
1	-3.375121000	2.706206000	0.283901000
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6	1.363060000	-0.284650000	-2.232045000
1	1.926069000	-0.916712000	-2.945382000
1	0.536439000	0.152941000	-2.831920000
6	2.210250000	0.841412000	-1.764421000
6	2.768060000	2.194817000	0.029434000
6	3.602698000	2.968669000	-0.753991000
6	3.747604000	2.645597000	-2.102638000
6	3.048011000	1.564150000	-2.610511000
6	1.136161000	0.688155000	2.137526000
6	0.079193000	-1.447951000	1.466315000
1	2.076102000	-2.315288000	-0.370978000
8	2.531972000	-3.109908000	-0.001567000
6	3.901212000	-3.049962000	-0.341783000
1	4.295072000	-4.069837000	-0.202995000
1	3.128457000	1.272376000	-3.655231000
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1	4.401484000	3.230986000	-2.744383000
1	0.063937000	-2.456041000	-2.449796000
1	2.639921000	2.413314000	1.087424000
6	4.078042000	-2.661628000	-1.803737000
1	3.435607000	-3.284703000	-2.438788000
1	3.807066000	-1.606958000	-1.954410000
1	5.115299000	-2.787643000	-2.133397000
6	4.692412000	-2.116772000	0.555481000
6	6.087299000	-2.080134000	0.457465000
6	4.067490000	-1.263381000	1.464061000
6	6.833166000	-1.197319000	1.230507000
6	4.810938000	-0.369517000	2.234136000
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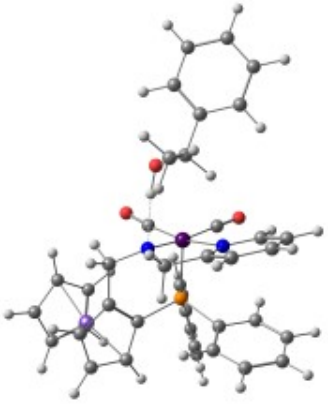
1	6.594721000	-2.756499000	-0.231275000
1	2.983501000	-1.297638000	1.577791000
1	7.917820000	-1.184681000	1.140876000
1	4.297852000	0.292427000	2.931185000
1	6.779576000	0.362842000	2.720440000

$[Mn(CO)_2(L^{-H})]$···HOCHPhMe (H-*R*)

E (BS1) = -2411.40360864

E (BS2) = -4598.52474391

G_{1M} = -4597.943570



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7	0.722752000	-0.702873000	-1.336694000
7	1.795465000	1.419907000	-0.332431000
6	-2.213597000	-0.000608000	-1.008701000
6	-1.672733000	-0.975895000	-1.921463000
6	-2.674916000	-1.243262000	-2.897614000
1	-2.582670000	-1.965648000	-3.703540000
6	-3.824022000	-0.449135000	-2.608855000
1	-4.762820000	-0.462182000	-3.152638000
6	-3.544649000	0.317888000	-1.444648000
1	-4.223146000	1.010951000	-0.957053000
6	-3.340220000	-2.592772000	0.799063000
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6	-3.024062000	-3.512975000	-0.240930000
1	-2.091434000	-4.057657000	-0.347986000
6	-4.130783000	-3.557403000	-1.138863000
1	-4.186714000	-4.137122000	-2.054027000

6	-5.128998000	-2.662038000	-0.653252000
1	-6.074577000	-2.441296000	-1.137055000
6	-4.638580000	-2.062333000	0.544223000
1	-5.148771000	-1.311805000	1.139382000
6	-1.141139000	2.526353000	-0.140040000
6	-0.714374000	3.444723000	0.827580000
1	-0.596113000	3.125274000	1.864383000
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1	-0.097667000	5.462636000	1.232909000
6	-0.551438000	5.164029000	-0.854767000
1	-0.319492000	6.189616000	-1.133752000
6	-0.977423000	4.258206000	-1.820785000
1	-1.083705000	4.574100000	-2.856526000
6	-1.275273000	2.943371000	-1.466073000
1	-1.609681000	2.241259000	-2.229538000
6	-2.478100000	0.850953000	1.750407000
6	-2.334249000	0.009442000	2.856689000
1	-1.495749000	-0.683067000	2.912614000
6	-3.261724000	0.044488000	3.895255000
1	-3.138695000	-0.616835000	4.750063000
6	-4.335844000	0.927537000	3.841728000
1	-5.057014000	0.958117000	4.655623000
6	-4.479790000	1.780731000	2.749590000
1	-5.311462000	2.480797000	2.708368000
6	-3.555732000	1.744780000	1.710995000
1	-3.669297000	2.427419000	0.869595000
6	-0.291480000	-1.594960000	-1.869009000
1	-0.310989000	-2.508965000	-1.260052000
6	1.080963000	0.302093000	-2.315849000
1	1.621524000	-0.128784000	-3.179956000
1	0.186208000	0.794411000	-2.754247000
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6	2.490626000	2.367259000	0.327086000
6	3.318826000	3.268730000	-0.314950000
6	3.440591000	3.196731000	-1.702117000
6	2.721271000	2.232413000	-2.388804000
6	0.987001000	0.432135000	2.163948000
6	0.106534000	-1.642407000	1.149966000
1	2.321800000	-1.550374000	-0.792724000
8	3.136997000	-1.914089000	-0.367064000
6	4.219252000	-1.050602000	-0.674626000
1	2.787510000	2.135047000	-3.470081000
1	3.861600000	4.009094000	0.265048000
1	4.090957000	3.885005000	-2.236292000
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1	2.377227000	2.390713000	1.408609000
6	5.400962000	-1.399039000	0.192332000
6	6.249803000	-0.388081000	0.645669000
6	5.702138000	-2.726871000	0.502641000
6	7.380154000	-0.694562000	1.398168000
6	6.828375000	-3.034858000	1.259853000
6	7.671214000	-2.020421000	1.708591000
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1	5.045083000	-3.520900000	0.151628000
1	8.031158000	0.104065000	1.748527000
1	7.050150000	-4.072955000	1.500351000
1	8.550944000	-2.262941000	2.301244000
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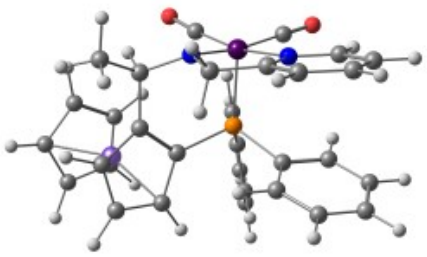
1	3.715990000	-0.895627000	-2.776720000
1	5.396803000	-0.454974000	-2.397440000
1	3.938933000	-0.005148000	-0.450937000

E. Catalytic cycles: catalyst I

[Mn(CO)$_2$(L^{-H})] (A)
E (BS1) = -2064.84418179
E (BS2) = -4251.83945811
G_{1M} = -4251.379680



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7	0.805284000	-2.123391000	0.955699000
7	2.967668000	-0.735319000	0.859767000
6	-0.854868000	-0.482949000	-0.951020000
6	-1.065475000	-1.873512000	-0.621918000
6	-1.886166000	-2.427772000	-1.649684000
1	-2.263908000	-3.444733000	-1.678689000
6	-2.188918000	-1.408706000	-2.599668000
1	-2.827641000	-1.517412000	-3.470014000
6	-1.557596000	-0.209523000	-2.173023000
1	-1.609232000	0.750475000	-2.676585000
6	-3.566573000	0.092989000	0.917513000
1	-2.959546000	0.617402000	1.647545000
6	-3.901024000	-1.290871000	0.952905000
1	-3.587811000	-2.002610000	1.710881000
6	-4.673239000	-1.586313000	-0.209170000
1	-5.050476000	-2.563193000	-0.492577000
6	-4.812881000	-0.383802000	-0.963021000
1	-5.314970000	-0.287914000	-1.919859000
6	-4.125182000	0.654789000	-0.268382000
1	-4.016591000	1.683060000	-0.598886000
6	1.522286000	1.122578000	-1.247552000
6	2.302521000	2.252862000	-0.973577000
1	2.062284000	2.884442000	-0.116796000
6	3.386320000	2.573849000	-1.781778000
1	3.981110000	3.458186000	-1.562795000
6	3.712078000	1.761302000	-2.866752000
1	4.561888000	2.010298000	-3.498642000
6	2.947718000	0.631075000	-3.139629000
1	3.196917000	-0.004975000	-3.986614000
6	1.855530000	0.310875000	-2.334525000
1	1.260799000	-0.574474000	-2.559590000
6	-0.734270000	2.221128000	0.109763000
6	-1.206062000	2.647223000	1.353732000
1	-0.985432000	2.070813000	2.249886000
6	-1.970472000	3.806774000	1.461628000
1	-2.331549000	4.125030000	2.437131000
6	-2.264258000	4.556562000	0.327303000
1	-2.858996000	5.463539000	0.411369000
6	-1.783818000	4.150040000	-0.916136000
1	-1.998141000	4.739826000	-1.804824000
6	-1.019647000	2.993369000	-1.024075000
1	-0.631205000	2.699753000	-1.998474000
6	-0.539933000	-2.588113000	0.616979000
1	-1.182487000	-2.298054000	1.458348000
6	1.804358000	-2.662114000	0.060513000
1	2.020855000	-3.728591000	0.250621000
1	1.477230000	-2.623369000	-1.000875000
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1	3.943442000	0.982255000	1.502685000
6	5.258568000	-0.260411000	0.341716000
1	6.101320000	0.418440000	0.432804000
6	5.360825000	-1.458717000	-0.365110000
6	4.250538000	-2.280673000	-0.449490000
1	4.277958000	-3.221813000	-0.994045000
6	1.640348000	1.068131000	2.520411000

6	-0.371016000	-0.333439000	2.616946000
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1	-0.175809000	-4.492524000	-0.413838000

$[Mn(CO)_2(L^{-H})]\cdots EtOH$ (B)
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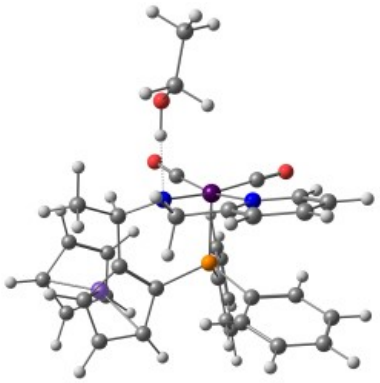
E (BS2) = -4406.86265741
G_{1M} = -4406.332272



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7	1.264852000	-1.594166000	-0.311672000
7	2.851305000	0.403777000	0.101727000
6	-1.194483000	-0.040683000	-1.120478000
6	-0.910272000	-1.416699000	-1.455249000
6	-1.741601000	-1.758097000	-2.563721000
1	-1.802868000	-2.735605000	-3.031205000
6	-2.532455000	-0.624865000	-2.914871000
1	-3.289347000	-0.591467000	-3.691604000
6	-2.199717000	0.434728000	-2.028770000
1	-2.639582000	1.426953000	-2.027590000
6	-3.458249000	-1.304761000	0.984971000
1	-2.876148000	-0.956620000	1.831507000
6	-3.376191000	-2.597402000	0.392739000
1	-2.716412000	-3.400747000	0.706428000
6	-4.272864000	-2.630692000	-0.715719000
1	-4.414431000	-3.463477000	-1.396356000
6	-4.907159000	-1.356824000	-0.808180000
1	-5.614726000	-1.052894000	-1.572242000
6	-4.400691000	-0.534418000	0.241162000
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6	0.485390000	2.277865000	-0.821728000
6	0.916704000	3.423068000	-0.140911000
1	0.673659000	3.553531000	0.914683000
6	1.656193000	4.397293000	-0.801371000
1	1.978953000	5.286946000	-0.264628000
6	1.985797000	4.232031000	-2.145549000
1	2.566524000	4.993369000	-2.661845000
6	1.570990000	3.090794000	-2.825299000
1	1.824939000	2.957767000	-3.874969000
6	0.822039000	2.116773000	-2.168064000
1	0.501203000	1.226581000	-2.709159000
6	-1.628873000	1.839631000	1.056080000
6	-1.915352000	1.510224000	2.383322000
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6	-2.938880000	2.159723000	3.069109000
1	-3.150028000	1.891159000	4.101806000
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6	-2.372079000	2.851117000	0.433199000
1	-2.144124000	3.147324000	-0.589954000
6	0.067619000	-2.326550000	-0.726533000
1	-0.419427000	-2.657780000	0.200906000
6	2.140222000	-1.298344000	-1.425121000
1	2.686340000	-2.186957000	-1.792039000
1	1.579223000	-0.921992000	-2.307712000
6	3.121865000	-0.250235000	-1.044340000
6	3.668662000	1.409966000	0.474401000
6	4.772024000	1.788676000	-0.265192000
6	5.060072000	1.098780000	-1.442594000
6	4.227201000	0.064460000	-1.832031000
6	1.429885000	0.804776000	2.480046000
6	0.027371000	-1.183469000	2.076506000
1	2.148547000	-2.675244000	0.889048000
8	2.699464000	-3.209693000	1.510939000
6	3.981313000	-3.336984000	0.922629000
1	4.359903000	-2.348322000	0.603120000
1	3.934492000	-3.968748000	0.017699000
1	4.408627000	-0.500695000	-2.743430000
1	5.395452000	2.608247000	0.079508000
6	4.925683000	-3.948897000	1.926156000
1	5.925307000	-4.076490000	1.496152000
1	5.011718000	-3.311477000	2.814482000
1	4.562720000	-4.932950000	2.247009000
1	5.924424000	1.368776000	-2.044311000
1	3.419678000	1.922226000	1.400832000
6	0.362622000	-3.591413000	-1.523678000
1	-0.546834000	-4.197790000	-1.622666000
1	0.735567000	-3.379936000	-2.533630000
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$[Mn(CO)_2(L^{-H})(\eta\text{-}H_2)]\cdots EtOH$ (C)
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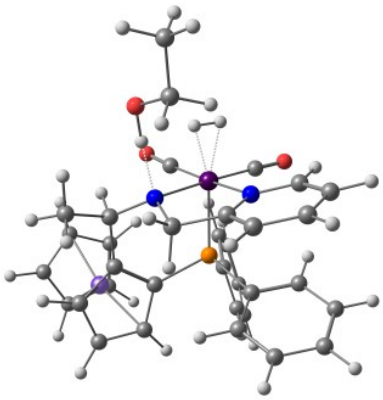
E (BS2) = -4408.03628307
G_{1M} = -4407.486987



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8	-0.929079000	-1.686564000	2.850650000
7	1.277306000	-1.638460000	-0.142118000
7	2.790057000	0.467672000	0.321739000
6	-1.216411000	-0.149899000	-1.071510000
6	-0.922384000	-1.539475000	-1.314960000
6	-1.748191000	-1.951150000	-2.404996000
1	-1.802986000	-2.954690000	-2.814384000
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1	-3.060964000	-0.762590000	1.900002000

6	-3.416808000	-2.567073000	0.623243000
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6	-4.252572000	-2.755516000	-0.516809000
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1	-5.604613000	-1.335868000	-1.603459000
6	-4.508739000	-0.577047000	0.200863000
1	-4.813096000	0.463316000	0.257246000
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6	1.879033000	4.133505000	-1.149902000
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6	2.022642000	3.940472000	-2.522979000
1	2.607015000	4.642618000	-3.113770000
6	1.411824000	2.851741000	-3.136176000
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6	-2.055632000	1.684467000	2.165934000
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6	4.995593000	1.193903000	-1.207062000
6	4.121766000	0.214707000	-1.648237000
6	1.161292000	1.043677000	2.594893000
6	-0.132024000	-1.087930000	2.236435000
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1	2.348324000	-2.771384000	0.527022000
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1	4.273996000	-0.296594000	-2.596330000
1	5.422186000	2.563571000	0.420790000
1	5.855993000	1.477956000	-1.808117000
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1	6.345353000	-3.472024000	1.171565000
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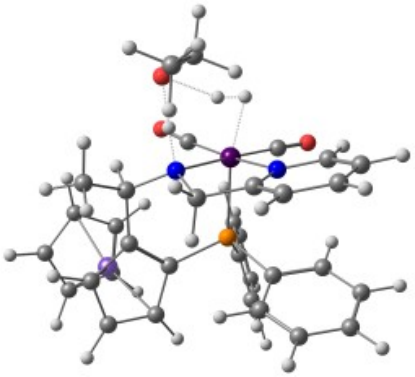
E (BS2) = -4408.03384959

G_{1M} = -4407.483857



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7	1.245075000	-1.710407000	0.018484000
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6	-1.149167000	-0.162811000	-1.083393000
6	-0.903120000	-1.576609000	-1.231636000
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6	-3.492738000	-2.394014000	0.675662000
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1	-4.385616000	-3.556375000	-1.021379000
6	-4.915346000	-1.385816000	-0.836321000
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6	-4.492893000	-0.394866000	0.098176000
1	-4.759692000	0.657060000	0.081788000
6	0.678445000	2.052145000	-1.082411000
6	1.308759000	3.169331000	-0.520136000
1	1.156336000	3.407060000	0.533841000
6	2.135746000	3.975092000	-1.293145000
1	2.620390000	4.839709000	-0.844481000
6	2.350318000	3.669505000	-2.636248000
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1	0.398698000	0.901137000	-2.889887000
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6	4.869095000	1.590057000	0.152874000
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1	2.130321000	-1.454731000	2.193492000
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1	6.068013000	1.064071000	-1.564138000
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6	0.351668000	-3.748530000	-1.097330000
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[MnH(CO)$_2$(L)]···EtOH (D)

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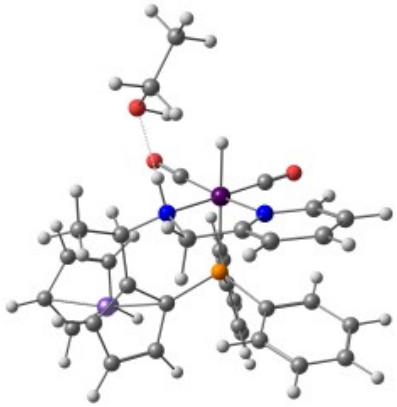
E (BS2) = -4408.06355481

G_{1M} = -4407.510481



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6	1.171924000	-0.114204000	-1.127310000
6	0.920480000	1.228316000	-1.598021000
6	1.777158000	1.449871000	-2.720231000
1	1.864472000	2.375625000	-3.279177000
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6	4.292967000	2.459539000	-0.919651000
1	4.489862000	3.193033000	-1.694271000
6	4.890061000	1.168798000	-0.817015000
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1	3.120035000	-1.475605000	4.212553000
6	3.600623000	-2.941115000	2.707938000
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6	3.285455000	-3.439702000	1.445296000
1	3.831640000	-4.289331000	1.040863000
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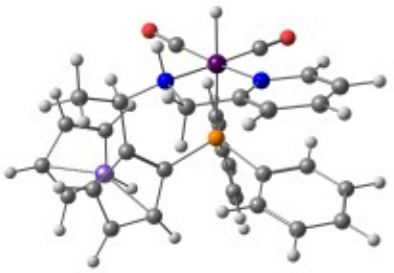
E (BS2) = -4253.04110075

G_{1M} = -4252.561954



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1	6.074290000	0.338819000	0.365354000
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[MnH(CO)$_2$(L)]···PhCOMe (F-*re*)

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E (BS2) = -4637.82839304

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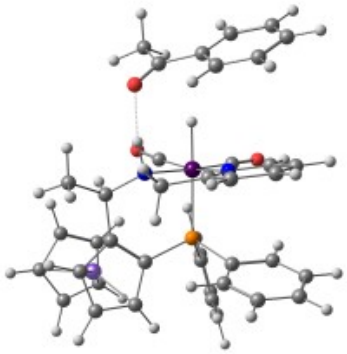

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[MnH(CO)$_2$(L)]···PhCOMe (F-*si*)
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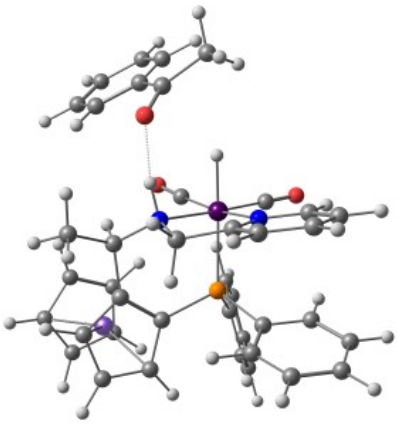
G_{1M} = -4637.221396



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1	-3.785039000	-1.436532000	-3.456670000
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6	1.341856000	-1.530119000	-3.130124000
1	2.433949000	-1.534213000	-3.026200000
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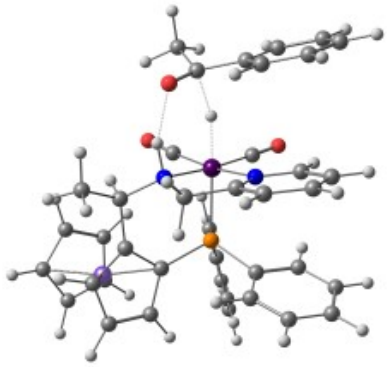
E (BS2) = -4637.82292119

G_{1M} = -4637.215637



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1	-2.934007000	-2.168751000	-3.254961000
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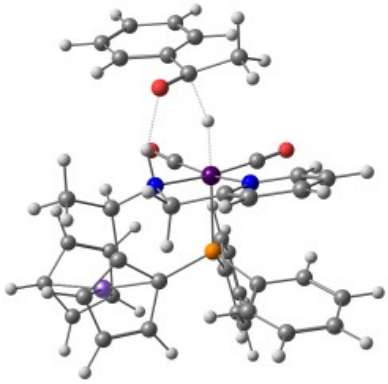
E (BS2) = -4637.82054981

G_{1M} = -4637.213903



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6	2.843040000	4.309138000	-1.510587000
6	2.338778000	3.263693000	-2.268815000
1	2.320076000	3.307713000	-3.355320000
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6	4.945822000	0.490374000	0.138935000
6	4.500889000	-2.104008000	1.599853000
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1	4.753735000	-3.442363000	3.261950000
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1	4.800194000	-1.231345000	2.177889000
1	4.769006000	0.652572000	1.206965000
1	6.012665000	0.264749000	-0.002540000
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$[Mn(CO)_2(L)]^+\cdots PhCH(Me)O^-$ (G-*S*)

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E (BS2) = -4637.83167065

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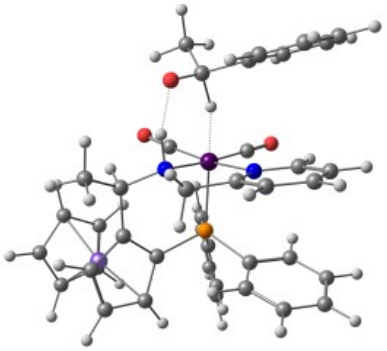

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$[Mn(CO)_2(L)]^+\cdots PhCH(Me)O^-$ (G-*R*)

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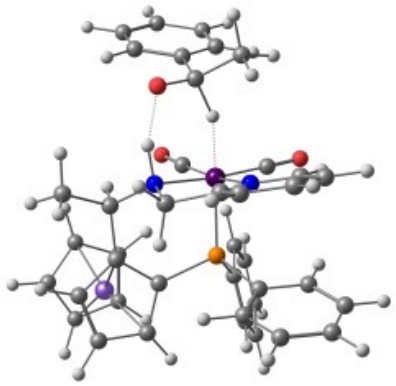
E (BS2) = -4637.82884767

G_{1M} = -4637.216726



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E (BS2) = -4637.82726983
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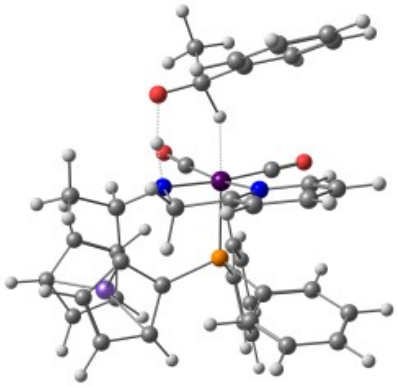

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1	0.496709000	-3.965519000	-1.839879000
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TS_{GH} (*R*)
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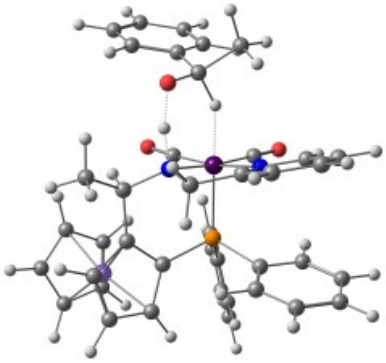
E (BS2) = -4637.82447546
G_{1M} = -4637.216889



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1	-3.690372000	-3.705206000	-2.645731000
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1	-5.567338000	-2.377834000	-1.232103000
6	-3.990847000	-2.238175000	0.357433000
1	-4.477465000	-1.660588000	1.137269000
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6	-1.617253000	-0.502145000	2.867868000
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1	-2.158171000	-1.593309000	4.639433000
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6	-3.985782000	0.908522000	3.244655000
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6	2.519343000	2.916852000	0.482307000
6	3.076853000	4.068545000	-0.041519000
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6	2.445441000	3.295970000	-2.216139000
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1	5.854180000	-0.315068000	-0.706270000
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[Mn(CO)$_2$(L^{-H})]···HOCHPhMe (H-*S*)

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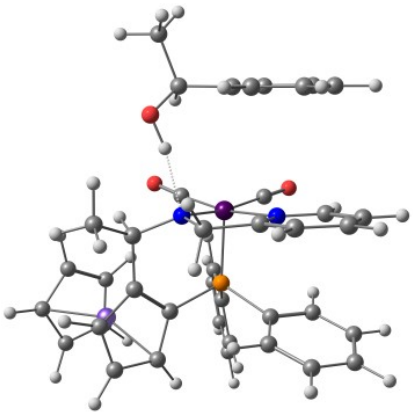
E (BS2) = -4637.8236555
G_{1M} = -4637.218075



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6	-1.889926000	0.175373000	-1.028284000
6	-1.531913000	-1.022170000	-1.750930000
6	-2.534575000	-1.223968000	-2.747055000
1	-2.585076000	-2.063229000	-3.433127000
6	-3.501190000	-0.180813000	-2.649400000
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6	-0.014593000	4.046074000	-2.350434000
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1	3.601136000	-1.646320000	2.967128000
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1	3.296016000	-5.403326000	1.027168000
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6	-0.096503000	-2.896050000	-2.613141000
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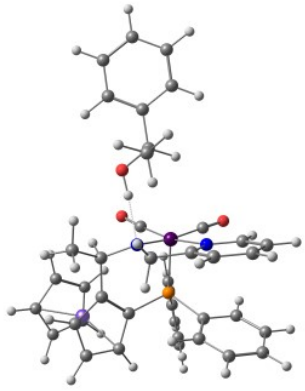
1	0.028365000	-2.394930000	-3.581146000

[Mn(CO)$_2$(L^{-H})]···HOCHPhMe (H-*R*)

E (BS1) = -2450.68881326

E (BS2) = -4637.8236555

G_{1M} = -4637.218075



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6	-1.186991000	-1.118558000	-1.852585000
6	-2.012929000	-1.656265000	-2.884466000
1	-1.682898000	-2.320483000	-3.676724000
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1	-1.840564000	-2.729995000	1.600487000
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6	-2.302505000	5.067770000	-0.722018000
1	-2.450745000	6.113786000	-0.981430000
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1	-2.375933000	4.388135000	-2.764692000
6	-2.074008000	2.759316000	-1.392525000
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6	-2.669889000	0.314779000	1.775968000
6	-2.266490000	-0.398587000	2.907363000
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6	-3.180186000	-0.703718000	3.913582000
1	-2.851743000	-1.260504000	4.788377000
6	-4.504249000	-0.291990000	3.802044000
1	-5.216799000	-0.527372000	4.589533000
6	-4.913238000	0.434086000	2.685228000
1	-5.944123000	0.770681000	2.599191000
6	-4.001615000	0.739706000	1.680603000
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6	0.308995000	-1.329673000	-1.675412000
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1	1.825712000	0.673760000	-2.957736000
1	0.115098000	1.021874000	-2.762661000
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6	1.410862000	3.456964000	0.382409000
6	1.775504000	4.604086000	-0.295063000
6	1.958384000	4.539009000	-1.676350000
6	1.758718000	3.330445000	-2.320683000
6	0.745579000	1.143997000	2.274583000
6	0.590590000	-1.125371000	1.333829000
1	2.584220000	-0.859436000	-0.627740000
8	3.392545000	-1.324463000	-0.299720000
6	4.421035000	-0.356421000	-0.217319000
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1	1.918101000	5.530470000	0.253252000
1	2.252204000	5.422644000	-2.237523000
1	1.268091000	3.470830000	1.460490000
6	0.953258000	-1.893904000	-2.936383000
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1	0.749140000	-1.285460000	-3.826284000
1	2.040757000	-1.957859000	-2.800016000
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6	6.537008000	-0.183348000	1.125233000
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6	7.705544000	-0.724187000	1.652140000
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1	6.306789000	0.872122000	1.276415000
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1	8.388187000	-0.092400000	2.217214000
1	7.332428000	-3.928307000	0.592486000
1	8.906314000	-2.500357000	1.879305000
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6	4.743130000	0.198364000	-1.597799000
1	5.052241000	-0.618509000	-2.263734000
1	3.863464000	0.689178000	-2.035577000
1	5.555503000	0.934076000	-1.552391000

A. Reoptimized enantiodetermining TS_{FG} with the method of ref. 19.

F.1. Catalyst 5a.

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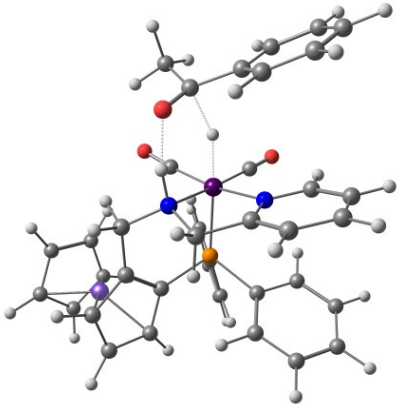
E (BS2) = -4597.24246395
G_{1M} = -4596.683772



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6	-1.690828000	-0.988188000	-1.864065000
6	-2.686073000	-1.097630000	-2.903401000
1	-2.707211000	-1.873508000	-3.681270000
6	-3.653456000	-0.048007000	-2.729247000
1	-4.545423000	0.116963000	-3.348436000
6	-3.267138000	0.725797000	-1.581009000
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6	-3.586900000	-2.374797000	0.654109000
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6	-3.856927000	-3.182090000	-0.506240000
1	-3.261675000	-4.038580000	-0.850630000
6	-5.030620000	-2.654390000	-1.153827000
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1	-4.656882000	-0.557767000	1.486024000
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6	0.358124000	4.772182000	0.196279000
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6	0.138682000	5.189774000	-1.130759000
1	0.425283000	6.205419000	-1.446647000
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1	-1.431918000	-0.475030000	2.896877000
6	-3.042337000	0.598606000	3.879842000
1	-3.033686000	-0.061308000	4.761982000
6	-3.951089000	1.669210000	3.807907000
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6	-3.945179000	2.511088000	2.680220000
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6	-3.037928000	2.281016000	1.631228000
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1	-0.683028000	-2.686802000	-0.951277000
6	1.205941000	-0.247512000	-2.341071000
1	1.581719000	-0.750986000	-3.259645000
1	0.329715000	0.364823000	-2.653328000
6	2.242823000	0.675387000	-1.763810000
6	3.055426000	1.714555000	0.160516000
6	3.973223000	2.468915000	-0.578154000
1	4.638180000	3.172264000	-0.055732000
6	4.028620000	2.303456000	-1.972297000
6	3.151206000	1.385203000	-2.566925000
1	3.154946000	1.217228000	-3.654526000
6	1.280110000	0.278141000	2.188888000
6	0.091580000	-1.747982000	1.389745000
1	1.509213000	-1.961010000	-1.259536000
1	2.219781000	-1.365577000	0.768428000
6	3.277744000	-2.661439000	0.154048000
6	4.542012000	-1.851998000	0.372024000
6	2.875509000	-3.649121000	1.247101000
6	5.054145000	-1.543539000	1.654378000
6	5.271227000	-1.438652000	-0.765972000
6	6.262350000	-0.840064000	1.791538000
6	6.481542000	-0.740083000	-0.630401000
1	4.866021000	-1.694297000	-1.756849000
6	6.982049000	-0.437768000	0.650055000
1	6.646210000	-0.604324000	2.797074000
1	7.041581000	-0.432042000	-1.528116000
8	2.887601000	-2.873172000	-1.029858000
1	4.743394000	2.875127000	-2.583574000
1	7.932030000	0.109460000	0.759605000
1	4.500524000	-1.842357000	2.557569000
1	2.924316000	-3.235590000	2.271557000
1	1.851577000	-4.019164000	1.056953000
1	3.575213000	-4.513419000	1.192341000
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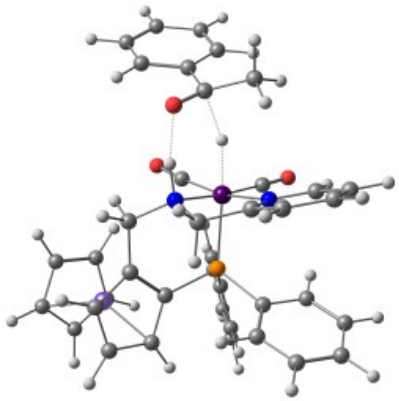
E (BS2) = -4597.24069533
G_{1M} = -4596.682740



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8	1.726990000	0.909408000	3.176388000
8	1.100176000	-2.555803000	1.020392000
7	1.046788000	-0.002900000	-1.725877000
7	1.707054000	2.164637000	-0.325684000
6	-1.990943000	-0.007146000	-0.942076000

6	-1.356246000	-0.668949000	-2.078702000
6	-2.380678000	-0.915234000	-3.064933000
1	-2.223071000	-1.412979000	-4.031855000
6	-3.636538000	-0.432745000	-2.557118000
1	-4.607278000	-0.500007000	-3.066393000
6	-3.404212000	0.120618000	-1.250951000
1	-4.165229000	0.569257000	-0.599614000
6	-2.151972000	-3.301319000	-0.019293000
1	-1.213789000	-3.255555000	0.548892000
6	-2.303713000	-3.822973000	-1.351978000
1	-1.505140000	-4.248886000	-1.974346000
6	-3.682385000	-3.664614000	-1.739094000
1	-4.117182000	-3.943970000	-2.708165000
6	-4.383935000	-3.046433000	-0.643118000
1	-5.447550000	-2.773046000	-0.630852000
6	-3.438785000	-2.819535000	0.418689000
1	-3.652479000	-2.345621000	1.385353000
6	-1.497475000	2.527711000	0.376608000
6	-1.151885000	3.342100000	1.482662000
1	-0.711821000	2.883644000	2.383608000
6	-1.370864000	4.728845000	1.448057000
1	-1.105737000	5.345116000	2.322092000
6	-1.923672000	5.330179000	0.300700000
1	-2.093959000	6.418136000	0.272701000
6	-2.254819000	4.533086000	-0.808356000
1	-2.687850000	4.993585000	-1.710888000
6	-2.044046000	3.140866000	-0.772073000
1	-2.324915000	2.529897000	-1.644017000
6	-2.044238000	0.205353000	1.969286000
6	-1.554335000	-0.802549000	2.827436000
1	-0.579733000	-1.268844000	2.625040000
6	-2.306065000	-1.223436000	3.940031000
1	-1.907717000	-2.010831000	4.599603000
6	-3.556067000	-0.639886000	4.212358000
1	-4.142907000	-0.967631000	5.085176000
6	-4.049399000	0.371991000	3.367862000
1	-5.024043000	0.841295000	3.577090000
6	-3.297639000	0.794669000	2.257685000
1	-3.688184000	1.601641000	1.618051000
6	0.106178000	-1.026385000	-2.249342000
1	0.350052000	-1.973178000	-1.729935000
6	0.932144000	1.282950000	-2.444616000
1	1.324520000	1.215047000	-3.483665000
1	-0.146954000	1.544775000	-2.529891000
6	1.622140000	2.372708000	-1.672831000
6	2.248187000	3.153283000	0.435830000
6	2.726839000	4.353885000	-0.099722000
1	3.154238000	5.112300000	0.572651000
6	2.658649000	4.558364000	-1.488259000
6	2.098028000	3.546008000	-2.281420000
1	2.019388000	3.657157000	-3.373427000
6	1.485629000	0.672439000	2.040120000
6	1.067247000	-1.403773000	0.743890000
1	2.026225000	-0.359422000	-1.907841000
1	2.751797000	-0.063765000	0.172476000
6	4.139560000	-0.465948000	-0.837676000
6	4.493178000	-1.686276000	-0.006175000
6	4.878894000	0.835677000	-0.533790000
6	5.094384000	-1.605853000	1.271580000
6	4.255277000	-2.962837000	-0.563456000
6	5.443117000	-2.772978000	1.972152000
6	4.605541000	-4.129680000	0.133514000
1	3.796550000	-3.009928000	-1.563042000
6	5.201024000	-4.038987000	1.405979000
1	5.908322000	-2.693926000	2.967844000
1	4.416179000	-5.117233000	-0.317566000
8	3.667140000	-0.636868000	-1.999191000
1	3.035660000	5.486237000	-1.944557000
1	5.477348000	-4.952869000	1.955880000
1	4.420984000	1.660097000	-1.111728000
1	5.285428000	-0.625420000	1.733828000
1	4.897984000	1.107113000	0.538265000
1	5.931776000	0.720562000	-0.876906000
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F.2. Catalyst I.

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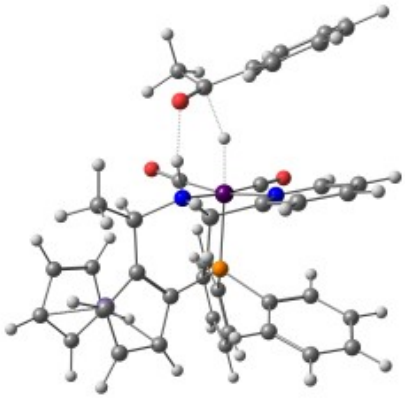
E (BS2) = -4636.52525285
G_{1M} = -4635.940804



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8	1.586795000	1.212319000	3.183201000
8	-0.345628000	-2.335489000	2.363153000
7	0.749170000	-1.323599000	-1.088383000
7	2.191956000	0.831780000	-0.470872000
6	-2.021728000	0.085331000	-0.992093000
6	-1.687639000	-1.174884000	-1.656409000
6	-2.686241000	-1.397944000	-2.677149000
1	-2.738282000	-2.265241000	-3.347078000
6	-3.630966000	-0.314931000	-2.647356000
1	-4.518389000	-0.217167000	-3.286971000
6	-3.232068000	0.595180000	-1.610322000
1	-3.750999000	1.522240000	-1.335257000
6	-3.615775000	-2.150873000	1.027306000
1	-2.780802000	-2.189986000	1.738940000
6	-3.885501000	-3.116626000	-0.005111000
1	-3.298300000	-4.021379000	-0.212602000
6	-5.047191000	-2.677361000	-0.735137000
1	-5.496642000	-3.184595000	-1.599358000
6	-5.497942000	-1.440180000	-0.150653000
1	-6.351565000	-0.839331000	-0.491983000
6	-4.612419000	-1.112523000	0.936353000
1	-4.671911000	-0.220296000	1.572982000
6	-0.597458000	2.578553000	-0.585807000
6	-0.009028000	3.592775000	0.208702000
1	0.161275000	3.416370000	1.283609000
6	0.353584000	4.826407000	-0.355931000
1	0.800062000	5.607444000	0.280206000
6	0.150801000	5.063749000	-1.729256000
1	0.436347000	6.030849000	-2.172692000
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1	-0.578992000	4.232793000	-3.605598000
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6	3.054966000	1.788437000	-0.035764000
6	3.959503000	2.440749000	-0.880216000
1	4.628008000	3.209148000	-0.464953000
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6	0.113053000	-1.477212000	1.683499000
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6	4.557700000	-1.720936000	0.650487000
6	2.895474000	-3.389882000	1.759637000
6	5.080768000	-1.254119000	1.879519000
6	5.277103000	-1.453484000	-0.536371000
6	6.289051000	-0.538326000	1.916861000
6	6.486931000	-0.742038000	-0.500197000
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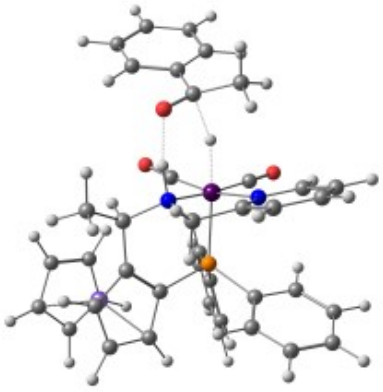
E (BS2) = -4636.52370747

G_{1M} = -4635.939627



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6	-1.372787000	-0.734165000	-1.987959000
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1	-2.112798000	6.443056000	0.157798000
6	-2.259316000	4.529419000	-0.874072000
1	-2.686227000	4.964391000	-1.792051000
6	-2.044849000	3.139307000	-0.799083000
1	-2.316787000	2.504912000	-1.656968000
6	-2.045420000	0.285396000	2.031767000
6	-1.549136000	-0.689617000	2.923543000
1	-0.571415000	-1.155917000	2.737069000
6	-2.297514000	-1.076952000	4.050521000
1	-1.893971000	-1.839179000	4.735987000
6	-3.550661000	-0.491851000	4.304077000
1	-4.135119000	-0.793425000	5.187856000
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1	-5.026753000	0.959831000	3.621175000
6	-3.301370000	0.877868000	2.302240000
1	-3.696616000	1.661458000	1.637008000
6	0.090759000	-1.138850000	-2.125354000
1	0.287987000	-1.977155000	-1.427987000
6	0.895895000	1.201044000	-2.433522000
1	1.300534000	1.107994000	-3.464416000
1	-0.185366000	1.447002000	-2.537343000
6	1.571794000	2.330192000	-1.705364000
6	2.205918000	3.204537000	0.363864000
6	2.661683000	4.389459000	-0.223753000
1	3.083778000	5.180435000	0.413546000
6	2.577788000	4.536808000	-1.618668000
6	2.025412000	3.485146000	-2.364807000
1	1.936012000	3.550802000	-3.459686000
6	1.488767000	0.782842000	2.073617000
6	1.072193000	-1.346267000	0.872316000
1	2.001247000	-0.410031000	-1.825590000
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6	4.127051000	-0.466488000	-0.766931000
6	4.524109000	-1.605357000	0.155867000
6	4.838464000	0.872904000	-0.581512000
6	5.151852000	-1.403908000	1.407333000
6	4.302469000	-2.929561000	-0.284397000
6	5.542319000	-2.499234000	2.196264000
6	4.694624000	-4.024947000	0.500679000
1	3.821900000	-3.073020000	-1.264122000
6	5.316376000	-3.813740000	1.745980000
1	6.027989000	-2.325459000	3.169915000
1	4.517216000	-5.051131000	0.140014000
8	3.644793000	-0.742034000	-1.904214000
1	2.936792000	5.450890000	-2.115521000
1	5.625523000	-4.671418000	2.364640000

1	4.353250000	1.635901000	-1.218585000
1	5.331743000	-0.383880000	1.779533000
1	4.864656000	1.232383000	0.464140000
1	5.889201000	0.754444000	-0.930001000
1	2.273647000	3.054530000	1.450749000
6	0.438092000	-1.627093000	-3.542275000
1	1.517484000	-1.872536000	-3.604011000
1	-0.128909000	-2.548572000	-3.781798000
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Crystal Data, Data Collection and Structure Refinement for 5a

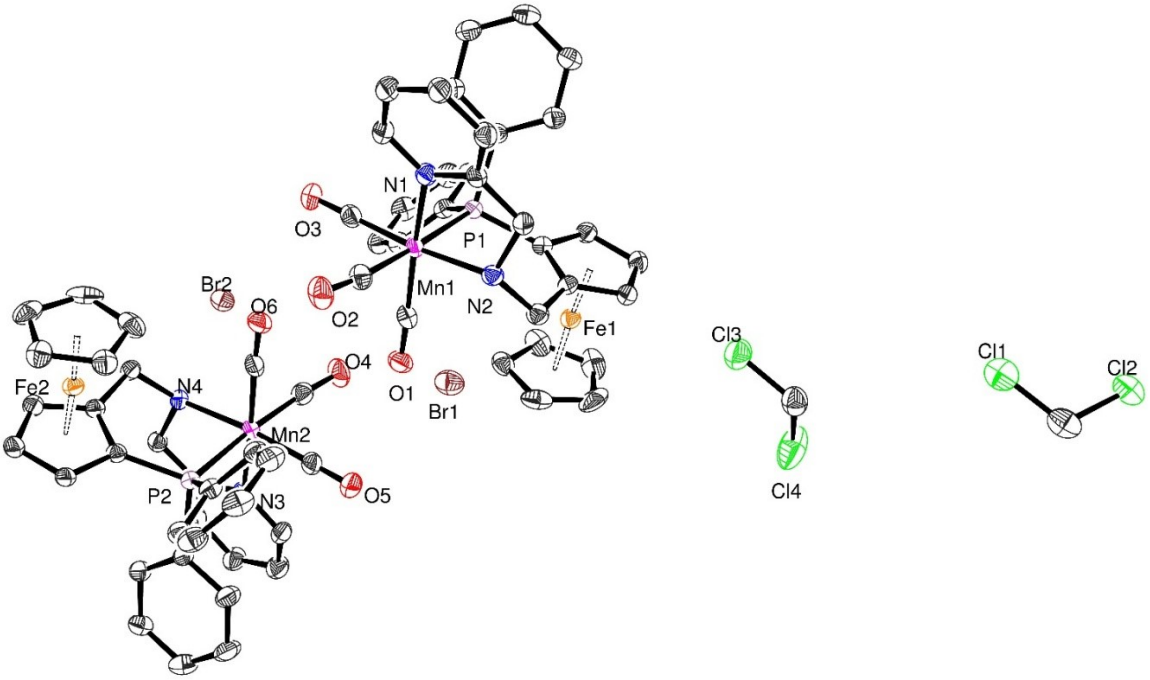

Figure S36 : Asymmetric Unit

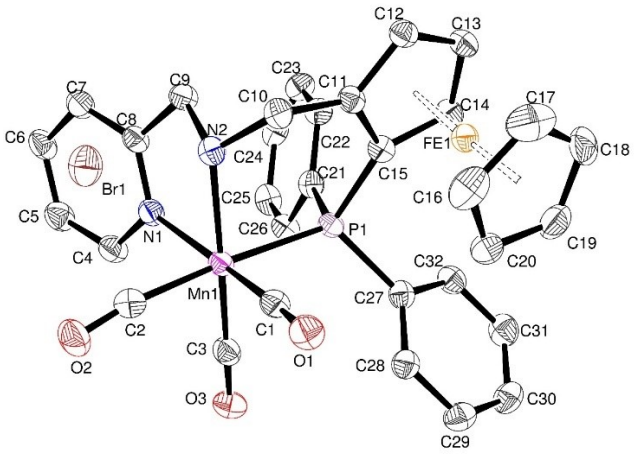

Figure S37 : Compound

Table S1. Crystal data and structure refinement for **5a** (20240924-Vickie_Mn).

Identification code	20240924-Vickie_Mn
Empirical formula	C33 H29 Br Cl2 Fe Mn N2 O3 P
Formula weight	794.15
Temperature	103(2) K
Wavelength	1.54184 A
Crystal system, space group	Orthorhombic, P 21 21 21
Unit cell dimensions	a = 14.75840(10) A alpha = 90 deg.
	b = 15.39170(10) A beta = 90 deg.
	c = 28.80400(10) A gamma = 90 deg.
Volume	6543.03(7) A^3
Z, Calculated density	8, 1.612 Mg/m^3
Absorption coefficient	10.393 mm^-1
F(000)	3200
Crystal size	0.2 x 0.2 x 0.2 mm
Theta range for data collection	3.068 to 80.235 deg.
Limiting indices	-18<=h<=17, -19<=k<=18, -36<=l<=36
Reflections collected / unique	141040 / 14175 [R(int) = 0.0520]
Completeness to theta = 67.684	100.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	14175 / 0 / 801
Goodness-of-fit on F^2	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0334, wR2 = 0.0888
R indices (all data)	R1 = 0.0339, wR2 = 0.0891
Absolute structure parameter	0.0005(12)
Largest diff. peak and hole	1.488 and -0.745 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5a** (20240924-Vickie_Mn). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	3392(3)	8353(3)	7119(1)	27(1)
C(2)	4359(3)	9516(3)	7481(2)	30(1)
C(3)	3531(3)	9900(3)	6747(1)	28(1)
C(4)	5502(3)	10595(3)	6714(2)	30(1)
C(5)	6316(3)	11040(3)	6717(2)	33(1)
C(6)	7120(3)	10582(3)	6756(2)	31(1)
C(7)	7084(3)	9682(3)	6788(2)	30(1)
C(8)	6241(3)	9267(3)	6784(1)	24(1)
C(9)	6154(3)	8302(3)	6809(1)	25(1)
C(10)	5081(3)	7125(3)	6958(1)	25(1)
C(11)	4908(3)	6864(2)	6463(1)	22(1)
C(12)	5168(3)	6058(3)	6264(1)	24(1)
C(13)	4862(3)	6023(3)	5795(1)	26(1)
C(14)	4398(3)	6815(3)	5698(1)	25(1)
C(15)	4425(3)	7346(2)	6111(1)	22(1)
C(16)	3064(3)	5840(4)	6811(2)	40(1)
C(17)	3286(4)	5097(3)	6534(3)	52(2)
C(18)	2891(3)	5221(3)	6087(2)	47(1)
C(19)	2438(3)	6031(4)	6093(2)	37(1)
C(20)	2537(3)	6410(3)	6535(2)	31(1)
C(21)	4914(3)	8961(3)	5732(1)	25(1)
C(22)	5654(3)	8507(3)	5553(1)	27(1)
C(23)	6263(3)	8917(3)	5256(2)	30(1)
C(24)	6139(3)	9784(3)	5136(1)	30(1)
C(25)	5406(3)	10241(3)	5315(2)	31(1)
C(26)	4792(3)	9833(3)	5608(2)	29(1)
C(27)	3021(3)	8570(3)	5867(1)	24(1)
C(28)	2240(3)	8721(3)	6126(2)	27(1)
C(29)	1395(3)	8783(3)	5913(2)	32(1)
C(30)	1328(3)	8688(3)	5438(2)	34(1)
C(31)	2096(3)	8534(3)	5173(2)	34(1)
C(32)	2941(3)	8483(3)	5382(1)	28(1)
C(33)	722(3)	8466(3)	7367(2)	30(1)
C(34)	1482(3)	7998(3)	8113(2)	27(1)
C(35)	1669(3)	9565(3)	7780(1)	26(1)
C(36)	-497(3)	7333(3)	8155(2)	29(1)
C(37)	-1310(3)	6887(3)	8179(2)	34(1)
C(38)	-2114(3)	7347(3)	8120(2)	34(1)
C(39)	-2073(3)	8236(3)	8042(2)	29(1)
C(40)	-1232(3)	8644(3)	8030(1)	24(1)
C(41)	-1145(3)	9608(3)	7986(1)	24(1)
C(42)	-37(3)	10784(2)	7969(1)	23(1)
C(43)	22(3)	10944(2)	8484(1)	21(1)
C(44)	460(3)	10404(2)	8831(1)	21(1)
C(45)	394(3)	10847(2)	9267(1)	24(1)
C(46)	-68(3)	11645(3)	9193(1)	26(1)
C(47)	-300(3)	11698(3)	8714(1)	24(1)
C(48)	1728(3)	12284(4)	8277(2)	40(1)
C(49)	2264(3)	11571(3)	8414(2)	35(1)
C(50)	2451(3)	11646(3)	8896(2)	31(1)
C(51)	2031(3)	12423(3)	9058(2)	33(1)
C(52)	1579(3)	12818(3)	8678(2)	38(1)

C(53)	107(3)	8647(2)	9093(1)	23(1)
C(54)	-786(3)	8885(3)	9175(1)	26(1)
C(55)	-1377(3)	8311(3)	9391(2)	30(1)
C(56)	-1076(3)	7503(3)	9530(2)	37(1)
C(57)	-191(3)	7256(3)	9448(2)	38(1)
C(58)	413(3)	7823(3)	9233(2)	32(1)
C(59)	1933(3)	9254(3)	9034(1)	25(1)
C(60)	1953(3)	9314(3)	9520(2)	30(1)
C(61)	2770(3)	9312(3)	9756(2)	35(1)
C(62)	3572(3)	9218(3)	9521(2)	35(1)
C(63)	3573(3)	9129(3)	9038(2)	34(1)
C(64)	2754(3)	9153(3)	8794(2)	28(1)
C(65)	8164(4)	116(4)	5713(2)	47(1)
C(66)	4415(4)	2531(4)	5663(2)	45(1)
N(1)	5460(2)	9720(2)	6751(1)	24(1)
N(2)	5277(2)	8067(2)	7026(1)	23(1)
N(3)	-451(2)	8199(2)	8080(1)	24(1)
N(4)	-225(2)	9862(2)	7839(1)	22(1)
O(1)	2829(2)	7945(2)	7289(1)	32(1)
O(2)	4314(3)	9895(2)	7820(1)	41(1)
O(3)	3050(2)	10454(2)	6653(1)	34(1)
O(4)	824(3)	8152(2)	7011(1)	39(1)
O(5)	1953(2)	7437(2)	8207(1)	35(1)
O(6)	2249(2)	9968(2)	7634(1)	32(1)
Mn(1)	4295(1)	9024(1)	6897(1)	21(1)
Mn(2)	734(1)	8888(1)	7964(1)	21(1)
Fe(1)	3786(1)	6200(1)	6239(1)	23(1)
Fe(2)	1076(1)	11595(1)	8787(1)	22(1)
P(1)	4130(1)	8475(1)	6151(1)	21(1)
P(2)	851(1)	9317(1)	8733(1)	21(1)
Cl(1)	7805(1)	1185(1)	5575(1)	53(1)
Cl(2)	8665(1)	-413(1)	5229(1)	52(1)
Cl(3)	4093(1)	3590(1)	5521(1)	56(1)
Cl(4)	3489(1)	1823(1)	5665(1)	81(1)
Br(1)	5398(1)	7911(1)	8134(1)	34(1)
Br(2)	-408(1)	10059(1)	6722(1)	30(1)

Table S3. Bond lengths [A] and angles [deg] for **5a** (20240924-Vickie_Mn).

C(1)-O(1)	1.151(5)
C(1)-Mn(1)	1.803(4)
C(2)-O(2)	1.138(6)
C(2)-Mn(1)	1.847(5)
C(3)-O(3)	1.143(5)
C(3)-Mn(1)	1.810(4)
C(4)-N(1)	1.352(5)
C(4)-C(5)	1.383(6)
C(4)-H(4)	0.9500
C(5)-C(6)	1.386(7)
C(5)-H(5)	0.9500
C(6)-C(7)	1.389(6)
C(6)-H(6)	0.9500
C(7)-C(8)	1.398(6)
C(7)-H(7)	0.9500
C(8)-N(1)	1.351(5)
C(8)-C(9)	1.494(5)
C(9)-N(2)	1.481(5)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-N(2)	1.491(5)
C(10)-C(11)	1.505(5)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.418(5)
C(11)-C(15)	1.444(5)
C(11)-Fe(1)	2.049(4)
C(12)-C(13)	1.427(6)
C(12)-Fe(1)	2.053(4)
C(12)-H(12)	1.0000
C(13)-C(14)	1.426(6)
C(13)-Fe(1)	2.057(4)
C(13)-H(13)	1.0000
C(14)-C(15)	1.444(5)
C(14)-Fe(1)	2.035(4)
C(14)-H(14)	1.0000
C(15)-P(1)	1.795(4)
C(15)-Fe(1)	2.033(4)
C(16)-C(20)	1.416(7)
C(16)-C(17)	1.432(9)
C(16)-Fe(1)	2.039(5)
C(16)-H(16)	1.0000
C(17)-C(18)	1.426(10)
C(17)-Fe(1)	2.038(5)
C(17)-H(17)	1.0000
C(18)-C(19)	1.415(8)
C(18)-Fe(1)	2.051(4)
C(18)-H(18)	1.0000
C(19)-C(20)	1.406(7)
C(19)-Fe(1)	2.050(4)
C(19)-H(19)	1.0000
C(20)-Fe(1)	2.057(4)
C(20)-H(20)	1.0000
C(21)-C(22)	1.395(6)
C(21)-C(26)	1.401(6)
C(21)-P(1)	1.833(4)
C(22)-C(23)	1.393(6)
C(22)-H(22)	0.9500

C(23)-C(24)	1.389(6)
C(23)-H(23)	0.9500
C(24)-C(25)	1.389(7)
C(24)-H(24)	0.9500
C(25)-C(26)	1.389(6)
C(25)-H(25)	0.9500
C(26)-H(26)	0.9500
C(27)-C(28)	1.393(6)
C(27)-C(32)	1.408(6)
C(27)-P(1)	1.835(4)
C(28)-C(29)	1.393(6)
C(28)-H(28)	0.9500
C(29)-C(30)	1.381(7)
C(29)-H(29)	0.9500
C(30)-C(31)	1.387(7)
C(30)-H(30)	0.9500
C(31)-C(32)	1.387(6)
C(31)-H(31)	0.9500
C(32)-H(32)	0.9500
C(33)-O(4)	1.144(6)
C(33)-Mn(2)	1.839(5)
C(34)-O(5)	1.141(5)
C(34)-Mn(2)	1.811(4)
C(35)-O(6)	1.139(5)
C(35)-Mn(2)	1.809(4)
C(36)-N(3)	1.353(5)
C(36)-C(37)	1.384(6)
C(36)-H(36)	0.9500
C(37)-C(38)	1.392(6)
C(37)-H(37)	0.9500
C(38)-C(39)	1.388(6)
C(38)-H(38)	0.9500
C(39)-C(40)	1.391(6)
C(39)-H(39)	0.9500
C(40)-N(3)	1.348(5)
C(40)-C(41)	1.495(5)
C(41)-N(4)	1.475(5)
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
C(42)-N(4)	1.495(5)
C(42)-C(43)	1.506(5)
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(43)-C(47)	1.417(5)
C(43)-C(44)	1.452(5)
C(43)-Fe(2)	2.046(4)
C(44)-C(45)	1.433(5)
C(44)-P(2)	1.792(4)
C(44)-Fe(2)	2.050(4)
C(45)-C(46)	1.421(6)
C(45)-Fe(2)	2.061(4)
C(45)-H(45)	1.0000
C(46)-C(47)	1.424(6)
C(46)-Fe(2)	2.056(4)
C(46)-H(46)	1.0000
C(47)-Fe(2)	2.048(4)
C(47)-H(47)	1.0000
C(48)-C(49)	1.410(8)
C(48)-C(52)	1.435(8)
C(48)-Fe(2)	2.053(4)
C(48)-H(48)	1.0000

C(49)-C(50)	1.420(7)
C(49)-Fe(2)	2.057(4)
C(49)-H(49)	1.0000
C(50)-C(51)	1.425(6)
C(50)-Fe(2)	2.054(4)
C(50)-H(50)	1.0000
C(51)-C(52)	1.418(7)
C(51)-Fe(2)	2.053(4)
C(51)-H(51)	1.0000
C(52)-Fe(2)	2.049(4)
C(52)-H(52)	1.0000
C(53)-C(54)	1.387(6)
C(53)-C(58)	1.406(6)
C(53)-P(2)	1.828(4)
C(54)-C(55)	1.390(6)
C(54)-H(54)	0.9500
C(55)-C(56)	1.380(7)
C(55)-H(55)	0.9500
C(56)-C(57)	1.380(7)
C(56)-H(56)	0.9500
C(57)-C(58)	1.393(6)
C(57)-H(57)	0.9500
C(58)-H(58)	0.9500
C(59)-C(60)	1.403(6)
C(59)-C(64)	1.404(6)
C(59)-P(2)	1.820(4)
C(60)-C(61)	1.383(6)
C(60)-H(60)	0.9500
C(61)-C(62)	1.372(7)
C(61)-H(61)	0.9500
C(62)-C(63)	1.397(7)
C(62)-H(62)	0.9500
C(63)-C(64)	1.399(6)
C(63)-H(63)	0.9500
C(64)-H(64)	0.9500
C(65)-Cl(1)	1.773(7)
C(65)-Cl(2)	1.776(6)
C(65)-H(65A)	0.9900
C(65)-H(65B)	0.9900
C(66)-Cl(3)	1.746(6)
C(66)-Cl(4)	1.747(6)
C(66)-H(66A)	0.9900
C(66)-H(66B)	0.9900
N(1)-Mn(1)	2.068(3)
N(2)-Mn(1)	2.099(3)
N(2)-H(2)	0.86(5)
N(3)-Mn(2)	2.071(3)
N(4)-Mn(2)	2.093(3)
N(4)-H(4A)	0.92(5)
Mn(1)-P(1)	2.3224(11)
Mn(2)-P(2)	2.3170(11)

O(1)-C(1)-Mn(1)	175.5(4)
O(2)-C(2)-Mn(1)	170.8(4)
O(3)-C(3)-Mn(1)	179.8(5)
N(1)-C(4)-C(5)	122.2(4)
N(1)-C(4)-H(4)	118.9
C(5)-C(4)-H(4)	118.9
C(4)-C(5)-C(6)	119.5(4)
C(4)-C(5)-H(5)	120.3
C(6)-C(5)-H(5)	120.3

C(5)-C(6)-C(7)	118.7(4)
C(5)-C(6)-H(6)	120.7
C(7)-C(6)-H(6)	120.7
C(6)-C(7)-C(8)	119.3(4)
C(6)-C(7)-H(7)	120.3
C(8)-C(7)-H(7)	120.3
N(1)-C(8)-C(7)	121.6(4)
N(1)-C(8)-C(9)	116.3(3)
C(7)-C(8)-C(9)	122.1(4)
N(2)-C(9)-C(8)	109.8(3)
N(2)-C(9)-H(9A)	109.7
C(8)-C(9)-H(9A)	109.7
N(2)-C(9)-H(9B)	109.7
C(8)-C(9)-H(9B)	109.7
H(9A)-C(9)-H(9B)	108.2
N(2)-C(10)-C(11)	114.6(3)
N(2)-C(10)-H(10A)	108.6
C(11)-C(10)-H(10A)	108.6
N(2)-C(10)-H(10B)	108.6
C(11)-C(10)-H(10B)	108.6
H(10A)-C(10)-H(10B)	107.6
C(12)-C(11)-C(15)	107.5(3)
C(12)-C(11)-C(10)	124.7(4)
C(15)-C(11)-C(10)	127.8(3)
C(12)-C(11)-Fe(1)	69.9(2)
C(15)-C(11)-Fe(1)	68.7(2)
C(10)-C(11)-Fe(1)	124.7(3)
C(11)-C(12)-C(13)	109.2(3)
C(11)-C(12)-Fe(1)	69.6(2)
C(13)-C(12)-Fe(1)	69.8(2)
C(11)-C(12)-H(12)	125.4
C(13)-C(12)-H(12)	125.4
Fe(1)-C(12)-H(12)	125.4
C(14)-C(13)-C(12)	107.8(3)
C(14)-C(13)-Fe(1)	68.8(2)
C(12)-C(13)-Fe(1)	69.5(2)
C(14)-C(13)-H(13)	126.1
C(12)-C(13)-H(13)	126.1
Fe(1)-C(13)-H(13)	126.1
C(13)-C(14)-C(15)	108.0(3)
C(13)-C(14)-Fe(1)	70.4(2)
C(15)-C(14)-Fe(1)	69.1(2)
C(13)-C(14)-H(14)	126.0
C(15)-C(14)-H(14)	126.0
Fe(1)-C(14)-H(14)	126.0
C(14)-C(15)-C(11)	107.5(3)
C(14)-C(15)-P(1)	126.5(3)
C(11)-C(15)-P(1)	124.9(3)
C(14)-C(15)-Fe(1)	69.3(2)
C(11)-C(15)-Fe(1)	69.9(2)
P(1)-C(15)-Fe(1)	135.6(2)
C(20)-C(16)-C(17)	108.0(5)
C(20)-C(16)-Fe(1)	70.4(3)
C(17)-C(16)-Fe(1)	69.4(3)
C(20)-C(16)-H(16)	126.0
C(17)-C(16)-H(16)	126.0
Fe(1)-C(16)-H(16)	126.0
C(18)-C(17)-C(16)	107.6(4)
C(18)-C(17)-Fe(1)	70.1(3)
C(16)-C(17)-Fe(1)	69.5(3)
C(18)-C(17)-H(17)	126.2

C(16)-C(17)-H(17)	126.2
Fe(1)-C(17)-H(17)	126.2
C(19)-C(18)-C(17)	107.4(5)
C(19)-C(18)-Fe(1)	69.8(3)
C(17)-C(18)-Fe(1)	69.1(3)
C(19)-C(18)-H(18)	126.3
C(17)-C(18)-H(18)	126.3
Fe(1)-C(18)-H(18)	126.3
C(20)-C(19)-C(18)	109.2(5)
C(20)-C(19)-Fe(1)	70.2(3)
C(18)-C(19)-Fe(1)	69.9(3)
C(20)-C(19)-H(19)	125.4
C(18)-C(19)-H(19)	125.4
Fe(1)-C(19)-H(19)	125.4
C(19)-C(20)-C(16)	107.9(4)
C(19)-C(20)-Fe(1)	69.7(3)
C(16)-C(20)-Fe(1)	69.1(3)
C(19)-C(20)-H(20)	126.1
C(16)-C(20)-H(20)	126.1
Fe(1)-C(20)-H(20)	126.1
C(22)-C(21)-C(26)	119.1(4)
C(22)-C(21)-P(1)	122.2(3)
C(26)-C(21)-P(1)	118.5(3)
C(23)-C(22)-C(21)	120.3(4)
C(23)-C(22)-H(22)	119.9
C(21)-C(22)-H(22)	119.9
C(24)-C(23)-C(22)	120.2(4)
C(24)-C(23)-H(23)	119.9
C(22)-C(23)-H(23)	119.9
C(25)-C(24)-C(23)	119.8(4)
C(25)-C(24)-H(24)	120.1
C(23)-C(24)-H(24)	120.1
C(24)-C(25)-C(26)	120.3(4)
C(24)-C(25)-H(25)	119.8
C(26)-C(25)-H(25)	119.8
C(25)-C(26)-C(21)	120.3(4)
C(25)-C(26)-H(26)	119.9
C(21)-C(26)-H(26)	119.9
C(28)-C(27)-C(32)	118.6(4)
C(28)-C(27)-P(1)	120.8(3)
C(32)-C(27)-P(1)	120.6(3)
C(29)-C(28)-C(27)	121.1(4)
C(29)-C(28)-H(28)	119.5
C(27)-C(28)-H(28)	119.5
C(30)-C(29)-C(28)	119.6(4)
C(30)-C(29)-H(29)	120.2
C(28)-C(29)-H(29)	120.2
C(29)-C(30)-C(31)	120.3(4)
C(29)-C(30)-H(30)	119.8
C(31)-C(30)-H(30)	119.8
C(30)-C(31)-C(32)	120.4(4)
C(30)-C(31)-H(31)	119.8
C(32)-C(31)-H(31)	119.8
C(31)-C(32)-C(27)	120.0(4)
C(31)-C(32)-H(32)	120.0
C(27)-C(32)-H(32)	120.0
O(4)-C(33)-Mn(2)	170.8(4)
O(5)-C(34)-Mn(2)	179.9(5)
O(6)-C(35)-Mn(2)	175.2(4)
N(3)-C(36)-C(37)	122.6(4)
N(3)-C(36)-H(36)	118.7

C(37)-C(36)-H(36)	118.7
C(36)-C(37)-C(38)	118.8(4)
C(36)-C(37)-H(37)	120.6
C(38)-C(37)-H(37)	120.6
C(39)-C(38)-C(37)	119.0(4)
C(39)-C(38)-H(38)	120.5
C(37)-C(38)-H(38)	120.5
C(38)-C(39)-C(40)	119.2(4)
C(38)-C(39)-H(39)	120.4
C(40)-C(39)-H(39)	120.4
N(3)-C(40)-C(39)	122.1(4)
N(3)-C(40)-C(41)	116.1(4)
C(39)-C(40)-C(41)	121.8(4)
N(4)-C(41)-C(40)	111.5(3)
N(4)-C(41)-H(41A)	109.3
C(40)-C(41)-H(41A)	109.3
N(4)-C(41)-H(41B)	109.3
C(40)-C(41)-H(41B)	109.3
H(41A)-C(41)-H(41B)	108.0
N(4)-C(42)-C(43)	114.4(3)
N(4)-C(42)-H(42A)	108.7
C(43)-C(42)-H(42A)	108.7
N(4)-C(42)-H(42B)	108.7
C(43)-C(42)-H(42B)	108.7
H(42A)-C(42)-H(42B)	107.6
C(47)-C(43)-C(44)	107.3(3)
C(47)-C(43)-C(42)	125.1(3)
C(44)-C(43)-C(42)	127.5(3)
C(47)-C(43)-Fe(2)	69.8(2)
C(44)-C(43)-Fe(2)	69.4(2)
C(42)-C(43)-Fe(2)	122.9(3)
C(45)-C(44)-C(43)	107.5(3)
C(45)-C(44)-P(2)	127.2(3)
C(43)-C(44)-P(2)	124.7(3)
C(45)-C(44)-Fe(2)	70.0(2)
C(43)-C(44)-Fe(2)	69.1(2)
P(2)-C(44)-Fe(2)	133.0(2)
C(46)-C(45)-C(44)	108.2(3)
C(46)-C(45)-Fe(2)	69.6(2)
C(44)-C(45)-Fe(2)	69.2(2)
C(46)-C(45)-H(45)	125.9
C(44)-C(45)-H(45)	125.9
Fe(2)-C(45)-H(45)	125.9
C(45)-C(46)-C(47)	108.1(3)
C(45)-C(46)-Fe(2)	70.0(2)
C(47)-C(46)-Fe(2)	69.4(2)
C(45)-C(46)-H(46)	126.0
C(47)-C(46)-H(46)	126.0
Fe(2)-C(46)-H(46)	126.0
C(43)-C(47)-C(46)	109.0(3)
C(43)-C(47)-Fe(2)	69.7(2)
C(46)-C(47)-Fe(2)	70.0(2)
C(43)-C(47)-H(47)	125.5
C(46)-C(47)-H(47)	125.5
Fe(2)-C(47)-H(47)	125.5
C(49)-C(48)-C(52)	107.8(4)
C(49)-C(48)-Fe(2)	70.1(3)
C(52)-C(48)-Fe(2)	69.4(3)
C(49)-C(48)-H(48)	126.1
C(52)-C(48)-H(48)	126.1
Fe(2)-C(48)-H(48)	126.1

C(48)-C(49)-C(50)	108.6(4)
C(48)-C(49)-Fe(2)	69.8(3)
C(50)-C(49)-Fe(2)	69.7(2)
C(48)-C(49)-H(49)	125.7
C(50)-C(49)-H(49)	125.7
Fe(2)-C(49)-H(49)	125.7
C(49)-C(50)-C(51)	107.7(4)
C(49)-C(50)-Fe(2)	69.9(3)
C(51)-C(50)-Fe(2)	69.7(2)
C(49)-C(50)-H(50)	126.2
C(51)-C(50)-H(50)	126.2
Fe(2)-C(50)-H(50)	126.2
C(52)-C(51)-C(50)	108.2(4)
C(52)-C(51)-Fe(2)	69.6(2)
C(50)-C(51)-Fe(2)	69.7(2)
C(52)-C(51)-H(51)	125.9
C(50)-C(51)-H(51)	125.9
Fe(2)-C(51)-H(51)	125.9
C(51)-C(52)-C(48)	107.7(4)
C(51)-C(52)-Fe(2)	70.0(3)
C(48)-C(52)-Fe(2)	69.7(2)
C(51)-C(52)-H(52)	126.2
C(48)-C(52)-H(52)	126.2
Fe(2)-C(52)-H(52)	126.2
C(54)-C(53)-C(58)	119.7(4)
C(54)-C(53)-P(2)	121.2(3)
C(58)-C(53)-P(2)	118.5(3)
C(53)-C(54)-C(55)	120.3(4)
C(53)-C(54)-H(54)	119.9
C(55)-C(54)-H(54)	119.9
C(56)-C(55)-C(54)	120.1(4)
C(56)-C(55)-H(55)	120.0
C(54)-C(55)-H(55)	120.0
C(55)-C(56)-C(57)	120.2(4)
C(55)-C(56)-H(56)	119.9
C(57)-C(56)-H(56)	119.9
C(56)-C(57)-C(58)	120.6(4)
C(56)-C(57)-H(57)	119.7
C(58)-C(57)-H(57)	119.7
C(57)-C(58)-C(53)	119.1(4)
C(57)-C(58)-H(58)	120.4
C(53)-C(58)-H(58)	120.4
C(60)-C(59)-C(64)	118.8(4)
C(60)-C(59)-P(2)	119.4(3)
C(64)-C(59)-P(2)	121.8(3)
C(61)-C(60)-C(59)	120.5(4)
C(61)-C(60)-H(60)	119.8
C(59)-C(60)-H(60)	119.8
C(62)-C(61)-C(60)	120.7(4)
C(62)-C(61)-H(61)	119.7
C(60)-C(61)-H(61)	119.7
C(61)-C(62)-C(63)	120.1(4)
C(61)-C(62)-H(62)	119.9
C(63)-C(62)-H(62)	119.9
C(62)-C(63)-C(64)	119.8(4)
C(62)-C(63)-H(63)	120.1
C(64)-C(63)-H(63)	120.1
C(63)-C(64)-C(59)	120.0(4)
C(63)-C(64)-H(64)	120.0
C(59)-C(64)-H(64)	120.0
Cl(1)-C(65)-Cl(2)	112.0(3)

Cl(1)-C(65)-H(65A)	109.2
Cl(2)-C(65)-H(65A)	109.2
Cl(1)-C(65)-H(65B)	109.2
Cl(2)-C(65)-H(65B)	109.2
H(65A)-C(65)-H(65B)	107.9
Cl(3)-C(66)-Cl(4)	111.8(3)
Cl(3)-C(66)-H(66A)	109.3
Cl(4)-C(66)-H(66A)	109.3
Cl(3)-C(66)-H(66B)	109.3
Cl(4)-C(66)-H(66B)	109.3
H(66A)-C(66)-H(66B)	107.9
C(8)-N(1)-C(4)	118.7(4)
C(8)-N(1)-Mn(1)	115.4(3)
C(4)-N(1)-Mn(1)	124.7(3)
C(9)-N(2)-C(10)	110.6(3)
C(9)-N(2)-Mn(1)	111.0(2)
C(10)-N(2)-Mn(1)	121.7(2)
C(9)-N(2)-H(2)	108(3)
C(10)-N(2)-H(2)	104(3)
Mn(1)-N(2)-H(2)	100(3)
C(40)-N(3)-C(36)	118.3(4)
C(40)-N(3)-Mn(2)	116.4(3)
C(36)-N(3)-Mn(2)	124.9(3)
C(41)-N(4)-C(42)	110.5(3)
C(41)-N(4)-Mn(2)	112.5(2)
C(42)-N(4)-Mn(2)	120.8(2)
C(41)-N(4)-H(4A)	106(3)
C(42)-N(4)-H(4A)	104(3)
Mn(2)-N(4)-H(4A)	101(3)
C(1)-Mn(1)-C(3)	92.92(19)
C(1)-Mn(1)-C(2)	87.16(19)
C(3)-Mn(1)-C(2)	86.83(19)
C(1)-Mn(1)-N(1)	169.42(17)
C(3)-Mn(1)-N(1)	94.80(16)
C(2)-Mn(1)-N(1)	86.07(17)
C(1)-Mn(1)-N(2)	92.59(16)
C(3)-Mn(1)-N(2)	174.20(16)
C(2)-Mn(1)-N(2)	95.27(16)
N(1)-Mn(1)-N(2)	79.97(13)
C(1)-Mn(1)-P(1)	92.34(13)
C(3)-Mn(1)-P(1)	89.09(13)
C(2)-Mn(1)-P(1)	175.85(14)
N(1)-Mn(1)-P(1)	95.00(10)
N(2)-Mn(1)-P(1)	88.86(10)
C(35)-Mn(2)-C(34)	92.27(18)
C(35)-Mn(2)-C(33)	86.37(19)
C(34)-Mn(2)-C(33)	87.73(19)
C(35)-Mn(2)-N(3)	170.36(16)
C(34)-Mn(2)-N(3)	95.18(16)
C(33)-Mn(2)-N(3)	87.83(17)
C(35)-Mn(2)-N(4)	92.99(16)
C(34)-Mn(2)-N(4)	174.27(16)
C(33)-Mn(2)-N(4)	94.88(16)
N(3)-Mn(2)-N(4)	79.84(13)
C(35)-Mn(2)-P(2)	93.36(13)
C(34)-Mn(2)-P(2)	86.76(14)
C(33)-Mn(2)-P(2)	174.47(14)
N(3)-Mn(2)-P(2)	93.15(10)
N(4)-Mn(2)-P(2)	90.65(9)
C(15)-Fe(1)-C(14)	41.59(15)
C(15)-Fe(1)-C(17)	165.1(2)

C(14)-Fe(1)-C(17)	150.3(2)
C(15)-Fe(1)-C(16)	128.64(19)
C(14)-Fe(1)-C(16)	167.8(2)
C(17)-Fe(1)-C(16)	41.1(3)
C(15)-Fe(1)-C(11)	41.43(15)
C(14)-Fe(1)-C(11)	69.57(16)
C(17)-Fe(1)-C(11)	125.2(2)
C(16)-Fe(1)-C(11)	107.63(19)
C(15)-Fe(1)-C(19)	121.59(19)
C(14)-Fe(1)-C(19)	109.52(19)
C(17)-Fe(1)-C(19)	68.1(2)
C(16)-Fe(1)-C(19)	67.8(2)
C(11)-Fe(1)-C(19)	155.75(18)
C(15)-Fe(1)-C(18)	153.8(2)
C(14)-Fe(1)-C(18)	117.7(2)
C(17)-Fe(1)-C(18)	40.8(3)
C(16)-Fe(1)-C(18)	68.6(2)
C(11)-Fe(1)-C(18)	162.4(2)
C(19)-Fe(1)-C(18)	40.4(2)
C(15)-Fe(1)-C(12)	68.79(15)
C(14)-Fe(1)-C(12)	68.66(16)
C(17)-Fe(1)-C(12)	104.83(19)
C(16)-Fe(1)-C(12)	117.45(18)
C(11)-Fe(1)-C(12)	40.46(15)
C(19)-Fe(1)-C(12)	163.39(19)
C(18)-Fe(1)-C(12)	124.68(19)
C(15)-Fe(1)-C(20)	110.77(17)
C(14)-Fe(1)-C(20)	129.99(18)
C(17)-Fe(1)-C(20)	68.5(2)
C(16)-Fe(1)-C(20)	40.5(2)
C(11)-Fe(1)-C(20)	121.00(17)
C(19)-Fe(1)-C(20)	40.06(19)
C(18)-Fe(1)-C(20)	68.07(19)
C(12)-Fe(1)-C(20)	153.16(18)
C(15)-Fe(1)-C(13)	69.19(16)
C(14)-Fe(1)-C(13)	40.79(16)
C(17)-Fe(1)-C(13)	115.4(2)
C(16)-Fe(1)-C(13)	150.4(2)
C(11)-Fe(1)-C(13)	68.81(16)
C(19)-Fe(1)-C(13)	127.27(18)
C(18)-Fe(1)-C(13)	105.49(19)
C(12)-Fe(1)-C(13)	40.65(16)
C(20)-Fe(1)-C(13)	166.07(18)
C(43)-Fe(2)-C(47)	40.50(15)
C(43)-Fe(2)-C(52)	131.29(19)
C(47)-Fe(2)-C(52)	105.79(18)
C(43)-Fe(2)-C(44)	41.53(15)
C(47)-Fe(2)-C(44)	68.64(15)
C(52)-Fe(2)-C(44)	172.82(18)
C(43)-Fe(2)-C(48)	107.69(17)
C(47)-Fe(2)-C(48)	110.53(18)
C(52)-Fe(2)-C(48)	41.0(2)
C(44)-Fe(2)-C(48)	135.58(19)
C(43)-Fe(2)-C(51)	170.91(17)
C(47)-Fe(2)-C(51)	132.17(17)
C(52)-Fe(2)-C(51)	40.4(2)
C(44)-Fe(2)-C(51)	146.72(17)
C(48)-Fe(2)-C(51)	68.2(2)
C(43)-Fe(2)-C(50)	146.63(17)
C(47)-Fe(2)-C(50)	172.76(18)
C(52)-Fe(2)-C(50)	68.28(19)

C(44)-Fe(2)-C(50)	117.60(17)
C(48)-Fe(2)-C(50)	68.06(19)
C(51)-Fe(2)-C(50)	40.59(18)
C(43)-Fe(2)-C(46)	68.65(16)
C(47)-Fe(2)-C(46)	40.62(16)
C(52)-Fe(2)-C(46)	110.52(19)
C(44)-Fe(2)-C(46)	68.53(16)
C(48)-Fe(2)-C(46)	140.6(2)
C(51)-Fe(2)-C(46)	108.95(18)
C(50)-Fe(2)-C(46)	136.33(18)
C(43)-Fe(2)-C(49)	114.61(17)
C(47)-Fe(2)-C(49)	142.43(18)
C(52)-Fe(2)-C(49)	68.1(2)
C(44)-Fe(2)-C(49)	113.23(18)
C(48)-Fe(2)-C(49)	40.1(2)
C(51)-Fe(2)-C(49)	67.96(19)
C(50)-Fe(2)-C(49)	40.43(18)
C(46)-Fe(2)-C(49)	176.65(18)
C(43)-Fe(2)-C(45)	69.00(15)
C(47)-Fe(2)-C(45)	68.17(16)
C(52)-Fe(2)-C(45)	142.46(19)
C(44)-Fe(2)-C(45)	40.80(14)
C(48)-Fe(2)-C(45)	176.31(19)
C(51)-Fe(2)-C(45)	115.28(18)
C(50)-Fe(2)-C(45)	113.68(18)
C(46)-Fe(2)-C(45)	40.37(16)
C(49)-Fe(2)-C(45)	139.20(19)
C(15)-P(1)-C(21)	101.47(18)
C(15)-P(1)-C(27)	105.38(18)
C(21)-P(1)-C(27)	103.69(18)
C(15)-P(1)-Mn(1)	112.76(13)
C(21)-P(1)-Mn(1)	113.24(13)
C(27)-P(1)-Mn(1)	118.51(13)
C(44)-P(2)-C(59)	104.86(18)
C(44)-P(2)-C(53)	104.11(18)
C(59)-P(2)-C(53)	103.14(18)
C(44)-P(2)-Mn(2)	113.11(12)
C(59)-P(2)-Mn(2)	120.40(14)
C(53)-P(2)-Mn(2)	109.64(13)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for **5a** (20240924-Vickie_Mn). The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	26(2)	29(2)	24(2)	-4(2)	2(2)	3(2)
C(2)	27(2)	32(2)	33(2)	-2(2)	1(2)	2(2)
C(3)	28(2)	28(2)	26(2)	-5(2)	4(2)	-2(2)
C(4)	31(2)	24(2)	33(2)	-2(2)	3(2)	2(2)
C(5)	34(2)	24(2)	39(2)	-4(2)	6(2)	-4(2)
C(6)	33(2)	25(2)	37(2)	-7(2)	7(2)	-7(2)
C(7)	29(2)	27(2)	32(2)	-5(2)	3(2)	-1(2)
C(8)	27(2)	23(2)	22(2)	-3(1)	3(1)	0(1)
C(9)	25(2)	23(2)	27(2)	-1(1)	2(2)	2(1)
C(10)	28(2)	25(2)	23(2)	0(2)	1(1)	-1(1)
C(11)	24(2)	18(2)	25(2)	1(1)	2(1)	-2(1)
C(12)	24(2)	22(2)	26(2)	0(2)	2(1)	1(1)
C(13)	30(2)	24(2)	25(2)	-4(2)	2(2)	3(2)
C(14)	30(2)	24(2)	21(2)	0(1)	0(1)	0(2)
C(15)	24(2)	21(2)	22(2)	2(1)	2(1)	-1(1)
C(16)	32(2)	50(3)	37(2)	14(2)	4(2)	-11(2)
C(17)	34(2)	27(2)	95(5)	25(3)	12(3)	-5(2)
C(18)	32(2)	36(2)	71(4)	-24(2)	12(2)	-16(2)
C(19)	23(2)	48(3)	40(2)	-6(2)	-1(2)	-6(2)
C(20)	24(2)	34(2)	36(2)	-4(2)	6(2)	-3(2)
C(21)	28(2)	26(2)	20(2)	1(2)	0(1)	-2(2)
C(22)	28(2)	28(2)	25(2)	2(2)	0(2)	1(2)
C(23)	26(2)	36(2)	27(2)	4(2)	2(2)	0(2)
C(24)	28(2)	38(2)	23(2)	7(2)	-2(2)	-7(2)
C(25)	40(2)	26(2)	27(2)	3(2)	1(2)	-6(2)
C(26)	33(2)	26(2)	28(2)	-1(2)	3(2)	2(2)
C(27)	28(2)	22(2)	24(2)	2(1)	-1(2)	-2(1)
C(28)	27(2)	27(2)	26(2)	0(2)	-1(2)	0(2)
C(29)	27(2)	32(2)	37(2)	4(2)	0(2)	3(2)
C(30)	29(2)	37(2)	35(2)	4(2)	-8(2)	0(2)
C(31)	41(2)	37(2)	25(2)	0(2)	-7(2)	2(2)
C(32)	33(2)	27(2)	24(2)	-1(2)	1(2)	2(2)
C(33)	29(2)	26(2)	35(2)	1(2)	1(2)	-1(2)
C(34)	28(2)	24(2)	29(2)	-3(2)	3(2)	-1(2)
C(35)	27(2)	29(2)	22(2)	-3(2)	2(2)	6(2)
C(36)	31(2)	21(2)	34(2)	1(2)	2(2)	2(2)
C(37)	34(2)	26(2)	42(2)	0(2)	3(2)	-2(2)
C(38)	30(2)	26(2)	45(3)	1(2)	4(2)	-4(2)
C(39)	28(2)	29(2)	31(2)	-4(2)	2(2)	0(2)
C(40)	27(2)	24(2)	23(2)	-1(1)	1(1)	1(1)
C(41)	26(2)	24(2)	22(2)	-1(1)	-1(1)	2(1)
C(42)	28(2)	20(2)	22(2)	0(1)	-2(1)	0(1)
C(43)	22(2)	21(2)	21(2)	1(1)	1(1)	-2(1)
C(44)	23(2)	21(2)	20(2)	0(1)	1(1)	-3(1)
C(45)	29(2)	21(2)	22(2)	0(1)	5(2)	-4(2)
C(46)	30(2)	24(2)	23(2)	-3(2)	3(2)	-2(2)
C(47)	23(2)	24(2)	27(2)	0(1)	1(1)	0(1)
C(48)	36(2)	53(3)	32(2)	18(2)	-2(2)	-22(2)
C(49)	28(2)	43(2)	34(2)	-7(2)	9(2)	-13(2)
C(50)	25(2)	32(2)	35(2)	-1(2)	1(2)	-4(2)
C(51)	30(2)	31(2)	37(2)	-5(2)	-4(2)	-6(2)
C(52)	31(2)	26(2)	56(3)	8(2)	1(2)	-10(2)
C(53)	28(2)	20(2)	22(2)	2(1)	1(1)	0(1)

C(54)	30(2)	25(2)	24(2)	1(1)	1(2)	-1(2)
C(55)	28(2)	35(2)	28(2)	4(2)	2(2)	-2(2)
C(56)	38(2)	35(2)	37(2)	10(2)	1(2)	-10(2)
C(57)	45(3)	26(2)	42(3)	14(2)	1(2)	-1(2)
C(58)	32(2)	27(2)	37(2)	9(2)	1(2)	2(2)
C(59)	26(2)	22(2)	27(2)	4(1)	-2(2)	0(1)
C(60)	31(2)	31(2)	29(2)	4(2)	-1(2)	1(2)
C(61)	41(2)	33(2)	31(2)	7(2)	-9(2)	-2(2)
C(62)	28(2)	36(2)	42(2)	10(2)	-11(2)	-4(2)
C(63)	26(2)	30(2)	46(3)	10(2)	-1(2)	-1(2)
C(64)	27(2)	27(2)	29(2)	5(2)	-2(2)	2(2)
C(65)	44(3)	67(4)	30(2)	-3(2)	-5(2)	-7(3)
C(66)	48(3)	48(3)	38(3)	-5(2)	-3(2)	8(2)
N(1)	25(2)	23(2)	26(2)	-4(1)	3(1)	-2(1)
N(2)	26(2)	23(2)	20(2)	1(1)	0(1)	-1(1)
N(3)	25(2)	24(2)	24(2)	-1(1)	3(1)	-1(1)
N(4)	26(2)	20(1)	22(2)	-2(1)	1(1)	1(1)
O(1)	33(2)	34(2)	30(2)	0(1)	8(1)	-4(1)
O(2)	50(2)	46(2)	28(2)	-12(1)	-5(1)	8(2)
O(3)	35(2)	28(2)	39(2)	-1(1)	2(1)	8(1)
O(4)	50(2)	42(2)	26(2)	-13(1)	0(1)	7(2)
O(5)	35(2)	27(2)	42(2)	3(1)	6(1)	7(1)
O(6)	32(2)	31(2)	32(2)	-1(1)	9(1)	-6(1)
Mn(1)	22(1)	21(1)	20(1)	-2(1)	2(1)	1(1)
Mn(2)	23(1)	20(1)	20(1)	-1(1)	3(1)	1(1)
Fe(1)	23(1)	20(1)	26(1)	0(1)	1(1)	-2(1)
Fe(2)	24(1)	21(1)	21(1)	1(1)	0(1)	-3(1)
P(1)	23(1)	19(1)	19(1)	0(1)	2(1)	1(1)
P(2)	23(1)	19(1)	20(1)	2(1)	1(1)	1(1)
Cl(1)	54(1)	55(1)	51(1)	-10(1)	-1(1)	-13(1)
Cl(2)	48(1)	63(1)	44(1)	-3(1)	10(1)	0(1)
Cl(3)	47(1)	46(1)	76(1)	6(1)	7(1)	8(1)
Cl(4)	59(1)	43(1)	141(2)	-13(1)	-14(1)	4(1)
Br(1)	39(1)	39(1)	24(1)	1(1)	-2(1)	-4(1)
Br(2)	32(1)	35(1)	23(1)	-1(1)	-2(1)	-1(1)

Crystal Data, Data Collection and Structure Refinement for 5b

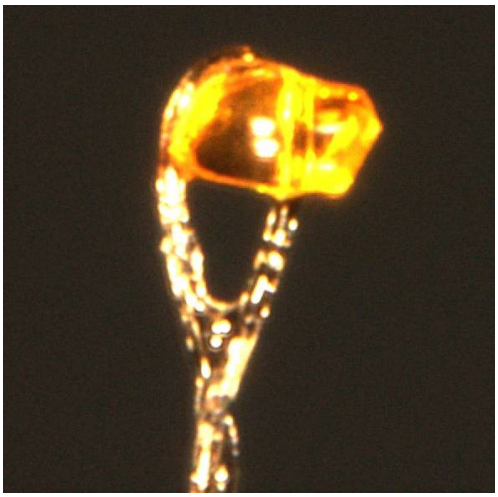

Figure S38 : Sample

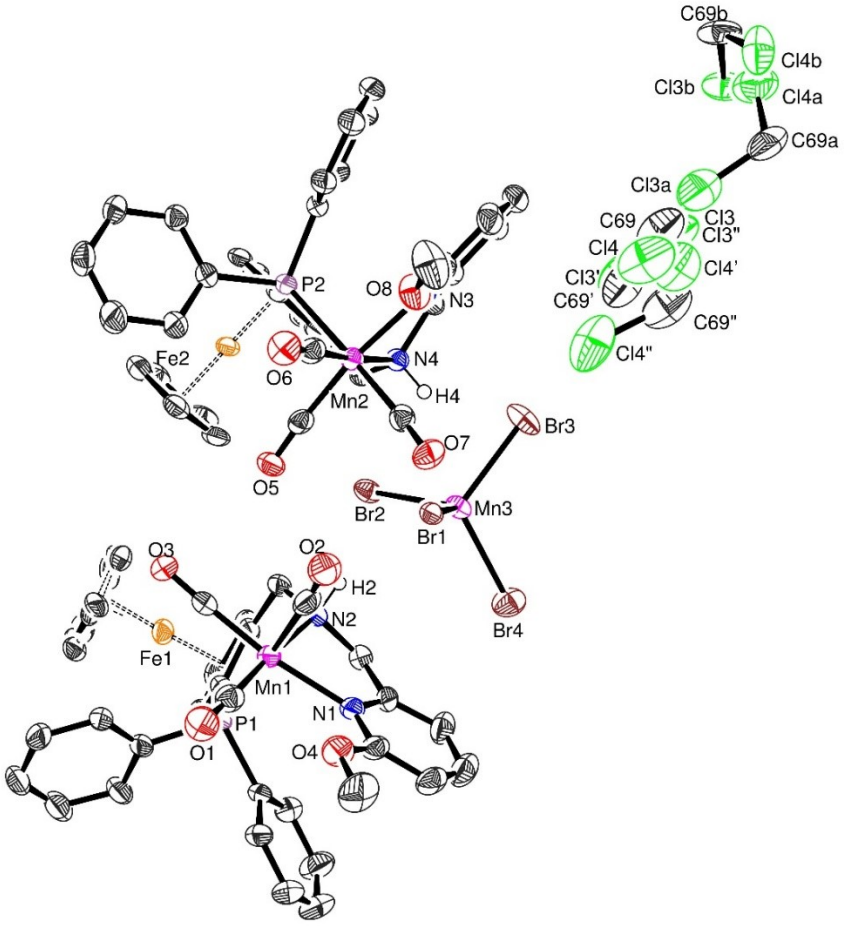

Figure S39 : Asymmetric Unit

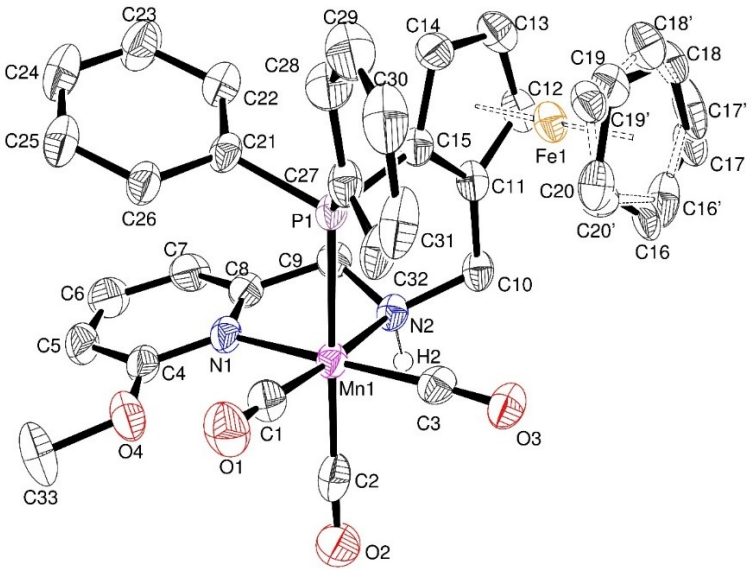

Figure S40 : Compound.

Table S5. Crystal data and structure refinement for **5b** (20241015-Vickie).

Identification code	20241015-Vickie
Empirical formula	2(C33 H29 Fe Mn N2 O4 P), Br4 Mn, C H2 Cl2
Formula weight	1778.15
Temperature	100(2) K
Wavelength	1.54184 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 13.9449(2) A alpha = 83.0710(10) deg.
	b = 14.3934(2) A beta = 89.5920(10) deg.
	c = 22.72820(10) A gamma = 61.467(2) deg.
Volume	3971.86(11) A^3
Z, Calculated density	2, 1.487 Mg/m^3
Absorption coefficient	10.394 mm^-1
F(000)	1770
Crystal size	0.20 x 0.18 x 0.10 mm
Theta range for data collection	3.527 to 80.685 deg.
Limiting indices	-17<=h<=17, -18<=k<=16, -29<=l<=29
Reflections collected / unique	83136 / 16830 [R(int) = 0.0448]
Completeness to theta = 67.684	99.6 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	16830 / 453 / 994
Goodness-of-fit on F^2	1.048
Final R indices [I>2sigma(I)]	R1 = 0.0494, wR2 = 0.1374
R indices (all data)	R1 = 0.0512, wR2 = 0.1390
Largest diff. peak and hole	1.625 and -1.454 e.A^-3

Table S6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5b** (20241015-Vickie). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	3048(3)	8649(3)	5748(2)	38(1)
C(2)	2897(4)	6935(3)	6115(2)	41(1)
C(3)	2957(3)	8137(3)	6844(2)	32(1)
C(4)	4821(4)	6639(3)	5099(2)	37(1)
C(5)	5600(4)	5947(4)	4745(2)	47(1)
C(6)	6495(4)	5074(4)	5022(2)	52(1)
C(7)	6617(4)	4877(4)	5634(2)	44(1)
C(8)	5837(3)	5610(3)	5953(2)	33(1)
C(9)	5948(3)	5487(3)	6613(2)	33(1)
C(10)	4988(3)	6205(3)	7492(2)	31(1)
C(11)	5690(3)	6710(3)	7576(2)	30(1)
C(12)	6498(3)	6358(3)	8056(2)	37(1)
C(13)	7022(3)	6999(3)	7988(2)	40(1)
C(14)	6557(3)	7752(3)	7469(2)	35(1)
C(15)	5732(3)	7576(3)	7200(2)	30(1)
C(21)	6027(3)	7960(3)	5959(2)	31(1)
C(22)	7131(4)	7320(3)	6089(2)	41(1)
C(23)	7874(4)	7188(4)	5651(2)	55(1)
C(24)	7501(5)	7709(5)	5083(2)	60(1)
C(25)	6398(4)	8355(4)	4947(2)	47(1)
C(26)	5650(4)	8489(3)	5378(2)	37(1)
C(27)	4412(3)	9619(3)	6525(2)	33(1)
C(28)	5145(4)	10027(3)	6563(2)	43(1)
C(29)	4772(5)	11077(4)	6656(2)	51(1)
C(30)	3673(5)	11742(3)	6683(2)	53(1)
C(31)	2931(5)	11359(3)	6627(2)	50(1)
C(32)	3305(4)	10295(3)	6553(2)	38(1)
C(33)	3656(6)	7717(5)	4266(2)	69(2)
C(34)	2020(3)	5710(3)	7578(2)	30(1)
C(35)	231(3)	5756(3)	7299(2)	34(1)
C(36)	1938(3)	4558(3)	6849(2)	33(1)
C(37)	492(3)	3360(3)	7367(2)	36(1)
C(38)	323(3)	2473(3)	7445(2)	43(1)
C(39)	1019(4)	1609(3)	7845(2)	43(1)
C(40)	1877(3)	1620(3)	8140(2)	36(1)
C(41)	1996(3)	2528(3)	8031(2)	29(1)
C(42)	2904(3)	2583(3)	8339(2)	31(1)
C(43)	3672(3)	3743(3)	8485(2)	28(1)
C(44)	3113(3)	4102(3)	9047(2)	27(1)
C(45)	1964(3)	4741(3)	9122(2)	27(1)
C(46)	1837(3)	4895(3)	9741(2)	29(1)
C(47)	2891(3)	4345(3)	10037(2)	31(1)
C(48)	3675(3)	3854(3)	9613(2)	30(1)
C(49)	2327(4)	6905(3)	8834(2)	36(1)
C(50)	3465(4)	6209(3)	8811(2)	40(1)
C(51)	3959(4)	5968(4)	9395(2)	43(1)
C(52)	3123(4)	6509(4)	9780(2)	44(1)
C(53)	2112(4)	7086(3)	9436(2)	41(1)
C(54)	271(3)	4260(3)	8835(2)	27(1)
C(55)	717(3)	3443(3)	9311(2)	30(1)
C(56)	234(4)	2803(3)	9466(2)	36(1)
C(57)	-698(4)	2985(3)	9148(2)	39(1)

C(58)	-1151(3)	3796(3)	8675(2)	38(1)
C(59)	-669(3)	4436(3)	8519(2)	33(1)
C(60)	-168(3)	6419(3)	8667(2)	29(1)
C(61)	-876(3)	6554(3)	9126(2)	31(1)
C(62)	-1698(3)	7567(3)	9205(2)	34(1)
C(63)	-1823(4)	8449(3)	8833(2)	44(1)
C(64)	-1108(4)	8320(3)	8379(2)	54(1)
C(65)	-295(4)	7315(3)	8294(2)	40(1)
C(66)	-1036(5)	4291(4)	6669(3)	67(2)
N(1)	4949(3)	6496(3)	5696(1)	31(1)
N(2)	4868(3)	6093(2)	6857(1)	29(1)
N(3)	1295(3)	3408(2)	7662(1)	30(1)
N(4)	3036(2)	3497(2)	8060(1)	27(1)
O(1)	2508(3)	9411(3)	5431(1)	50(1)
O(2)	2293(3)	6696(3)	6029(2)	52(1)
O(3)	2349(2)	8549(2)	7197(1)	39(1)
O(4)	3887(3)	7495(3)	4893(1)	47(1)
O(5)	2337(2)	6321(2)	7510(1)	38(1)
O(6)	-588(3)	6432(2)	7086(1)	46(1)
O(7)	2051(3)	4555(3)	6352(1)	42(1)
O(8)	-125(2)	4244(2)	6988(1)	45(1)
Fe(1)	5369(1)	7947(1)	8041(1)	31(1)
C(16)	3866(11)	8385(16)	8397(8)	31(3)
C(17)	4691(13)	8022(14)	8860(5)	36(3)
C(18)	5194(11)	8687(18)	8782(8)	41(4)
C(19)	4696(16)	9448(11)	8271(11)	38(4)
C(20)	3879(11)	9267(13)	8037(8)	34(4)
C(16')	4034(14)	8340(13)	8541(9)	43(4)
C(17')	4941(17)	8238(11)	8887(4)	49(4)
C(18')	5239(11)	9009(12)	8614(7)	39(3)
C(19')	4541(13)	9558(8)	8098(7)	31(3)
C(20')	3813(10)	9146(12)	8045(8)	34(3)
Fe(2)	2810(1)	5476(1)	9371(1)	27(1)
Mn(1)	3846(1)	7477(1)	6280(1)	27(1)
Mn(2)	1557(1)	4734(1)	7624(1)	26(1)
Mn(3)	6340(1)	2639(1)	7677(1)	31(1)
P(1)	4979(1)	8187(1)	6497(1)	26(1)
P(2)	900(1)	5082(1)	8566(1)	25(1)
Br(1)	4641(1)	3841(1)	6989(1)	28(1)
Br(2)	6358(1)	3568(1)	8535(1)	35(1)
Br(3)	6137(1)	1055(1)	8046(1)	51(1)
Br(4)	7900(1)	2251(1)	7033(1)	50(1)
Cl(3)	410(20)	1620(30)	6032(14)	84(5)
C(69)	-430(50)	1260(40)	5760(30)	82(4)
Cl(4)	-1171(16)	2121(19)	5185(10)	94(5)
Cl(3')	615(8)	1422(10)	6064(6)	65(2)
C(69')	-308(18)	2093(19)	5538(9)	78(4)
Cl(4')	-877(8)	1717(8)	5074(4)	80(2)
Cl(3")	-255(12)	1076(13)	5720(7)	88(4)
C(69")	-160(50)	1780(20)	5117(14)	86(5)
Cl(4")	-416(9)	3033(12)	5120(7)	91(3)
Cl(3A)	-166(15)	314(14)	6021(8)	92(4)
C(69A)	-170(40)	-830(20)	6018(12)	74(7)
Cl(4A)	-97(18)	-1370(14)	6717(10)	88(5)
Cl(3B)	-18(3)	-1104(3)	6964(2)	55(1)
C(69B)	-1396(8)	-741(9)	6804(5)	54(3)
Cl(4B)	-1832(3)	-643(3)	6128(2)	66(1)

Table S7. Bond lengths [A] and angles [deg] for **5b** (20241015-Vickie).

C(1)-O(1)	1.149(5)
C(1)-Mn(1)	1.810(4)
C(2)-O(2)	1.077(6)
C(2)-Mn(1)	1.888(5)
C(3)-O(3)	1.156(5)
C(3)-Mn(1)	1.797(4)
C(4)-O(4)	1.331(6)
C(4)-N(1)	1.348(5)
C(4)-C(5)	1.402(6)
C(5)-C(6)	1.362(8)
C(5)-H(5)	0.9500
C(6)-C(7)	1.380(7)
C(6)-H(6)	0.9500
C(7)-C(8)	1.378(5)
C(7)-H(7)	0.9500
C(8)-N(1)	1.351(5)
C(8)-C(9)	1.489(5)
C(9)-N(2)	1.479(5)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-N(2)	1.490(5)
C(10)-C(11)	1.496(5)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.433(5)
C(11)-C(15)	1.450(5)
C(11)-Fe(1)	2.043(3)
C(12)-C(13)	1.420(6)
C(12)-Fe(1)	2.063(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.420(6)
C(13)-Fe(1)	2.054(4)
C(13)-H(13)	0.9500
C(14)-C(15)	1.445(5)
C(14)-Fe(1)	2.032(4)
C(14)-H(14)	0.9500
C(15)-P(1)	1.797(4)
C(15)-Fe(1)	2.043(4)
C(21)-C(22)	1.376(6)
C(21)-C(26)	1.409(5)
C(21)-P(1)	1.832(4)
C(22)-C(23)	1.395(6)
C(22)-H(22)	0.9500
C(23)-C(24)	1.378(7)
C(23)-H(23)	0.9500
C(24)-C(25)	1.377(8)
C(24)-H(24)	0.9500
C(25)-C(26)	1.386(6)
C(25)-H(25)	0.9500
C(26)-H(26)	0.9500
C(27)-C(32)	1.383(6)
C(27)-C(28)	1.409(6)
C(27)-P(1)	1.831(4)
C(28)-C(29)	1.387(6)
C(28)-H(28)	0.9500
C(29)-C(30)	1.371(8)
C(29)-H(29)	0.9500
C(30)-C(31)	1.399(8)

C(30)-H(30)	0.9500
C(31)-C(32)	1.394(6)
C(31)-H(31)	0.9500
C(32)-H(32)	0.9500
C(33)-O(4)	1.426(5)
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-O(5)	1.152(5)
C(34)-Mn(2)	1.799(4)
C(35)-O(6)	1.148(5)
C(35)-Mn(2)	1.813(4)
C(36)-O(7)	1.141(5)
C(36)-Mn(2)	1.848(4)
C(37)-O(8)	1.341(5)
C(37)-N(3)	1.343(5)
C(37)-C(38)	1.395(6)
C(38)-C(39)	1.379(7)
C(38)-H(37)	0.9500
C(39)-C(40)	1.383(6)
C(39)-H(38)	0.9500
C(40)-C(41)	1.387(5)
C(40)-H(39)	0.9500
C(41)-N(3)	1.355(5)
C(41)-C(42)	1.491(5)
C(42)-N(4)	1.482(4)
C(42)-H(41A)	0.9900
C(42)-H(41B)	0.9900
C(43)-N(4)	1.496(4)
C(43)-C(44)	1.505(5)
C(43)-H(42A)	0.9900
C(43)-H(42B)	0.9900
C(44)-C(48)	1.425(5)
C(44)-C(45)	1.439(5)
C(44)-Fe(2)	2.044(3)
C(45)-C(46)	1.447(5)
C(45)-P(2)	1.795(4)
C(45)-Fe(2)	2.043(3)
C(46)-C(47)	1.419(5)
C(46)-Fe(2)	2.036(3)
C(46)-H(45)	0.9500
C(47)-C(48)	1.428(5)
C(47)-Fe(2)	2.047(3)
C(47)-H(46)	0.9500
C(48)-Fe(2)	2.054(4)
C(48)-H(47)	0.9500
C(49)-C(50)	1.419(6)
C(49)-C(53)	1.427(6)
C(49)-Fe(2)	2.063(4)
C(49)-H(49)	0.9500
C(50)-C(51)	1.426(6)
C(50)-Fe(2)	2.036(4)
C(50)-H(48)	0.9500
C(51)-C(52)	1.420(7)
C(51)-Fe(2)	2.042(4)
C(51)-H(52)	0.9500
C(52)-C(53)	1.424(7)
C(52)-Fe(2)	2.056(4)
C(52)-H(51)	0.9500
C(53)-Fe(2)	2.065(4)
C(53)-H(50)	0.9500

C(54)-C(55)	1.396(5)
C(54)-C(59)	1.397(5)
C(54)-P(2)	1.830(3)
C(55)-C(56)	1.393(5)
C(55)-H(54)	0.9500
C(56)-C(57)	1.385(6)
C(56)-H(55)	0.9500
C(57)-C(58)	1.385(6)
C(57)-H(56)	0.9500
C(58)-C(59)	1.391(5)
C(58)-H(57)	0.9500
C(59)-H(58)	0.9500
C(60)-C(65)	1.392(5)
C(60)-C(61)	1.396(5)
C(60)-P(2)	1.827(4)
C(61)-C(62)	1.391(5)
C(61)-H(60)	0.9500
C(62)-C(63)	1.373(6)
C(62)-H(61)	0.9500
C(63)-C(64)	1.396(7)
C(63)-H(62)	0.9500
C(64)-C(65)	1.383(6)
C(64)-H(63)	0.9500
C(65)-H(64)	0.9500
C(66)-O(8)	1.438(5)
C(66)-H(65A)	0.9800
C(66)-H(65B)	0.9800
C(66)-H(65C)	0.9800
N(1)-Mn(1)	2.114(3)
N(2)-Mn(1)	2.098(3)
N(2)-H(2)	0.95(5)
N(3)-Mn(2)	2.100(3)
N(4)-Mn(2)	2.122(3)
N(4)-H(4)	0.92(5)
Fe(1)-C(20')	2.028(11)
Fe(1)-C(19)	2.037(11)
Fe(1)-C(20)	2.038(11)
Fe(1)-C(17')	2.043(9)
Fe(1)-C(16')	2.048(11)
Fe(1)-C(18)	2.052(9)
Fe(1)-C(19')	2.058(10)
C(16)-C(17)	1.421(13)
C(16)-C(20)	1.432(13)
C(16)-H(16)	0.9500
C(17)-C(18)	1.427(14)
C(17)-H(17)	0.9500
C(18)-C(19)	1.419(15)
C(18)-H(18)	0.9500
C(19)-C(20)	1.405(14)
C(19)-H(19)	0.9500
C(20)-H(20)	0.9500
C(16')-C(17')	1.432(15)
C(16')-C(20')	1.434(13)
C(16')-H(16')	0.9500
C(17')-C(18')	1.436(14)
C(17')-H(17')	0.9500
C(18')-C(19')	1.417(12)
C(18')-H(18')	0.9500
C(19')-C(20')	1.411(12)
C(19')-H(19')	0.9500
C(20')-H(20')	0.9500

Mn(1)-P(1)	2.3363(10)
Mn(2)-P(2)	2.3377(10)
Mn(3)-Br(3)	2.4759(7)
Mn(3)-Br(4)	2.4867(8)
Mn(3)-Br(2)	2.5014(7)
Mn(3)-Br(1)	2.5553(7)
Cl(3)-C(69)	1.651(17)
C(69)-Cl(4)	1.644(17)
C(69)-H(69A)	0.9900
C(69)-H(69B)	0.9900
Cl(3')-C(69')	1.605(14)
C(69')-Cl(4')	1.609(14)
C(69')-H(69C)	0.9900
C(69')-H(69D)	0.9900
Cl(3")-C(69")	1.648(16)
C(69")-Cl(4")	1.659(16)
C(69")-H(69E)	0.9900
C(69")-H(69F)	0.9900
Cl(3A)-C(69A)	1.649(17)
C(69A)-Cl(4A)	1.664(16)
C(69A)-H(69G)	0.9900
C(69A)-H(69H)	0.9900
Cl(3B)-C(69B)	1.762(9)
C(69B)-Cl(4B)	1.622(10)
C(69B)-H(69I)	0.9900
C(69B)-H(69J)	0.9900

O(1)-C(1)-Mn(1)	176.8(4)
O(2)-C(2)-Mn(1)	174.6(4)
O(3)-C(3)-Mn(1)	176.8(3)
O(4)-C(4)-N(1)	112.6(3)
O(4)-C(4)-C(5)	124.8(4)
N(1)-C(4)-C(5)	122.6(4)
C(6)-C(5)-C(4)	118.1(4)
C(6)-C(5)-H(5)	121.0
C(4)-C(5)-H(5)	121.0
C(5)-C(6)-C(7)	120.5(4)
C(5)-C(6)-H(6)	119.7
C(7)-C(6)-H(6)	119.7
C(8)-C(7)-C(6)	118.2(5)
C(8)-C(7)-H(7)	120.9
C(6)-C(7)-H(7)	120.9
N(1)-C(8)-C(7)	123.1(4)
N(1)-C(8)-C(9)	115.5(3)
C(7)-C(8)-C(9)	121.3(4)
N(2)-C(9)-C(8)	110.4(3)
N(2)-C(9)-H(9A)	109.6
C(8)-C(9)-H(9A)	109.6
N(2)-C(9)-H(9B)	109.6
C(8)-C(9)-H(9B)	109.6
H(9A)-C(9)-H(9B)	108.1
N(2)-C(10)-C(11)	111.9(3)
N(2)-C(10)-H(10A)	109.2
C(11)-C(10)-H(10A)	109.2
N(2)-C(10)-H(10B)	109.2
C(11)-C(10)-H(10B)	109.2
H(10A)-C(10)-H(10B)	107.9
C(12)-C(11)-C(15)	107.7(3)
C(12)-C(11)-C(10)	123.8(3)
C(15)-C(11)-C(10)	128.5(3)
C(12)-C(11)-Fe(1)	70.3(2)

C(15)-C(11)-Fe(1)	69.21(19)
C(10)-C(11)-Fe(1)	127.9(3)
C(13)-C(12)-C(11)	108.4(3)
C(13)-C(12)-Fe(1)	69.5(2)
C(11)-C(12)-Fe(1)	68.8(2)
C(13)-C(12)-H(12)	125.8
C(11)-C(12)-H(12)	125.8
Fe(1)-C(12)-H(12)	127.5
C(12)-C(13)-C(14)	108.6(4)
C(12)-C(13)-Fe(1)	70.2(2)
C(14)-C(13)-Fe(1)	68.8(2)
C(12)-C(13)-H(13)	125.7
C(14)-C(13)-H(13)	125.7
Fe(1)-C(13)-H(13)	126.9
C(13)-C(14)-C(15)	108.3(3)
C(13)-C(14)-Fe(1)	70.5(2)
C(15)-C(14)-Fe(1)	69.7(2)
C(13)-C(14)-H(14)	125.8
C(15)-C(14)-H(14)	125.8
Fe(1)-C(14)-H(14)	125.6
C(14)-C(15)-C(11)	107.0(3)
C(14)-C(15)-P(1)	128.3(3)
C(11)-C(15)-P(1)	124.5(3)
C(14)-C(15)-Fe(1)	68.8(2)
C(11)-C(15)-Fe(1)	69.22(19)
P(1)-C(15)-Fe(1)	131.7(2)
C(22)-C(21)-C(26)	119.5(4)
C(22)-C(21)-P(1)	124.3(3)
C(26)-C(21)-P(1)	116.3(3)
C(21)-C(22)-C(23)	120.5(4)
C(21)-C(22)-H(22)	119.8
C(23)-C(22)-H(22)	119.8
C(24)-C(23)-C(22)	119.8(5)
C(24)-C(23)-H(23)	120.1
C(22)-C(23)-H(23)	120.1
C(25)-C(24)-C(23)	120.3(4)
C(25)-C(24)-H(24)	119.8
C(23)-C(24)-H(24)	119.8
C(24)-C(25)-C(26)	120.6(4)
C(24)-C(25)-H(25)	119.7
C(26)-C(25)-H(25)	119.7
C(25)-C(26)-C(21)	119.4(4)
C(25)-C(26)-H(26)	120.3
C(21)-C(26)-H(26)	120.3
C(32)-C(27)-C(28)	119.0(4)
C(32)-C(27)-P(1)	122.6(3)
C(28)-C(27)-P(1)	118.2(3)
C(29)-C(28)-C(27)	120.7(5)
C(29)-C(28)-H(28)	119.7
C(27)-C(28)-H(28)	119.7
C(30)-C(29)-C(28)	119.9(5)
C(30)-C(29)-H(29)	120.1
C(28)-C(29)-H(29)	120.1
C(29)-C(30)-C(31)	120.1(4)
C(29)-C(30)-H(30)	119.9
C(31)-C(30)-H(30)	119.9
C(32)-C(31)-C(30)	120.2(5)
C(32)-C(31)-H(31)	119.9
C(30)-C(31)-H(31)	119.9
C(27)-C(32)-C(31)	120.0(4)
C(27)-C(32)-H(32)	120.0

C(31)-C(32)-H(32)	120.0
O(4)-C(33)-H(33A)	109.5
O(4)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
O(4)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
O(5)-C(34)-Mn(2)	175.4(3)
O(6)-C(35)-Mn(2)	176.9(4)
O(7)-C(36)-Mn(2)	171.6(4)
O(8)-C(37)-N(3)	113.4(3)
O(8)-C(37)-C(38)	123.5(4)
N(3)-C(37)-C(38)	123.1(4)
C(39)-C(38)-C(37)	118.0(4)
C(39)-C(38)-H(37)	121.0
C(37)-C(38)-H(37)	121.0
C(38)-C(39)-C(40)	120.2(4)
C(38)-C(39)-H(38)	119.9
C(40)-C(39)-H(38)	119.9
C(39)-C(40)-C(41)	118.1(4)
C(39)-C(40)-H(39)	120.9
C(41)-C(40)-H(39)	120.9
N(3)-C(41)-C(40)	122.9(3)
N(3)-C(41)-C(42)	116.7(3)
C(40)-C(41)-C(42)	120.3(3)
N(4)-C(42)-C(41)	111.1(3)
N(4)-C(42)-H(41A)	109.4
C(41)-C(42)-H(41A)	109.4
N(4)-C(42)-H(41B)	109.4
C(41)-C(42)-H(41B)	109.4
H(41A)-C(42)-H(41B)	108.0
N(4)-C(43)-C(44)	114.4(3)
N(4)-C(43)-H(42A)	108.7
C(44)-C(43)-H(42A)	108.7
N(4)-C(43)-H(42B)	108.7
C(44)-C(43)-H(42B)	108.7
H(42A)-C(43)-H(42B)	107.6
C(48)-C(44)-C(45)	107.7(3)
C(48)-C(44)-C(43)	124.0(3)
C(45)-C(44)-C(43)	128.3(3)
C(48)-C(44)-Fe(2)	70.0(2)
C(45)-C(44)-Fe(2)	69.38(19)
C(43)-C(44)-Fe(2)	125.7(2)
C(44)-C(45)-C(46)	107.5(3)
C(44)-C(45)-P(2)	124.7(3)
C(46)-C(45)-P(2)	127.2(3)
C(44)-C(45)-Fe(2)	69.40(19)
C(46)-C(45)-Fe(2)	68.97(19)
P(2)-C(45)-Fe(2)	134.32(18)
C(47)-C(46)-C(45)	107.9(3)
C(47)-C(46)-Fe(2)	70.1(2)
C(45)-C(46)-Fe(2)	69.47(18)
C(47)-C(46)-H(45)	126.0
C(45)-C(46)-H(45)	126.0
Fe(2)-C(46)-H(45)	126.0
C(46)-C(47)-C(48)	108.3(3)
C(46)-C(47)-Fe(2)	69.27(19)
C(48)-C(47)-Fe(2)	69.9(2)
C(46)-C(47)-H(46)	125.8
C(48)-C(47)-H(46)	125.8
Fe(2)-C(47)-H(46)	126.6

C(44)-C(48)-C(47)	108.5(3)
C(44)-C(48)-Fe(2)	69.3(2)
C(47)-C(48)-Fe(2)	69.4(2)
C(44)-C(48)-H(47)	125.7
C(47)-C(48)-H(47)	125.7
Fe(2)-C(48)-H(47)	127.2
C(50)-C(49)-C(53)	107.8(4)
C(50)-C(49)-Fe(2)	68.7(2)
C(53)-C(49)-Fe(2)	69.9(2)
C(50)-C(49)-H(49)	126.1
C(53)-C(49)-H(49)	126.1
Fe(2)-C(49)-H(49)	126.9
C(49)-C(50)-C(51)	108.3(4)
C(49)-C(50)-Fe(2)	70.7(2)
C(51)-C(50)-Fe(2)	69.7(2)
C(49)-C(50)-H(48)	125.9
C(51)-C(50)-H(48)	125.9
Fe(2)-C(50)-H(48)	125.3
C(52)-C(51)-C(50)	107.8(4)
C(52)-C(51)-Fe(2)	70.3(2)
C(50)-C(51)-Fe(2)	69.3(2)
C(52)-C(51)-H(52)	126.1
C(50)-C(51)-H(52)	126.1
Fe(2)-C(51)-H(52)	125.9
C(51)-C(52)-C(53)	108.2(4)
C(51)-C(52)-Fe(2)	69.2(2)
C(53)-C(52)-Fe(2)	70.1(2)
C(51)-C(52)-H(51)	125.9
C(53)-C(52)-H(51)	125.9
Fe(2)-C(52)-H(51)	126.4
C(52)-C(53)-C(49)	107.9(4)
C(52)-C(53)-Fe(2)	69.4(2)
C(49)-C(53)-Fe(2)	69.7(2)
C(52)-C(53)-H(50)	126.1
C(49)-C(53)-H(50)	126.1
Fe(2)-C(53)-H(50)	126.4
C(55)-C(54)-C(59)	119.4(3)
C(55)-C(54)-P(2)	123.3(3)
C(59)-C(54)-P(2)	117.2(3)
C(56)-C(55)-C(54)	120.1(4)
C(56)-C(55)-H(54)	119.9
C(54)-C(55)-H(54)	119.9
C(57)-C(56)-C(55)	119.8(4)
C(57)-C(56)-H(55)	120.1
C(55)-C(56)-H(55)	120.1
C(58)-C(57)-C(56)	120.7(3)
C(58)-C(57)-H(56)	119.7
C(56)-C(57)-H(56)	119.7
C(57)-C(58)-C(59)	119.7(4)
C(57)-C(58)-H(57)	120.1
C(59)-C(58)-H(57)	120.1
C(58)-C(59)-C(54)	120.3(4)
C(58)-C(59)-H(58)	119.9
C(54)-C(59)-H(58)	119.9
C(65)-C(60)-C(61)	118.9(3)
C(65)-C(60)-P(2)	121.1(3)
C(61)-C(60)-P(2)	120.0(3)
C(62)-C(61)-C(60)	120.4(3)
C(62)-C(61)-H(60)	119.8
C(60)-C(61)-H(60)	119.8
C(63)-C(62)-C(61)	120.5(4)

C(63)-C(62)-H(61)	119.7
C(61)-C(62)-H(61)	119.7
C(62)-C(63)-C(64)	119.3(4)
C(62)-C(63)-H(62)	120.4
C(64)-C(63)-H(62)	120.4
C(65)-C(64)-C(63)	120.7(4)
C(65)-C(64)-H(63)	119.7
C(63)-C(64)-H(63)	119.7
C(64)-C(65)-C(60)	120.2(4)
C(64)-C(65)-H(64)	119.9
C(60)-C(65)-H(64)	119.9
O(8)-C(66)-H(65A)	109.5
O(8)-C(66)-H(65B)	109.5
H(65A)-C(66)-H(65B)	109.5
O(8)-C(66)-H(65C)	109.5
H(65A)-C(66)-H(65C)	109.5
H(65B)-C(66)-H(65C)	109.5
C(4)-N(1)-C(8)	117.3(3)
C(4)-N(1)-Mn(1)	126.4(3)
C(8)-N(1)-Mn(1)	116.1(2)
C(9)-N(2)-C(10)	111.1(3)
C(9)-N(2)-Mn(1)	111.5(2)
C(10)-N(2)-Mn(1)	117.7(2)
C(9)-N(2)-H(2)	107(3)
C(10)-N(2)-H(2)	104(3)
Mn(1)-N(2)-H(2)	105(3)
C(37)-N(3)-C(41)	117.5(3)
C(37)-N(3)-Mn(2)	126.3(3)
C(41)-N(3)-Mn(2)	116.2(2)
C(42)-N(4)-C(43)	109.2(3)
C(42)-N(4)-Mn(2)	111.7(2)
C(43)-N(4)-Mn(2)	120.4(2)
C(42)-N(4)-H(4)	108(3)
C(43)-N(4)-H(4)	104(3)
Mn(2)-N(4)-H(4)	103(3)
C(4)-O(4)-C(33)	117.5(4)
C(37)-O(8)-C(66)	117.8(4)
C(20')-Fe(1)-C(14)	130.7(6)
C(14)-Fe(1)-C(19)	109.0(5)
C(14)-Fe(1)-C(20)	126.5(5)
C(19)-Fe(1)-C(20)	40.3(4)
C(20')-Fe(1)-C(17')	69.0(5)
C(14)-Fe(1)-C(17')	142.7(8)
C(20')-Fe(1)-C(15)	110.3(5)
C(14)-Fe(1)-C(15)	41.54(15)
C(19)-Fe(1)-C(15)	125.0(7)
C(20)-Fe(1)-C(15)	110.7(6)
C(17')-Fe(1)-C(15)	175.0(7)
C(20')-Fe(1)-C(11)	119.6(5)
C(14)-Fe(1)-C(11)	69.64(15)
C(19)-Fe(1)-C(11)	161.1(7)
C(20)-Fe(1)-C(11)	124.4(6)
C(17')-Fe(1)-C(11)	134.0(6)
C(15)-Fe(1)-C(11)	41.57(13)
C(20')-Fe(1)-C(16')	41.2(4)
C(14)-Fe(1)-C(16')	171.9(5)
C(17')-Fe(1)-C(16')	41.0(5)
C(15)-Fe(1)-C(16')	135.4(7)
C(11)-Fe(1)-C(16')	112.9(5)
C(14)-Fe(1)-C(18)	122.2(5)
C(19)-Fe(1)-C(18)	40.6(5)

C(20)-Fe(1)-C(18)	67.6(6)
C(15)-Fe(1)-C(18)	160.1(7)
C(11)-Fe(1)-C(18)	156.3(8)
C(20')-Fe(1)-C(13)	167.6(5)
C(14)-Fe(1)-C(13)	40.68(16)
C(19)-Fe(1)-C(13)	123.2(6)
C(20)-Fe(1)-C(13)	161.1(6)
C(17')-Fe(1)-C(13)	112.7(6)
C(15)-Fe(1)-C(13)	69.07(16)
C(11)-Fe(1)-C(13)	68.79(16)
C(16')-Fe(1)-C(13)	147.2(6)
C(18)-Fe(1)-C(13)	105.9(4)
C(20')-Fe(1)-C(19')	40.4(4)
C(14)-Fe(1)-C(19')	105.3(4)
C(17')-Fe(1)-C(19')	68.5(4)
C(15)-Fe(1)-C(19')	114.5(4)
C(11)-Fe(1)-C(19')	149.4(5)
C(16')-Fe(1)-C(19')	68.4(5)
C(13)-Fe(1)-C(19')	127.7(5)
C(20')-Fe(1)-C(12)	151.9(5)
C(14)-Fe(1)-C(12)	68.58(16)
C(19)-Fe(1)-C(12)	157.5(7)
C(20)-Fe(1)-C(12)	158.4(6)
C(17')-Fe(1)-C(12)	109.0(3)
C(15)-Fe(1)-C(12)	69.07(15)
C(11)-Fe(1)-C(12)	40.85(15)
C(16')-Fe(1)-C(12)	118.6(5)
C(18)-Fe(1)-C(12)	120.3(6)
C(13)-Fe(1)-C(12)	40.35(17)
C(19')-Fe(1)-C(12)	167.0(5)
C(17)-C(16)-C(20)	107.3(11)
C(17)-C(16)-Fe(1)	70.1(6)
C(20)-C(16)-Fe(1)	68.4(6)
C(17)-C(16)-H(16)	126.4
C(20)-C(16)-H(16)	126.4
Fe(1)-C(16)-H(16)	126.7
C(16)-C(17)-C(18)	107.5(10)
C(16)-C(17)-Fe(1)	69.8(6)
C(18)-C(17)-Fe(1)	69.0(6)
C(16)-C(17)-H(17)	126.3
C(18)-C(17)-H(17)	126.3
Fe(1)-C(17)-H(17)	126.5
C(19)-C(18)-C(17)	108.8(9)
C(19)-C(18)-Fe(1)	69.1(6)
C(17)-C(18)-Fe(1)	70.6(6)
C(19)-C(18)-H(18)	125.6
C(17)-C(18)-H(18)	125.6
Fe(1)-C(18)-H(18)	126.3
C(20)-C(19)-C(18)	107.3(10)
C(20)-C(19)-Fe(1)	69.9(6)
C(18)-C(19)-Fe(1)	70.3(6)
C(20)-C(19)-H(19)	126.4
C(18)-C(19)-H(19)	126.4
Fe(1)-C(19)-H(19)	125.1
C(19)-C(20)-C(16)	109.2(11)
C(19)-C(20)-Fe(1)	69.8(6)
C(16)-C(20)-Fe(1)	70.8(6)
C(19)-C(20)-H(20)	125.4
C(16)-C(20)-H(20)	125.4
Fe(1)-C(20)-H(20)	125.6
C(17')-C(16')-C(20')	107.2(9)

C(17')-C(16')-Fe(1)	69.3(6)
C(20')-C(16')-Fe(1)	68.7(6)
C(17')-C(16')-H(16')	126.4
C(20')-C(16')-H(16')	126.4
Fe(1)-C(16')-H(16')	127.2
C(16')-C(17')-C(18')	107.8(8)
C(16')-C(17')-Fe(1)	69.7(6)
C(18')-C(17')-Fe(1)	70.5(6)
C(16')-C(17')-H(17')	126.1
C(18')-C(17')-H(17')	126.1
Fe(1)-C(17')-H(17')	125.2
C(19')-C(18')-C(17')	107.9(9)
C(19')-C(18')-Fe(1)	69.5(6)
C(17')-C(18')-Fe(1)	68.6(5)
C(19')-C(18')-H(18')	126.0
C(17')-C(18')-H(18')	126.0
Fe(1)-C(18')-H(18')	127.4
C(20')-C(19')-C(18')	108.5(9)
C(20')-C(19')-Fe(1)	68.6(6)
C(18')-C(19')-Fe(1)	70.3(6)
C(20')-C(19')-H(19')	125.8
C(18')-C(19')-H(19')	125.7
Fe(1)-C(19')-H(19')	126.9
C(19')-C(20')-C(16')	108.5(10)
C(19')-C(20')-Fe(1)	71.0(6)
C(16')-C(20')-Fe(1)	70.2(6)
C(19')-C(20')-H(20')	125.7
C(16')-C(20')-H(20')	125.7
Fe(1)-C(20')-H(20')	124.7
C(50)-Fe(2)-C(46)	164.10(17)
C(50)-Fe(2)-C(51)	40.94(17)
C(46)-Fe(2)-C(51)	154.21(16)
C(50)-Fe(2)-C(45)	125.77(15)
C(46)-Fe(2)-C(45)	41.56(13)
C(51)-Fe(2)-C(45)	160.89(17)
C(50)-Fe(2)-C(44)	106.91(15)
C(46)-Fe(2)-C(44)	69.54(14)
C(51)-Fe(2)-C(44)	122.09(17)
C(45)-Fe(2)-C(44)	41.23(14)
C(50)-Fe(2)-C(47)	153.94(18)
C(46)-Fe(2)-C(47)	40.66(15)
C(51)-Fe(2)-C(47)	117.96(17)
C(45)-Fe(2)-C(47)	69.03(14)
C(44)-Fe(2)-C(47)	68.96(14)
C(50)-Fe(2)-C(48)	119.38(17)
C(46)-Fe(2)-C(48)	68.69(15)
C(51)-Fe(2)-C(48)	104.22(17)
C(45)-Fe(2)-C(48)	68.75(14)
C(44)-Fe(2)-C(48)	40.71(14)
C(47)-Fe(2)-C(48)	40.74(14)
C(50)-Fe(2)-C(52)	68.38(17)
C(46)-Fe(2)-C(52)	120.71(16)
C(51)-Fe(2)-C(52)	40.56(19)
C(45)-Fe(2)-C(52)	158.21(17)
C(44)-Fe(2)-C(52)	158.34(18)
C(47)-Fe(2)-C(52)	105.50(16)
C(48)-Fe(2)-C(52)	121.67(17)
C(50)-Fe(2)-C(49)	40.51(18)
C(46)-Fe(2)-C(49)	127.53(16)
C(51)-Fe(2)-C(49)	68.37(18)
C(45)-Fe(2)-C(49)	110.59(15)

C(44)-Fe(2)-C(49)	122.96(15)
C(47)-Fe(2)-C(49)	162.67(16)
C(48)-Fe(2)-C(49)	156.41(16)
C(52)-Fe(2)-C(49)	68.08(16)
C(50)-Fe(2)-C(53)	68.24(17)
C(46)-Fe(2)-C(53)	109.31(16)
C(51)-Fe(2)-C(53)	68.26(19)
C(45)-Fe(2)-C(53)	124.24(17)
C(44)-Fe(2)-C(53)	159.39(16)
C(47)-Fe(2)-C(53)	124.42(16)
C(48)-Fe(2)-C(53)	159.47(16)
C(52)-Fe(2)-C(53)	40.44(19)
C(49)-Fe(2)-C(53)	40.46(16)
C(3)-Mn(1)-C(1)	89.13(18)
C(3)-Mn(1)-C(2)	88.18(17)
C(1)-Mn(1)-C(2)	89.84(19)
C(3)-Mn(1)-N(2)	94.67(15)
C(1)-Mn(1)-N(2)	175.77(16)
C(2)-Mn(1)-N(2)	92.13(16)
C(3)-Mn(1)-N(1)	171.83(14)
C(1)-Mn(1)-N(1)	98.49(16)
C(2)-Mn(1)-N(1)	88.87(14)
N(2)-Mn(1)-N(1)	77.82(12)
C(3)-Mn(1)-P(1)	90.26(12)
C(1)-Mn(1)-P(1)	89.54(13)
C(2)-Mn(1)-P(1)	178.33(13)
N(2)-Mn(1)-P(1)	88.59(9)
N(1)-Mn(1)-P(1)	92.76(9)
C(34)-Mn(2)-C(35)	89.69(17)
C(34)-Mn(2)-C(36)	87.47(16)
C(35)-Mn(2)-C(36)	85.34(17)
C(34)-Mn(2)-N(3)	170.27(15)
C(35)-Mn(2)-N(3)	98.79(15)
C(36)-Mn(2)-N(3)	88.47(14)
C(34)-Mn(2)-N(4)	93.66(14)
C(35)-Mn(2)-N(4)	175.06(15)
C(36)-Mn(2)-N(4)	98.44(15)
N(3)-Mn(2)-N(4)	78.21(12)
C(34)-Mn(2)-P(2)	92.76(11)
C(35)-Mn(2)-P(2)	88.96(12)
C(36)-Mn(2)-P(2)	174.29(13)
N(3)-Mn(2)-P(2)	92.16(9)
N(4)-Mn(2)-P(2)	87.24(9)
Br(3)-Mn(3)-Br(4)	113.97(3)
Br(3)-Mn(3)-Br(2)	109.18(3)
Br(4)-Mn(3)-Br(2)	113.71(3)
Br(3)-Mn(3)-Br(1)	105.10(2)
Br(4)-Mn(3)-Br(1)	104.60(3)
Br(2)-Mn(3)-Br(1)	109.78(3)
C(15)-P(1)-C(27)	103.98(17)
C(15)-P(1)-C(21)	104.67(18)
C(27)-P(1)-C(21)	101.02(16)
C(15)-P(1)-Mn(1)	111.89(12)
C(27)-P(1)-Mn(1)	120.76(14)
C(21)-P(1)-Mn(1)	112.82(12)
C(45)-P(2)-C(60)	105.57(16)
C(45)-P(2)-C(54)	104.06(16)
C(60)-P(2)-C(54)	101.95(16)
C(45)-P(2)-Mn(2)	112.95(12)
C(60)-P(2)-Mn(2)	119.64(12)
C(54)-P(2)-Mn(2)	111.08(11)

Cl(4)-C(69)-Cl(3)	110(2)
Cl(4)-C(69)-H(69A)	109.6
Cl(3)-C(69)-H(69A)	109.6
Cl(4)-C(69)-H(69B)	109.6
Cl(3)-C(69)-H(69B)	109.6
H(69A)-C(69)-H(69B)	108.1
Cl(3')-C(69')-Cl(4')	131.1(17)
Cl(3')-C(69')-H(69C)	104.5
Cl(4')-C(69')-H(69C)	104.5
Cl(3')-C(69')-H(69D)	104.5
Cl(4')-C(69')-H(69D)	104.5
H(69C)-C(69')-H(69D)	105.6
Cl(3")-C(69")-Cl(4")	121(2)
Cl(3")-C(69")-H(69E)	107.0
Cl(4")-C(69")-H(69E)	107.0
Cl(3")-C(69")-H(69F)	107.0
Cl(4")-C(69")-H(69F)	107.0
H(69E)-C(69")-H(69F)	106.7
Cl(3A)-C(69A)-Cl(4A)	108.6(17)
Cl(3A)-C(69A)-H(69G)	110.0
Cl(4A)-C(69A)-H(69G)	110.0
Cl(3A)-C(69A)-H(69H)	110.0
Cl(4A)-C(69A)-H(69H)	110.0
H(69G)-C(69A)-H(69H)	108.4
Cl(4B)-C(69B)-Cl(3B)	120.2(7)
Cl(4B)-C(69B)-H(69I)	107.3
Cl(3B)-C(69B)-H(69I)	107.3
Cl(4B)-C(69B)-H(69J)	107.3
Cl(3B)-C(69B)-H(69J)	107.3
H(69I)-C(69B)-H(69J)	106.9

Symmetry transformations used to generate equivalent atoms:

Table S8. Anisotropic displacement parameters (A^2 x 10^3) for **5b** (20241015-Vickie). The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	41(2)	43(2)	32(2)	-6(2)	3(2)	-22(2)
C(2)	44(2)	39(2)	31(2)	-6(2)	14(2)	-14(2)
C(3)	36(2)	28(2)	36(2)	-3(1)	4(2)	-20(2)
C(4)	48(2)	49(2)	30(2)	-13(2)	11(2)	-34(2)
C(5)	64(3)	70(3)	31(2)	-23(2)	16(2)	-47(3)
C(6)	52(3)	69(3)	50(3)	-34(2)	19(2)	-35(2)
C(7)	42(2)	48(2)	48(2)	-25(2)	11(2)	-23(2)
C(8)	39(2)	32(2)	36(2)	-14(1)	10(2)	-23(2)
C(9)	38(2)	31(2)	35(2)	-9(1)	7(2)	-19(2)
C(10)	42(2)	24(2)	25(2)	2(1)	4(1)	-17(2)
C(11)	43(2)	23(2)	26(2)	-4(1)	5(1)	-16(2)
C(12)	45(2)	31(2)	29(2)	-5(1)	-1(2)	-12(2)
C(13)	39(2)	39(2)	37(2)	-11(2)	-2(2)	-13(2)
C(14)	37(2)	35(2)	36(2)	-11(2)	5(2)	-19(2)
C(15)	39(2)	25(2)	28(2)	-5(1)	6(1)	-18(2)
C(21)	43(2)	30(2)	30(2)	-5(1)	11(2)	-25(2)
C(22)	43(2)	40(2)	40(2)	-5(2)	11(2)	-20(2)
C(23)	43(2)	63(3)	50(3)	-4(2)	17(2)	-19(2)
C(24)	65(3)	72(3)	46(3)	-11(2)	30(2)	-34(3)
C(25)	60(3)	50(2)	34(2)	-2(2)	15(2)	-30(2)
C(26)	48(2)	39(2)	30(2)	-5(2)	11(2)	-27(2)
C(27)	49(2)	27(2)	25(2)	-3(1)	8(2)	-21(2)
C(28)	60(3)	33(2)	45(2)	-6(2)	6(2)	-30(2)
C(29)	84(4)	39(2)	44(2)	-7(2)	7(2)	-39(3)
C(30)	94(4)	30(2)	40(2)	-8(2)	17(2)	-33(2)
C(31)	71(3)	31(2)	38(2)	-5(2)	25(2)	-16(2)
C(32)	54(2)	26(2)	33(2)	-4(1)	17(2)	-18(2)
C(33)	95(4)	81(4)	25(2)	-4(2)	-3(2)	-37(3)
C(34)	35(2)	35(2)	20(2)	-3(1)	3(1)	-15(2)
C(35)	37(2)	41(2)	29(2)	-9(2)	6(2)	-22(2)
C(36)	34(2)	33(2)	35(2)	-7(1)	2(2)	-17(2)
C(37)	30(2)	37(2)	44(2)	-15(2)	5(2)	-16(2)
C(38)	35(2)	44(2)	59(3)	-23(2)	6(2)	-23(2)
C(39)	43(2)	41(2)	60(3)	-20(2)	15(2)	-28(2)
C(40)	42(2)	31(2)	41(2)	-13(2)	12(2)	-21(2)
C(41)	28(2)	29(2)	34(2)	-12(1)	10(1)	-15(1)
C(42)	37(2)	28(2)	31(2)	-4(1)	4(1)	-19(2)
C(43)	31(2)	35(2)	24(2)	-6(1)	4(1)	-20(2)
C(44)	34(2)	27(2)	27(2)	-3(1)	3(1)	-20(1)
C(45)	35(2)	27(2)	27(2)	-3(1)	5(1)	-22(1)
C(46)	40(2)	30(2)	26(2)	-2(1)	7(1)	-25(2)
C(47)	43(2)	34(2)	24(2)	1(1)	4(1)	-24(2)
C(48)	34(2)	32(2)	26(2)	-1(1)	2(1)	-18(2)
C(49)	56(2)	32(2)	31(2)	-1(1)	2(2)	-30(2)
C(50)	59(3)	45(2)	36(2)	-7(2)	16(2)	-41(2)
C(51)	50(2)	50(2)	48(2)	-1(2)	1(2)	-39(2)
C(52)	73(3)	48(2)	33(2)	-8(2)	2(2)	-46(2)
C(53)	58(3)	33(2)	41(2)	-9(2)	12(2)	-29(2)
C(54)	30(2)	26(2)	30(2)	-8(1)	7(1)	-16(1)
C(55)	39(2)	32(2)	28(2)	-8(1)	10(1)	-22(2)
C(56)	48(2)	35(2)	36(2)	-8(2)	12(2)	-27(2)
C(57)	47(2)	42(2)	46(2)	-17(2)	17(2)	-34(2)
C(58)	33(2)	39(2)	49(2)	-13(2)	8(2)	-22(2)

C(59)	29(2)	32(2)	41(2)	-8(2)	5(2)	-17(2)
C(60)	32(2)	26(2)	33(2)	-7(1)	4(1)	-16(1)
C(61)	36(2)	29(2)	28(2)	-5(1)	2(1)	-16(2)
C(62)	37(2)	36(2)	31(2)	-12(1)	5(2)	-16(2)
C(63)	49(2)	25(2)	41(2)	-6(2)	3(2)	-5(2)
C(64)	66(3)	26(2)	53(3)	3(2)	12(2)	-12(2)
C(65)	47(2)	26(2)	42(2)	-2(2)	12(2)	-14(2)
C(66)	51(3)	54(3)	95(4)	-13(3)	-31(3)	-24(2)
N(1)	43(2)	36(2)	27(1)	-9(1)	9(1)	-27(1)
N(2)	37(2)	25(1)	28(1)	-5(1)	7(1)	-18(1)
N(3)	31(2)	32(2)	31(2)	-10(1)	6(1)	-17(1)
N(4)	29(1)	29(1)	26(1)	-5(1)	3(1)	-16(1)
O(1)	52(2)	44(2)	40(2)	5(1)	-5(1)	-13(2)
O(2)	57(2)	63(2)	50(2)	-19(2)	9(2)	-39(2)
O(3)	42(2)	40(2)	39(1)	-11(1)	15(1)	-22(1)
O(4)	66(2)	52(2)	26(1)	-5(1)	1(1)	-32(2)
O(5)	51(2)	36(1)	35(1)	-4(1)	8(1)	-29(1)
O(6)	40(2)	44(2)	42(2)	2(1)	-6(1)	-14(1)
O(7)	49(2)	54(2)	25(1)	-8(1)	4(1)	-25(1)
O(8)	37(2)	45(2)	53(2)	-10(1)	-9(1)	-21(1)
Fe(1)	40(1)	28(1)	26(1)	-8(1)	3(1)	-16(1)
C(16)	46(5)	35(5)	20(6)	-14(4)	7(4)	-23(4)
C(17)	54(6)	34(6)	27(5)	-12(4)	5(4)	-23(5)
C(18)	50(6)	49(9)	34(7)	-26(6)	8(5)	-26(6)
C(19)	58(8)	34(6)	40(9)	-25(5)	17(7)	-33(6)
C(20)	38(6)	22(5)	32(6)	-6(4)	11(5)	-6(5)
C(16')	74(8)	32(5)	36(8)	-14(5)	27(6)	-34(6)
C(17')	90(10)	24(5)	21(4)	-6(3)	3(4)	-18(5)
C(18')	46(5)	35(6)	33(6)	-9(4)	1(4)	-15(4)
C(19')	45(5)	29(4)	23(5)	-5(3)	2(4)	-22(3)
C(20')	48(6)	33(6)	36(6)	-12(4)	7(4)	-31(5)
Fe(2)	38(1)	32(1)	21(1)	-4(1)	5(1)	-25(1)
Mn(1)	34(1)	29(1)	25(1)	-5(1)	6(1)	-19(1)
Mn(2)	30(1)	29(1)	23(1)	-5(1)	3(1)	-17(1)
Mn(3)	35(1)	30(1)	34(1)	0(1)	-1(1)	-20(1)
P(1)	35(1)	24(1)	24(1)	-3(1)	6(1)	-18(1)
P(2)	29(1)	25(1)	25(1)	-4(1)	5(1)	-16(1)
Br(1)	34(1)	28(1)	26(1)	-4(1)	3(1)	-18(1)
Br(2)	41(1)	40(1)	33(1)	-1(1)	-2(1)	-28(1)
Br(3)	59(1)	34(1)	67(1)	12(1)	-13(1)	-30(1)
Br(4)	38(1)	68(1)	51(1)	-11(1)	5(1)	-30(1)
Cl(3)	58(8)	89(9)	81(7)	-28(7)	28(6)	-13(7)
C(69)	62(7)	95(7)	67(6)	-11(6)	14(6)	-19(6)
Cl(4)	67(7)	102(9)	74(7)	18(7)	-1(6)	-15(7)
Cl(3')	36(4)	75(5)	80(4)	-40(4)	2(3)	-17(4)
C(69')	60(6)	92(7)	70(6)	-27(5)	11(5)	-23(6)
Cl(4')	79(5)	91(6)	56(4)	-2(3)	-11(3)	-31(4)
Cl(3")	58(6)	107(7)	78(6)	-5(5)	25(5)	-24(5)
C(69")	58(7)	102(7)	72(7)	-10(6)	12(6)	-19(7)
Cl(4")	36(5)	116(7)	99(8)	-46(6)	-4(5)	-12(5)
Cl(3A)	90(8)	89(8)	96(8)	-21(6)	36(7)	-39(7)
C(69A)	59(13)	72(12)	85(13)	-22(12)	42(13)	-24(11)
Cl(4A)	81(8)	58(7)	104(10)	4(7)	41(8)	-22(6)
Cl(3B)	38(1)	61(2)	58(2)	20(2)	-5(1)	-24(1)
C(69B)	32(4)	42(5)	68(5)	25(5)	12(4)	-8(4)
Cl(4B)	56(2)	56(2)	78(2)	-29(2)	-7(2)	-17(1)

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