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Bis[diphenylphosphino]methane and its bridge-substituted analogues as chemically non-innocent ligands for H_2 activation

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Electronic Supplementary Information

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Experimental part

All manipulations were carried out using Schlenk techniques under an atmosphere of dry nitrogen. Dry and oxygen-free organic solvents (THF, Et_2O, CH_2Cl_2, toluene, pentane) were obtained using LabSolv (Innovative Technology) solvent purification system. Deuterated solvents for NMR were deoxygenated by three freeze-pump-thaw cycles and kept over 3Å molecular sieves. High pressure experiments were carried out in non-stirred 'Autoclave Maxitech' autoclaves (50 mL). A liquid nitrogen/ethanol slush bath was used to maintain samples at the desired low temperature. Bridge-substituted diphosphinomethanes $Ph_2PCH(Me)PPh_2$[1] and $Ph_2PCH(Ph)PPh_2$[2] were prepared according to literature methods. Complex *fac*-[(κ^2-dppm)Mn(CO)$_3$Br] (*fac*-$\mathbf{1^H}$) was synthetized by a modification of previously described protocol.[3] Manganese hydride complex *fac*-[(κ^2-dppm)Mn(CO)$_3$H] (*fac*-$\mathbf{3^H}$) was prepared from $Mn_2(CO)_{10}$ and dppm using the synthetic approach described for other chelating diphosphines.[4] All other reagent grade chemicals purchased from commercial sources were used as received.

Solution IR spectra were recorded in 0.1 mm CaF_2 cells using a Perkin Elmer Frontier FT-IR spectrometer and given in cm^{-1} with relative intensity in parentheses. ^{1}H, ^{31}P, and ^{13}C NMR spectra were obtained on Bruker Avance 400, Avance III HD 400, and Bruker Avance NEO 600 spectrometers and referenced against the residual signals of deuterated solvents (^{1}H and ^{13}C)[5] and 85% H_3PO_4 (^{31}P, external standard), respectively. When necessary, signal attribution in ^{13}C spectra was based on decoupled ^{13}C{^{31}P, ^{1}H} and ^{13}C–^{1}H HMQC experiments. High-resolution mass-spectra (chemical ionization, methane) were obtained on a GCT Premier (Waters) instrument. Elemental analyses were carried out at the LCC-CNRS (Toulouse) using a Perkin Elmer 2400 series II analyzer.

General procedure for the synthesis of Mn(I) complexes *fac*-[(κ^2-Ph$_2$PCH(R)PPh$_2$)Mn(CO)$_3$Br] (*fac*-$\mathbf{1^H}$, *fac*-$\mathbf{1^{Me}}$, *fac*-$\mathbf{1^{Ph}}$). A solution of Mn(CO)$_5$Br (303 mg, 1.1 mmol) and dppm (423 mg, 1.1 mmol) in THF (10 mL) was heated at 50 °C during 1-2 h until the disappearance of ν_{CO} bands of the precursor (2136 (m), 2046 (vs), 2005 (s) cm^{-1}). The solution was cooled to room temperature, filtered through Celite and then nitrogen-saturated heptane (10 mL) was slowly added under stirring to induce the precipitation of the target product *fac*-$\mathbf{1^H}$. The resulting suspension was further concentrated under vacuum to *ca.* a half of its initial volume and cooled at −20°C overnight. The supernatant was removed by decantation and the yellow precipitate was washed with hexane (2×15 mL) and dried under vacuum to afford *fac*-$\mathbf{1^H}$ (612 mg, 92%) as yellow microcrystalline solid. Similarly, complexes *fac*-$\mathbf{1^{Me}}$ (396 mg, 90%) and *fac*-$\mathbf{1^{Ph}}$ (473 mg, 87%) were obtained as yellow powders from the substituted dppm derivatives $Ph_2PCH(Me)PPh_2$ (283 mg, 0.7 mmol) and $Ph_2PCH(Ph)PPh_2$ (368 mg, 0.8 mmol) and the equimolar amount of Mn(CO)$_5$Br (193 and 220 mg, respectively). Both latter complexes exist in solution as mixture of two isomers differing by the orientation of dppm backbone substituent *vs.* the Br atom (for all NMR description below major and minor isomers are depicted in parenthesis as **A** and **B**, respectively).

fac-$\mathbf{1^H}$: ^{1}H NMR (400.1 MHz, C_6D_6, 25 °C): δ 7.74−7.66 (m, 4H, CH_{Ph}), 7.36−7.28 (m, 4H, CH_{Ph}), 7.06−6.93 (m, 6H, CH_{Ph}), 6.88−6.82 (m, 6H, CH_{Ph}), 4.64 (dt, $^2J_{HH}$ = 14.7 Hz, $^2J_{PH}$ = 11.4 Hz, 1H, PCH_2P), 4.05 (dt, $^2J_{HH}$ = 14.7 Hz, $^2J_{PH}$ = 9.9 Hz, 1H, PCH_2P).

^{31}P{^{1}H} NMR (162.0 MHz, C_6D_6, 25 °C): δ 13.4 (br s).

$^{13}C\{^1H\}$ NMR (100.6 MHz, C_6D_6, 25 °C): δ 222.3 (br s, Mn–*C*O), 219.6 (br s, Mn–*C*O), 134.0 (vt, J_{CP} = 17.4 Hz, $C_{ipso\ PPh_2}$), 132.8 (vt, J_{CP} = 23.3 Hz, $C_{ipso\ PPh_2}$), 132.4 (vt, J_{CP} = 5.1 Hz, CH_{PPh_2}), 131.5 (vt, J_{CP} = 5.4 Hz, CH_{PPh_2}), 130.2, 129.9 (s, CH_{PPh_2}), 128.5 (vt overlapped with another vt signal, J_{CP} = 4.6 Hz, CH_{PPh_2}), 128.4 (vt overlapped with another vt signal, J_{CP} = 4.6 Hz, CH_{PPh_2}), 39.7 (t, $^1J_{CP}$ = 19.8 Hz, P*C*H_2P).

IR (THF, cm^{-1}): ν_{CO} 2020 (vs), 1950 (s), 1917 (s). Spectral data are in agreement with literature.[3]

fac-**1^{Me}** (20:1 ratio of isomers): ^1H NMR (400.1 MHz, $CDCl_3$, 25 °C): δ 7.89−7.81 (m, 0.2H, CH_{Ph} (**B**)), 7.68−7.61 (m, 4H, CH_{Ph} (**A**)), 7.61−7.55 (m, 0.2H, CH_{Ph} (**B**)), 7.50−7.38 (m, 12.6H, CH_{Ph} (**A**+**B**)), 7.37−7.30 (m, 4H, CH_{Ph} (**A**)), 5.42 (tq, $^2J_{PH}$ = 14.8 Hz, $^3J_{HH}$ = 7.4 Hz, 1H, PC*H*(CH_3)P (**A**)), 5.23−5.14 (m, 0.05H, PC*H*(CH_3)P (**B**)), 1.52 (td, $^3J_{PH}$ = 12.6 Hz, $^3J_{HH}$ = 7.4 Hz, 3H, PCH(CH_3)P (**A**)), 1.48 (td overlapped with another td signal, $^3J_{PH}$ = 15.2 Hz, $^3J_{HH}$ = 7.9 Hz, 0.15H, PCH(CH_3)P (**B**)).

$^1H\{^{31}P\}$ NMR (400.1 MHz, $CDCl_3$, 25 °C): δ 7.88−7.84 (m, CH_{Ph} (**B**)), 7.68−7.61 (m, CH_{Ph} (**A**)), 7.60−7.56 (m, CH_{Ph} (**B**)), 7.48−7.38 (m, CH_{Ph} (**A+B**)), 7.37−7.30 (m, CH_{Ph} (**A**)), 5.42 (q, $^3J_{HH}$ = 7.4 Hz, PC*H*(CH_3)P (**A**)), 5.19 (q, $^3J_{HH}$ = 7.9 Hz, PC*H*(CH_3)P (**B**)), 1.52 (d, $^3J_{HH}$ = 7.4 Hz, 3H, PCH(CH_3)P (**A**)), 1.48 (d, $^3J_{HH}$ = 7.9 Hz, PCH(CH_3)P (**B**)).

$^{31}P\{^1H\}$ NMR (162.0 MHz, $CDCl_3$, 25 °C): δ 33.0 (br s, (**A**)), 20.9 (br s, (**B**)).

$^{13}C\{^1H\}$ NMR (100.6 MHz, $CDCl_3$, 25 °C): δ 223.9 (br s, Mn–*C*O (**A**)), 218.7 (br s, Mn–*C*O, (**A**)), 135.9 (vt, J_{CP} = 4.6 Hz, CH_{PPh_2} (**B**)), 134.3 (vt, J_{CP} = 5.2 Hz, CH_{PPh_2} (**A**)), 132.4 (vt, J_{CP} = 4.5 Hz, CH_{PPh_2} (**A**)), 132.0 (vt, J_{CP} = 24.7 Hz, $C_{ipso\ PPh_2}$ (**A**)), 131.5 (vt, J_{CP} = 15.6 Hz, $C_{ipso\ PPh_2}$ (**A**)), 131.3 (vt, J_{CP} = 5.4 Hz, CH_{PPh_2} (**B**)), 131.0 (s, CH_{PPh_2} (**B**)), 130.9, 130.7 (s, CH_{PPh_2} (**A**)), 130.4 (s, CH_{PPh_2} (**B**)), 129.0 (vt, J_{CP} = 4.8 Hz, CH_{PPh_2} (**B**)), 128.8 (vt overlapped with another vt signal, J_{CP} = 4.3 Hz, CH_{PPh_2} (**A**)), 128.4 (vt overlapped with another vt signal, J_{CP} = 5.1 Hz, CH_{PPh_2} (**A**)), 128.5 (vt, J_{CP} = 5.1 Hz, CH_{PPh_2} (**B**)), 49.3 (t overlapped with another t signal, $^1J_{CP}$ = 18.3 Hz, P*C*H(CH_3)P (**B**)), 48.9 (t overlapped with another t signal, $^1J_{CP}$ = 17.7 Hz, P*C*H(CH_3)P (**A**)), 15.5 (t, $^2J_{CP}$ = 5.7 Hz, PCH(*C*H_3)P (**A**)), 14.3 (s, PCH(*C*H_3)P (**B**)).

IR (THF, cm^{-1}): ν_{CO} 2021 (vs), 1953 (s), 1910 (s).

Anal. Found: C, 56.65; H, 3.75. Calcd. for $C_{29}H_{24}BrMnO_3P_2$ (M = 617.3) C, 56.45; H, 3.9.

fac-**1^{Ph}** (4.5:1 ratio of isomers): ^1H NMR (400.1 MHz, C_6D_6, 25 °C): δ 7.76−7.63 (m, 5.7H, CH_{Ph} (**A**+**B**)), 7.61−7.54 (m, 4H, CH_{Ph} (**A**)), 7.26 (d, $^3J_{HH}$ = 6.7 Hz, 0.45H, CH_{Ph} (**B**)), 7.06−6.94 (m, 8H, CH_{Ph} + PC*H*(Ph)P (**A** at δ_H 6.99 from ^{13}C−^1H HMBC)), 6.92−6.66 (m, 11.7H, CH_{Ph} + PC*H*(Ph)P (**B** at δ_H 6.79 from ^{13}C−^1H HMBC)), 6.46 (d, $^3J_{HH}$ = 7.1 Hz, 2H, CH_{Ph} (**B**)).

$^{31}P\{^1H\}$ NMR (162.0 MHz, C_6D_6, 25 °C): δ 41.4 (br s, (**A**)), 25.2 (br s, (**B**)).

$^{13}C\{^1H\}$ NMR (100.6 MHz, C_6D_6, 25 °C): δ 225.4 (br s, Mn–*C*O (**A**)), 219.5 (br s, Mn–*C*O, (**A**)), 138.6 (vt, J_{CP} = 18.6 Hz, $C_{ipso\ PPh_2}$ (**B**)), 136.3 (vt, J_{CP} = 4.4 Hz, CH_{PPh_2} (**B**)), 135.4 (vt, J_{CP} = 5.3 Hz, CH_{PPh_2} (**A**)), 134.7 (t, $^3J_{CP}$ = 7.9 Hz, CH_{Ph} (**A**)), 134.0 (t, $^3J_{CP}$ = 7.1 Hz, CH_{Ph} (**B**)), 133.0 (vt, J_{CP} = 25.0 Hz, $C_{ipso\ PPh_2}$ (**A**)), 132.6 (vt, J_{CP} = 3.6 Hz, CH_{PPh_2} (**A**)), 131.3 (vt, J_{CP} = 14.8 Hz, $C_{ipso\ PPh_2}$ (**A**)), 130.9 (vt overlapped with s signal, J_{CP} = 3.6 Hz, CH_{PPh_2} (**B**)), 130.9 (s, CH_{PPh_2} (**A**)), 130.7 (vt, J_{CP} = 3.6 Hz, CH_{PPh_2} (**B**)), 130.4 (s, CH_{PPh_2} (**B**)), 130.2 (s, CH_{PPh_2} (**A**)), 129.9 (s, CH_{PPh_2} (**B**)), 129.0 (vt, J_{CP} = 4.5 Hz, CH_{PPh_2} (**B**)), 128.4 (s, CH_{Ph} (**A**)), 128.2 (vt overlapped with another vt signal, J_{CP} = 5.1 Hz, CH_{PPh_2} (**A**)), 128.15 (vt overlapped with another vt signal, J_{CP} = 4.4 Hz, CH_{PPh_2} (**A**)), 128.0 (s, CH_{Ph} (**A**)), 127.6 (t, J_{CP} = 2.0 Hz, CH_{Ph} (**B**)), 67.5 (t, $^1J_{CP}$ = 16.2 Hz, P*C*H(Ph)P (**B**)), 60.6 (t, $^1J_{CP}$ = 13.7 Hz, P*C*H(Ph)P (**A**)).

IR (THF, cm^{-1}): ν_{CO} 2023 (vs), 1958 (s), 1915 (sh), 1901 (m, br).

Anal. Found: C, 60.0; H, 3.45. Calcd. for $C_{34}H_{26}BrMnO_3P_2$ (M = 679.4) C, 60.1; H, 3.85.

Synthesis of Mn(I) complex *fac*-[(κ^2-Ph$_2$PCH$_2$PPh$_2$)Mn(CO)$_3$H] (*fac*-3^H). A yellow suspension of $Mn_2(CO)_{10}$ (292 mg, 0.75 mmol) and dppm (577 mg, 1.5 mmol) in 1-butanol (15 mL) was heated to 125 °C. Initially yellow solution gradually turned orange and the evolution of CO was observed. The reaction mixture was refluxed with IR monitoring until the ν_{CO} bands of the product *fac*-**3^H** (1998 (s), 1920 (vs) cm^{-1}) ceased to increase (*ca.* 6h). The resulting orange suspension was cooled to room temperature and the volatiles were removed under vacuum. The waxy orange residue was washed with hexane (2×15 mL) and then extracted with 1:2 THF/heptane mixture (5×5 mL). The combined extracts were filtered through Celite, concentrated to *ca.* 75% of the initial volume and kept at −20 °C overnight. The supernatant was removed by decantation and the precipitate was washed with hexane (20 mL) and dried under vacuum to afford *fac*-**3^H** (233 mg, 30%) as yellow-orange solid.

fac-**3^H**: ^{1}H NMR (400.1 MHz, C_6D_6, 25 °C): δ 7.73−7.65 (m, 4H, Ph), 7.48−7.41 (m, 4H, CH_{Ph}), 7.05−6.90 (m, 12H, CH_{Ph}), 3.92 (dtd, $^2J_{HH}$ = 15.1 Hz, $^2J_{PH}$ = 9.3 Hz, $^4J_{HH}$ = 5.8 Hz, 1H, PC*H*$_2$P), 3.64 (dt, $^2J_{HH}$ = 15.1 Hz, $^2J_{PH}$ = 11.0 Hz, 1H, PC*H*$_2$P), −5.10 (td, $^2J_{PH}$ = 43.9 Hz, $^4J_{HH}$ = 5.8 Hz, 1H, Mn−*H*). According to 1D NOESY experiment (Figure S13) the signals at 3.92 and 3.64 ppm belong to the CH_2 protons of dppm being in *anti* and *syn* position to the hydride ligand, respectively.

^{31}P{^{1}H} NMR (162.0 MHz, C_6D_6, 25 °C): δ 34.5 (br s).

^{13}C{^{1}H} NMR (150.9 MHz, C_6D_6, 25 °C): δ 225.0 (br s, Mn–*C*O), 222.5 (br s, Mn–*C*O), 138.1 (vt, J_{CP} = 24.0 Hz, $C_{ipso\,PPh_2}$), 136.0 (vt, J_{CP} = 15.4 Hz, $C_{ipso\,PPh_2}$), 132.1, 130.3, 130.1, 128.8 (s, CH_{PPh_2}), 48.5 (t, $^1J_{CP}$ = 21.1 Hz, P*C*H$_2$P).

IR (THF, cm^{-1}): ν_{CO} 1995 (s), 1913 (vs). Spectral data are in agreement with literature.[6]

Anal. Found: C, 64.1; H, 4.1; Calcd. for $C_{28}H_{23}MnO_3P_2$ (M = 524.4) C, 64.15; H, 4.4.

Synthesis of Mn(I) diphosphinomethanide complex *fac*-[(κ^3*P,C,P*-Ph$_2$PCHPPh$_2$)Mn(CO)$_3$] (*fac*-2^H) and its reactivity with dihydrogen. A solution of KHMDS (0.33 mL of 0.5M in toluene, 0.165 mmol) was added to a yellow suspension of complex *fac*-**1^H** (90 mg, 0.15 mmol) in toluene (5 mL) at room temperature. The reaction mixture immediately changed the color to orange and IR monitoring (Figure S48) revealed the complete transformation ν_{CO} bands of starting complex *fac*-**1^H** (2023 (vs), 1955 (s), 1918 (s) cm^{-1}) into those of the product *fac*-**2^H** (1997 (vs), 1919 (s), 1906 (s) cm^{-1}). Hydrogen gas was bubbled through the solution during 1-2 min and the resulting mixture was kept under H_2 atmosphere overnight. IR analysis of the reaction mixture showed the disappearance of characteristic bands of *fac*-**2^H** and the presence of a variety of ν_{CO} bands with overall low intensity. The orange solution was filtered through Celite, evaporated under vacuum and the residue was analyzed by ^{1}H and ^{31}P NMR spectroscopy evidencing the formation of the very complex mixture (Figures S15-S16). Only traces of the expected hydride complex *fac*-[(κ^2-Ph$_2$PCH$_2$PPh$_2$)Mn(CO)$_3$H] (*fac*-**3^H**) were detected by the presence of the characteristic signals at δ_P 34.5 and at δ_H −5.10 (td, $^2J_{PH}$ = 43.9 Hz, $^4J_{HH}$ = 5.8 Hz) perfectly matching with the data for independently prepared sample (see below).

In a second experiment, a solution of *fac*-**2^{H}** in toluene prepared as described above was transferred to the autoclave, purged three times with hydrogen and then pressurized to 50 atm. The reaction mixture was stirred at 50 °C for 16 h, cooled to room temperature and H_2 pressure was released. IR analysis of the resulting solution (Figure S48) evidenced the formation of *fac*-**3^{H}** as a major product (ν_{CO} 1998 (vs), 1914 (vs) cm^{-1},), which was then confirmed by NMR data of the aliquot (Figures S17-S18). The solution was filtered through Celite, evaporated under vacuum and the residue was purified by crystallization from THF/heptane mixture as described above to afford complex *fac*-**3^{H}** (40 mg, 50%).

Synthesis of Mn(I) complex *fac*-[(κ^3*P,C,P*-$Ph_2PC(Me)PPh_2$)$Mn(CO)_3$] (*fac*-2^{Me}) and its reactions with H_2. A solution of KHMDS (0.22 mL of 0.5M in toluene, 0.11 mmol) was added to a yellow suspension of complex *fac*-**1^{Me}** (62 mg, 0.1 mmol) in toluene (5 mL) at room temperature. The reaction mixture immediately changed the color to orange and IR monitoring (Figure S49) revealed the quantitative formation of *fac*-**2^{Me}** (ν_{CO} 1994 (vs), 1913 (s), 1903 (s) cm^{-1}). The resulting solution was stirred for 1 h under H_2 atmosphere at room temperature. IR spectrum of the resulting red solution revealed the formation of hydride complex *fac*-**3^{Me}** as a main product (ν_{CO} 1997 (vs), 1917 (vs) cm^{-1}), which was then confirmed by ^{1}H and ^{31}P NMR spectroscopy (Figures S26-S27).

In a second experiment, a solution of *fac*-**2^{Me}** in toluene (15 mL) prepared as described above from *fac*-**1^{Me}** (154 mg, 0.25 mmol) and KHMDS (0.55 mL of 0.5M in toluene, 0.275 mmol) was transferred to the autoclave, purged three times with hydrogen and then pressurized to 50 atm. After stirring for 1 h, excessive H_2 pressure was released and a quantitative formation of *fac*-**3^{Me}** was evidenced by IR (Figure S49) and NMR spectroscopy (Figures S28-S29). The volatiles were removed under vacuum, the residue was again re-dissolved in warm toluene (4 mL) and the resulting solution was filtered through Celite. The solution was slowly (1 h) concentrated under vacuum to *ca.* 25% of initial volume inducing the crystallization of *fac*-**3^{Me}** finished at −20 °C overnight. The supernatant was removed by decantation and the precipitate was washed with hexane (3×1 mL) and dried under vacuum to afford *fac*-**3^{Me}** (134 mg, 92%) as light yellow microcrystalline solid containing 0.5 molecule of toluene according to microanalysis and NMR data.

fac-**3^{Me}** (5:1 ratio of isomers): ^{1}H NMR (400.1 MHz, C_6D_6, 25 °C): δ 7.92−7.85 (m, 4H, CH_{Ph} (**A**)), 7.66−7.59 (m, 0.8H, CH_{Ph} (**B**)), 7.57−7.51 (m, 0.8H, CH_{Ph} (**B**)), 7.51−7.44 (m, 4H, CH_{Ph} (**A**)), 7.14−7.11 (m, 0.7H, CH_{Tol}), 7.08−6.91 (m, 15.6H, CH_{Ph} (**A**+**B**) + CH_{Tol}), 4.62−4.49 (m, 1H, PC*H*(CH_3)P (**A**)), 5.49−5.37 (m, 0.2H, PC*H*(CH_3)P (**B**)), 2.11 (s, 1.6H, CH_{3Tol}), 0.74 (td overlapped with another td, $^3J_{PH}$ = 13.6 Hz, $^3J_{HH}$ = 7.5 Hz, 0.6H, PCH(CH_3)P (**B**)), 0.65 (td overlapped with another td signal, $^3J_{PH}$ = 15.4 Hz, $^3J_{HH}$ = 7.8 Hz, 3H, PCH(CH_3)P (**A**)), −5.01 (td, $^2J_{PH}$ = 41.9 Hz, $^4J_{HH}$ = 3.9 Hz, 1H, Mn−*H* (**A**)), −5.83 (t, $^2J_{PH}$ = 44.4 Hz, 0.15H, Mn−*H* (**B**)). According to 1D NOESY experiments (Figures S34-S35) **A** and **B** were attributed to *fac,anti-* and *fac,syn*-isomers of complex *fac*-**3^{Me}**, respectively.

^{1}H{^{31}P} NMR (400.1 MHz, C_6D_6, 25 °C): δ 7.91−7.86 (m, CH_{Ph} (**A**)), 7.65−7.61 (m, CH_{Ph} (**B**)), 7.56−7.52 (m, CH_{Ph} (**B**)), 7.14−7.11 (m, CH_{Tol}), 7.08−6.91 (m, CH_{Ph} (**A**+**B**) + CH_{Tol}), 4.56 (qd, $^3J_{HH}$ = 7.8 Hz, $^4J_{HH}$ = 4.0 Hz PC*H*(CH_3)P (**A**)), 4.44 (q, $^3J_{HH}$ = 7.5 Hz, PC*H*(CH_3)P (**B**)), 2.11 (s, CH_{3Tol}), 0.74 (d, $^3J_{HH}$ = 7.5 Hz, PCH(CH_3)P (**B**)), 0.65 (d, $^3J_{HH}$ = 7.8 Hz, PCH(CH_3)P (**A**)), −5.01 (d, $^4J_{HH}$ = 4.0 Hz, Mn−*H* (**A**)), −5.83 (s, Mn−*H* (**B**)).

^{31}P{^{1}H} NMR (162.0 MHz, C_6D_6, 25 °C): δ 52.4 (br s, (**B**)), 51.7 (br s, (**A**)).

$^{13}C\{^1H\}$ NMR (100.6 MHz, C_6D_6, 25 °C): δ 225.2 (br s, Mn–*C*O (**A**)), 224.6 (br s, Mn–*C*O (**B**)), 218.7 (br s, Mn–*C*O, (**A**)), 221.9 (br s, Mn–*C*O, (**A**+**B**)), 138.5 (vt, J_{CP} = 26.7 Hz, $C_{ipso\ PPh_2}$ (**A**)), 136.8 (vt, J_{CP} = 16.7 Hz, $C_{ipso\ PPh_2}$ (**A**)), 135.0 (vt, J_{CP} = 5.4 Hz, CH_{PPh_2} (**A**)), 134.7 (vt, J_{CP} = 5.9 Hz, CH_{PPh_2} (**B**)), 133.2 (vt, J_{CP} = 12.0 Hz, $C_{ipso\ PPh_2}$ (**B**)), 132.0 (s, CH_{PPh_2} (**B**)), 131.8 (vt, J_{CP} = 5.4 Hz, CH_{PPh_2} (**A**)), 131.6 (s, CH_{PPh_2} (**B**)), 131.3 (vt, J_{CP} = 5.1 Hz, CH_{PPh_2} (**B**)), 130.7 (s, CH_{PPh_2} (**A**)), 130.5 (s, CH_{PPh_2} (**B**)), 130.0 (s, CH_{PPh_2} (**B**)), 129.9 (s, CH_{PPh_2} (**A**)), 129.3 (s, CH_{PPh_2} (**B**)), 128.9 (vt overlapped with another vt signal, J_{CP} = 5.6 Hz, CH_{PPh_2} (**B**)), 128.8 (vt overlapped with another vt signal, J_{CP} = 4.7 Hz, CH_{PPh_2} (**A**)), 128.4 (vt overlapped with solvent signal, J_{CP} = 5.0 Hz, CH_{PPh_2} (**A**)), 55.6 (t, $^1J_{CP}$ = 21.2 Hz, P*C*H(CH_3)P (**B**)), 51.6 (t, $^1J_{CP}$ = 20.9 Hz, P*C*H(CH_3)P (**A**)), 15.7 (t, $^2J_{CP}$ = 5.4 Hz, PCH(*C*H_3)P (**B**)), 15.1 (t, $^2J_{CP}$ = 5.0 Hz, PCH(*C*H_3)P (**A**)).

IR (toluene, cm^{-1}): ν_{CO} 1997 (vs), 1917 (vs).

Anal. Found: C, 66.35; H, 4.85; Calcd. for $C_{29}H_{25}MnO_3P_2$•0.5toluene (M = 538.4) C, 66.8; H, 5.0.

Synthesis of Mn(I) complex *fac*-[(κ^3*P,C,P*-$Ph_2PC(Ph)PPh_2$)Mn(CO)$_3$] (*fac*-2^{Ph}) and its reactions with H_2. A solution of KHMDS (0.44 mL of 0.5M in toluene, 0.22 mmol) was added to a yellow suspension of complex *fac*-**1**^{Ph} (136 mg, 0.2 mmol) in toluene (5 mL) at room temperature. The reaction mixture immediately changed the color to orange and IR monitoring revealed the quantitative formation of *fac*-**2**^{Ph} (ν_{CO} 1995 (vs), 1918 (s), 1905 (s) cm^{-1}). Hydrogen gas was bubbled through the solution during 1-2 min and the solution was stirred for additional 5 min. IR spectrum of the reaction aliquot (Figure S50) showed the complete conversion of *fac*-**2**^{Ph} into the hydride product *fac*-**3**^{Ph} (ν_{CO} 1998 (vs), 1918 (vs) cm^{-1}). The volatiles were removed under vacuum, the residue was again re-dissolved in warm toluene (3 mL) and the resulting solution was filtered through Celite. The solution was slowly (1 h) concentrated under vacuum to *ca.* 30% of initial volume and left overnight at 0 °C. The resulting yellow crystals, some of them being suitable for X-ray diffraction, were separated from the solution, washed with hexane (2×1 mL) and dried under vacuum to afford *fac*-**3**^{Ph} (106 mg, 89%) as light yellow crystals.

fac-**3**^{Ph} (5.3:1 ratio of isomers): ^1H NMR (400.1 MHz, C_6D_6, 25 °C): δ 7.86−7.78 (m, 4H, C*H*$_{Ph}$ (**A**)), 7.78−7.71 (m, 4H, C*H*$_{Ph}$ (**A**)), 7.71−7.65 (m, 0.75H, C*H*$_{Ph}$ (**B**)), 7.63−7.57 (m, 0.75H, C*H*$_{Ph}$ (**B**)), 7.07−6.77 (m, 14.7H, C*H*$_{Ph}$ (**A**+**B**)), 6.75−6.52 (m, 3.6H, C*H*$_{Ph}$ (**A**+**B**)), 6.32 (td overlapped with m signal, $^2J_{PH}$ = 13.9 Hz, $^4J_{HH}$ = 3.3 Hz, 1H, PC*H*(Ph)P (**A**)), 6.31−6.27 (m overlapped with td signal, 2H, C*H*$_{Ph}$ (**A**)), 6.16−6.11 (m overlapped with t signal, 0.35H, C*H*$_{Ph}$ (**B**)), 6.08 (t, $^2J_{PH}$ = 13.2 Hz, 0.18H, PC*H*(Ph)P (**B**)), −4.70 (td, $^2J_{PH}$ = 42.6 Hz, $^4J_{HH}$ = 3.3 Hz, 1H, Mn−*H* (**A**)), −5.64 (t, $^2J_{PH}$ = 44.3 Hz, 0.17H, Mn−*H* (**B**)). According to 1D NOESY experiments (Figure S46-S47) **A** and **B** were attributed to *fac,anti*- and *fac,syn*-isomers of complex *fac*-**3**^{Ph}, respectively.

$^{31}P\{^1H\}$ NMR (162.0 MHz, C_6D_6, 25 °C): δ 58.7 (br s, (**B**)), 54.1 (br s, (**B**)).

$^{13}C\{^1H\}$ NMR (100.6 MHz, C_6D_6, 25 °C): δ 225.1 (br s, Mn–*C*O (**A**)), 224.5 (br s, Mn–*C*O (**B**)), 221.5 (br t, $^2J_{PC}$ = 12.5 Hz, Mn–*C*O, (**A**+**B**)), 139.9 (vt, J_{CP} = 26.5 Hz, $C_{ipso\ PPh_2}$ (**B**)), 139.7 (vt, J_{CP} = 17.2 Hz, $C_{ipso\ PPh_2}$ (**A**)), 135.9 (vt, J_{CP} = 5.4 Hz, CH_{PPh_2} (**A**)), 135.8 (vt, J_{CP} = 6.1 Hz, CH_{PPh_2} (**B**)), 135.3 (t, $^2J_{CP}$ = 7.6 Hz, $C_{ipso\ Ph}$ (**B**)), 134.9 (vt, J_{CP} = 8.2 Hz, CH_{Ph} (**B**)), 132.4 (t, $^2J_{CP}$ = 11.6 Hz, $C_{ipso\ Ph}$ (**A**)), 131.2 (vt overlapped with another vt signal, J_{CP} = 10.7 Hz, $C_{ipso\ PPh_2}$ (**A**)), 131.1 (vt, J_{CP} = 5.3 Hz, CH_{PPh_2} (**A**)), 130.1, 130.9 (s, CH_{PPh_2} (**B**)), 130.6 (s, CH_{PPh_2} (**A**)), 130.4 (vt, J_{CP} = 3.7 Hz, CH_{PPh_2} (**B**)), 130.0 (s, CH_{PPh_2} (**A**)), 129.8 (vt, J_{CP}

= 3.8 Hz, $C\mathrm{H_{PPh_2}}$ (**A**)), 129.0 (vt, J_{CP} = 4.6 Hz, $C\mathrm{H_{PPh_2}}$ (**A**)), 128.9 (vt, J_{CP} = 4.9 Hz, $C\mathrm{H_{PPh_2}}$ (**B**)), 128.0, 127.9 (s, $\mathrm{C}H_{\mathrm{Ph}}$ (**A**)), 127.3 (br s, $\mathrm{C}H_{\mathrm{Ph}}$ (**B**)), 127.3 (br t, J_{PC} = 2.5 Hz, $\mathrm{C}H_{\mathrm{Ph}}$ (**A**)), 68.6 (t, $^1J_{CP}$ = 16.6 Hz, P*C*H(Ph)P (**A**)), 68.3 (t, $^1J_{CP}$ = 17.4 Hz, P*C*H(Ph)P (**B**)).

IR (toluene, cm^{-1}): ν_{CO} 1998 (vs), 1918 (vs).

Anal. Found: C, 68.2; H, 4.15. Calcd. for $C_{34}H_{27}MnO_3P_2$ (M = 600.5) C, 68.0; H, 4.5.

Preparation of Mn(I) diphosphinomethanide complexes *fac*-[(κ^3*P,C,P*-$Ph_2PC(R)PPh_2$)$Mn(CO)_3$] (*fac*-2^R) for NMR characterization. A solution of KHMDS (0.15 mL of 0.5M in toluene, 0.077 mmol) was added to suspension of 0.07 mmol of complex *fac*-**1**^{R} (*fac*-**1^H**, 42 mg; *fac*-**1^{Me}**, 43 mg; *fac*-**1^{Ph}**, 47 mg) in toluene (2 mL). After complete formation of complex *fac*-**2^R** evidenced by IR spectroscopy, all volatiles were removed under vacuum. The residue was dissolved in dry C_6D_6 and the resulting solution was filtered through Celite directly to the NMR tube.

fac-**2^H**: ^{1}H NMR (400.1 MHz, C_6D_6, 25 °C): δ 7.30−7.19 (m, 4H, $\mathrm{C}H_{\mathrm{Ph}}$), 7.14−6.69 (m, 10H, $\mathrm{C}H_{\mathrm{Ph}}$ + $\mathrm{C}H_{\mathrm{Tol}}$), 6.71 (t, $^3J_{HH}$ = 6.8 Hz, 2H, $\mathrm{C}H_{\mathrm{Ph}}$), 6.57 (t, $^3J_{HH}$ = 6.8 Hz, 4H, $\mathrm{C}H_{\mathrm{Ph}}$), 1.65 (s, 1H, PC*H*P).

^{31}P{^{1}H} NMR (162.0 MHz, C_6D_6, 25 °C): δ 12.4 (br s).

^{13}C{^{1}H} NMR (100.6 MHz, C_6D_6, 25 °C): δ 224.0 (br s, Mn–*C*O), 135.0 (vt, J_{CP} = 6.9 Hz, $C\mathrm{H_{PPh_2}}$), 134.8 (vt, J_{CP} = 38.8 Hz, $C_{ipso\ \mathrm{PPh_2}}$), 132.0 (vt, J_{CP} = 5.3 Hz, $C\mathrm{H_{PPh_2}}$), 130.1, 130.0 (s, $C\mathrm{H_{PPh_2}}$), 129.0 (vt, J_{CP} = 18.7 Hz, $C_{ipso\ \mathrm{PPh_2}}$), 128.5 (vt overlapped with residual solvent protons, J_{CP} = 6.4 Hz (obtained from DEPT 135 experiment), $C\mathrm{H_{PPh_2}}$), 128.0 (vt overlapped with residual solvent protons, J_{CP} = 5.7 Hz (obtained from DEPT 135 experiment), $C\mathrm{H_{PPh_2}}$), −10.1 (t, $^1J_{CP}$ = 5.3 Hz, P*C*HP).

IR (toluene, cm^{-1}): ν_{CO} 1997 (vs), 1919 (s), 1906 (s).

HRMS (CI, positive mode): *m/z* 522.0353 (M$^+$), 523.0425 (M+H$^+$); Calcd. for $C_{28}H_{21}MnP_2O_3$ (M$^+$): *m/z* 522.0346 (ε_r = 1.3 ppm), for $C_{28}H_{21}MnP_2O_3$ (M–H$^+$): *m/z* 523.0425 (ε_r = 0.0 ppm).

fac-**2^{Me}**: ^{1}H NMR (400.1 MHz, C_6D_6, 25 °C): δ 7.38−7.28 (m, 4H, $\mathrm{C}H_{\mathrm{Ph}}$), 7.10−6.69 (m, 10H, $\mathrm{C}H_{\mathrm{Ph}}$ + $\mathrm{C}H_{\mathrm{Tol}}$), 6.74 (t, $^3J_{HH}$ = 7.3 Hz, 2H, $\mathrm{C}H_{\mathrm{Ph}}$), 6.59 (t, $^3J_{HH}$ = 7.3 Hz, 4H, $\mathrm{C}H_{\mathrm{Ph}}$), 1.77 (t, $^3J_{PH}$ = 8.8 Hz, 3H, PC(CH_3)P).

^{31}P{^{1}H} NMR (162.0 MHz, C_6D_6, 25 °C): δ 20.4 (br s).

^{13}C{^{1}H} NMR (100.6 MHz, C_6D_6, 25 °C): δ 226.0 (br s, Mn–*C*O), 134.7 (vt, J_{CP} = 6.7 Hz, $C\mathrm{H_{PPh_2}}$), 134.1 (vt, J_{CP} = 5.3 Hz, $C\mathrm{H_{PPh_2}}$), 133.1 (vdd, J_{CP} = 36.8 Hz, J_{CP} = 39.7 Hz, $C_{ipso\ \mathrm{PPh_2}}$), 130.1, 129.9 (s, $C\mathrm{H_{PPh_2}}$), 129.3 (vdd, J_{CP} = 20.7 Hz, J_{CP} = 17.9 Hz, $C_{ipso\ \mathrm{PPh_2}}$), 128.3 (vt overlapped with residual solvent protons, J_{CP} = 5.4 Hz (obtained from DEPT 135 experiment), $C\mathrm{H_{PPh_2}}$), 128.3 (vt overlapped with residual solvent protons, J_{CP} = 5.4 Hz (obtained from DEPT 135 experiment), $C\mathrm{H_{PPh_2}}$), 128.1 (vt overlapped with residual solvent protons, J_{CP} = 5.6 Hz (obtained from DEPT 135 experiment), 10.7 (t, $^2J_{CP}$ = 2.8 Hz, PC(*C*H$_3$)P), 0.2 (s, P*C*(CH$_3$)P).

IR (toluene, cm^{-1}): ν_{CO} 1994 (vs), 1913 (s), 1903 (s).

HRMS (CI, positive mode): *m/z* 536.0482 (M$^+$), 537.0555 (M+H$^+$); Calcd. for $C_{29}H_{23}MnP_2O_3$ (M$^+$): *m/z* 536.0503 (ε_r = 3.9 ppm), for $C_{29}H_{24}MnP_2O_3$ (M–H$^+$): *m/z* 537.0581 (ε_r = 4.8 ppm).

fac-**2**^{Ph}: ^{1}H NMR (400.1 MHz, C_6D_6, 25 °C): δ 7.44−7.18 (m, 10H, CH_{Ph}), 6.99−6.94 (m, 3H, CH_{Ph}), 6.85−6.53 (m, 12H, CH_{Ph}).

^{31}P{^{1}H} NMR (162.0 MHz, C_6D_6, 25 °C): δ 17.6 (br s).

^{13}C{^{1}H} NMR (100.6 MHz, C_6D_6, 25 °C): δ 225.8 (br s, Mn–*C*O), 137.2 (vt, J_{CP} = 23.8 Hz, $C_{ipso\ PPh_2}$), 136.3 (vt, J_{CP} = 3.8 Hz, CH_{Ph}), 135.0 (s, CH_{PPh_2}), 134.6, 134.0 (br s, CH_{PPh_2}), 131.4 (vt, J_{CP} = 4.9 Hz, CH_{Ph}), 130.7 (vt, J_{CP} = 18.5 Hz, $C_{ipso\ PPh_2}$), 130.0, 129.9 (br s, CH_{PPh_2}), 129.0 (vt, J_{CP} = 5.4 Hz, CH_{Ph}), 128.2 (vt overlapped with residual solvent signal, J_{CP} = 5.8 Hz, CH_{PPh_2}), 126.3 (s, CH_{Ph}), 123.7 (t, $^{2}J_{CP}$ = 10.7 Hz, $C_{ipso\ Ph}$), 12.8 (br t, $^{1}J_{CP}$ = 2.4 Hz, P*C*(Ph)P).

IR (toluene, cm^{-1}): ν_{CO} 1995 (vs), 1918 (s), 1905 (s).

HRMS (CI, positive mode): *m/z* 598.0649 (M^+), 599.0718 ($M+H^+$); Calcd. for $C_{34}H_{25}MnP_2O_3$ (M^+): *m/z* 598.0659 (ε_r = 1.7 ppm), for $C_{34}H_{26}MnP_2O_3$ ($M–H^+$): *m/z* 599.0738 (ε_r = 3.3 ppm).

Synthesis of Mn(I) diphosphinomethanide complex *fac*-[(κ^3*P,C,P*-$Ph_2PC(Ph)PPh_2$)Mn(CO)$_3$] (*fac*-2^{Ph}). A solution of KHMDS (0.22 mL of 0.5M in toluene, 0.11 mmol) was added to a yellow suspension of complex *fac*-**1**^{Ph} (68 mg, 0.1 mmol) in toluene (3 mL) at room temperature. The reaction mixture immediately changed the color to orange and IR monitoring revealed the quantitative formation of *fac*-**2**^{Ph} (ν_{CO} 1995 (vs), 1918 (s), 1905 (s) cm^{-1}). The volatiles were removed under vacuum, the residue was again re-dissolved in toluene (3 mL). The resulting solution was filtered through Celite and concentrated under vacuum to *ca.* half of the initial volume and cooled overnight at −20 °C to induce the formation of yellow crystals of *fac*-**2**^{Ph}, some of them being suitable for X-ray diffraction. The solution was removed by decantation, the precipitate was washed with toluene (1 mL) at −20°C and dried under vacuum to afford *fac*-**2**^{Ph} (38 mg, 60%) as light yellow microcrystals analyzing as *fac*-**2**^{Ph}•0.5toluene.

Anal. Found: C, 66.6; H, 4.85; Calcd. for $C_{29}H_{25}MnO_3P_2$•0.5toluene (M = 644.1) C, 66.9; H, 4.5.

Figure S1. ¹H NMR spectrum of complex *fac*-$\mathbf{1^H}$ (400.1 MHz, C_6D_6, 25 °C)

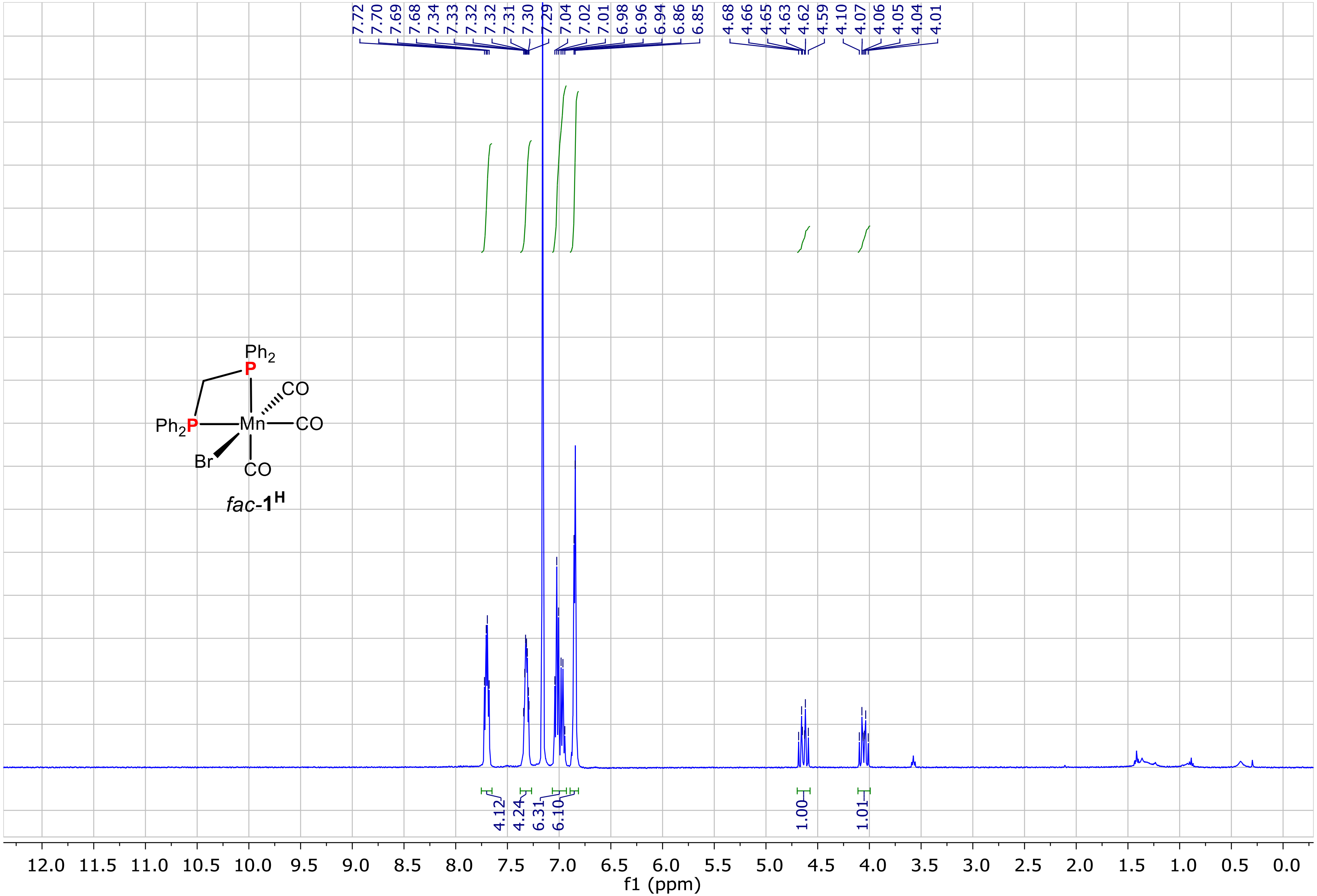


Figure S2. $^{31}P\{^1H\}$ NMR spectrum of complex *fac*-**1^H** (162.0 MHz, C_6D_6, 25 °C)

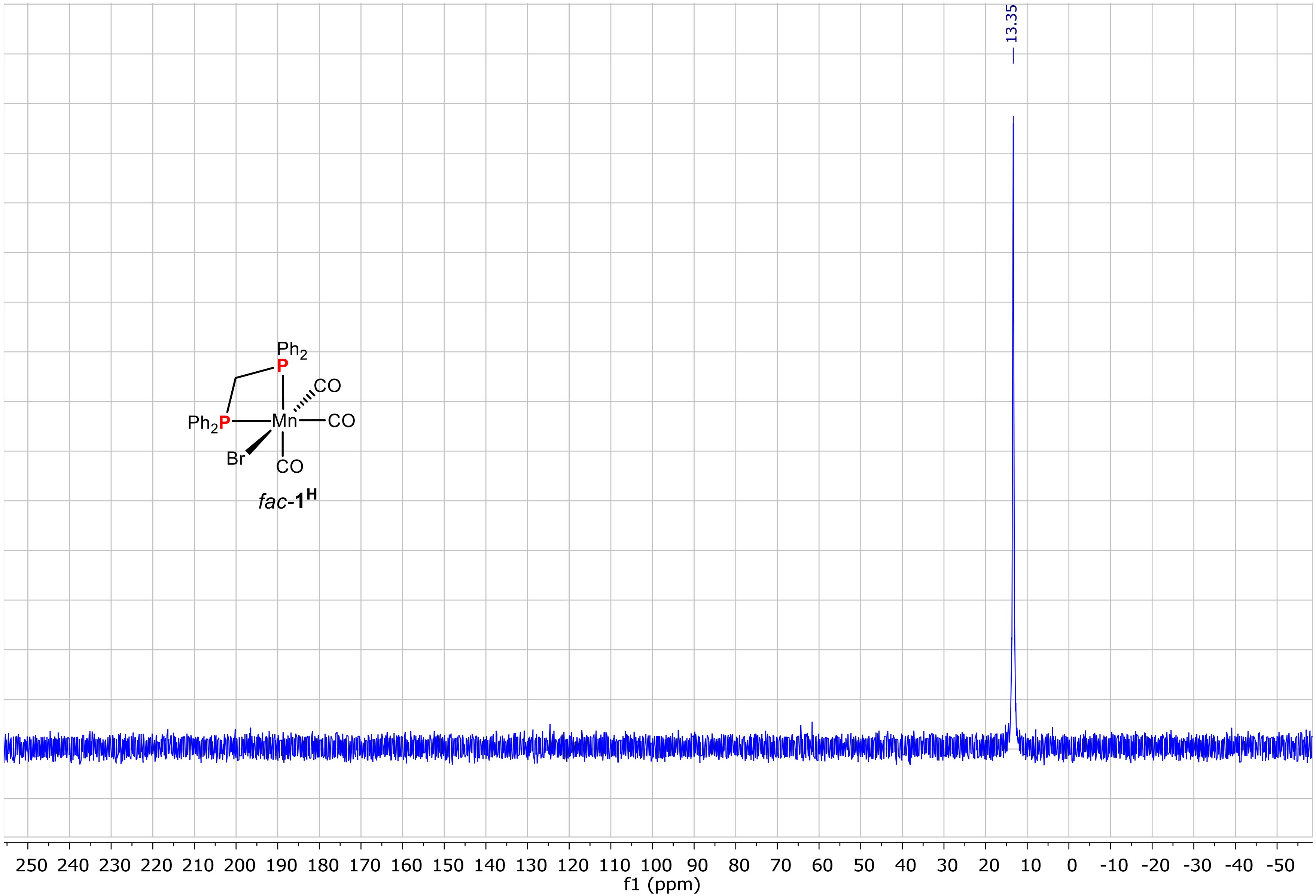


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of complex *fac*-$\mathbf{1^H}$ (100.6 MHz, C_6D_6, 25 °C)

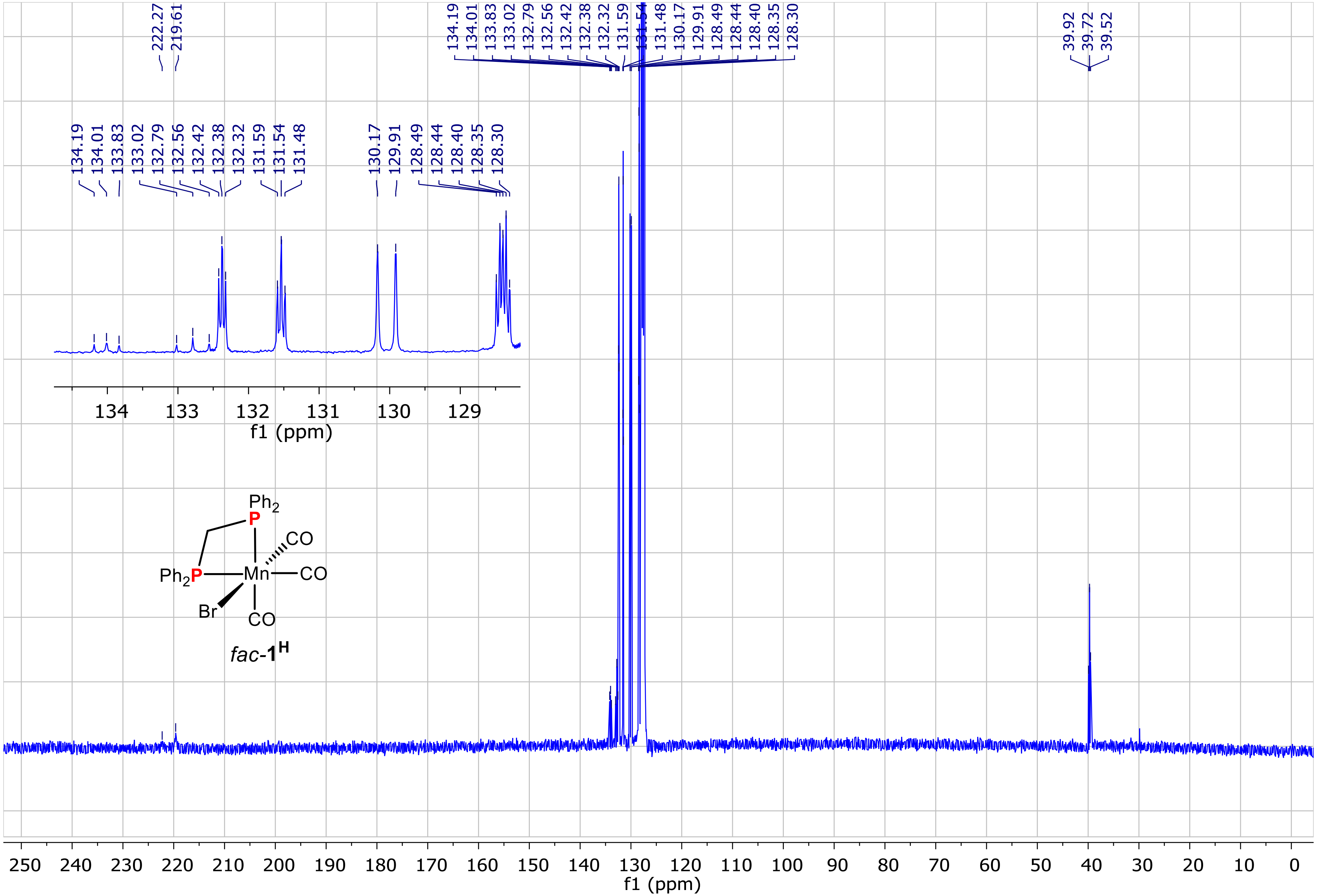


Figure S4. ^{1}H NMR spectrum of complex *fac*-**1**$^{\mathbf{Me}}$ (400.1 MHz, $CDCl_3$, 25 °C), traces of THF are marked with asterisk

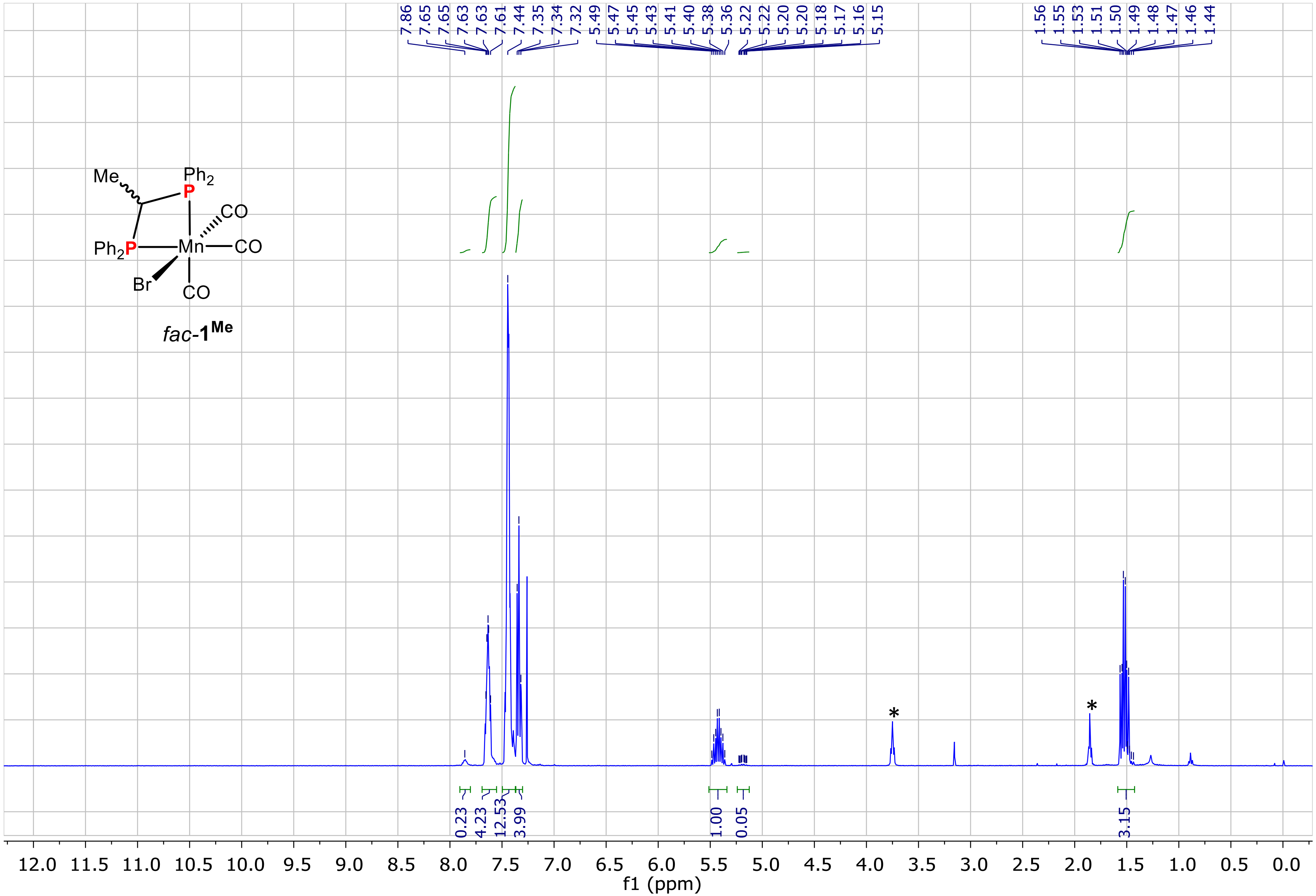


Figure S5. $^1H\{^{31}P\}$ NMR spectrum of complex *fac*-**1**$^{\mathbf{Me}}$ (400.1 MHz, $CDCl_3$, 25 °C), traces of THF are marked with asterisk

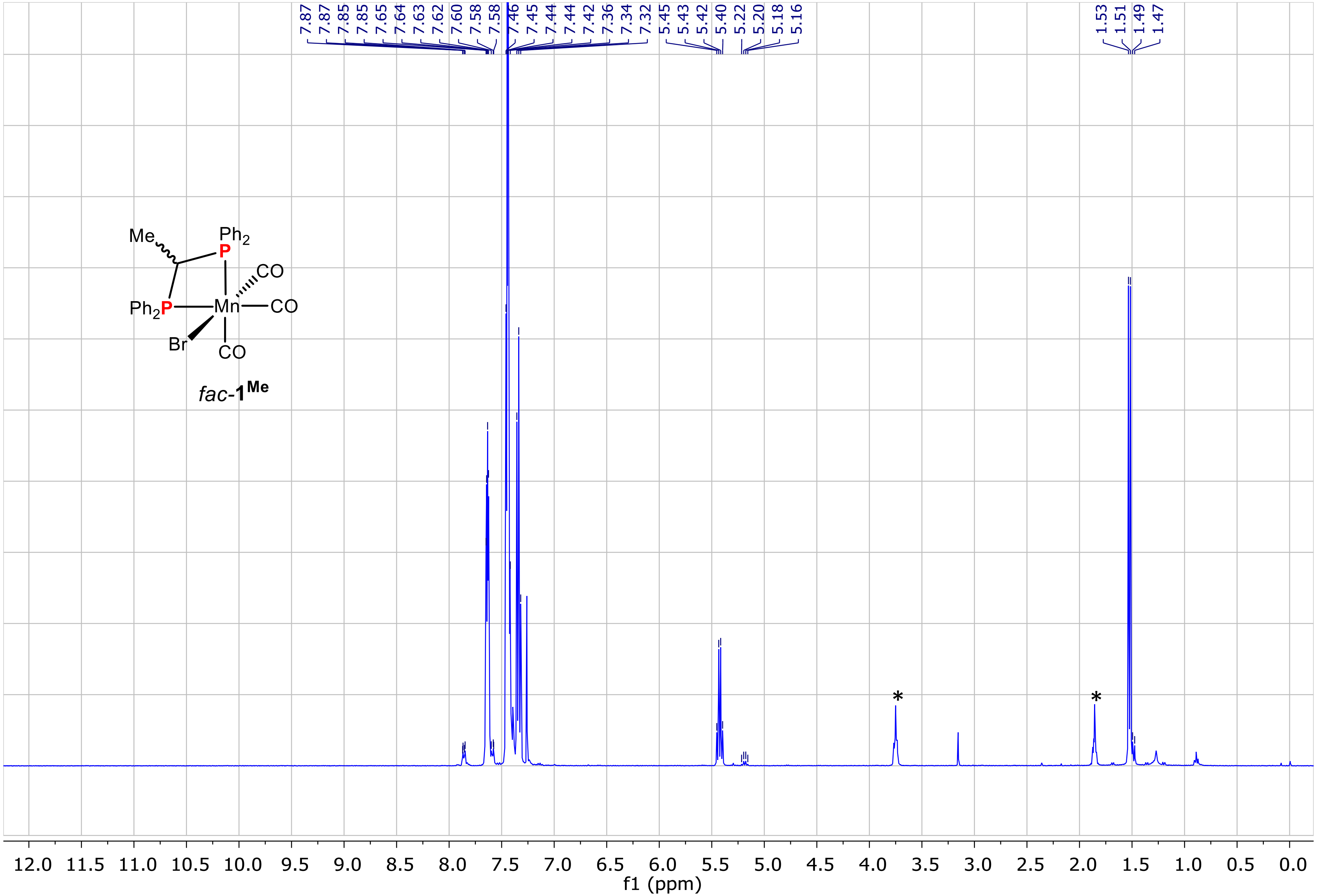


Figure S6. $^{31}P\{^1H\}$ NMR spectrum of complex *fac*-**1^{Me}** (162.0 MHz, $CDCl_3$, 25 °C)

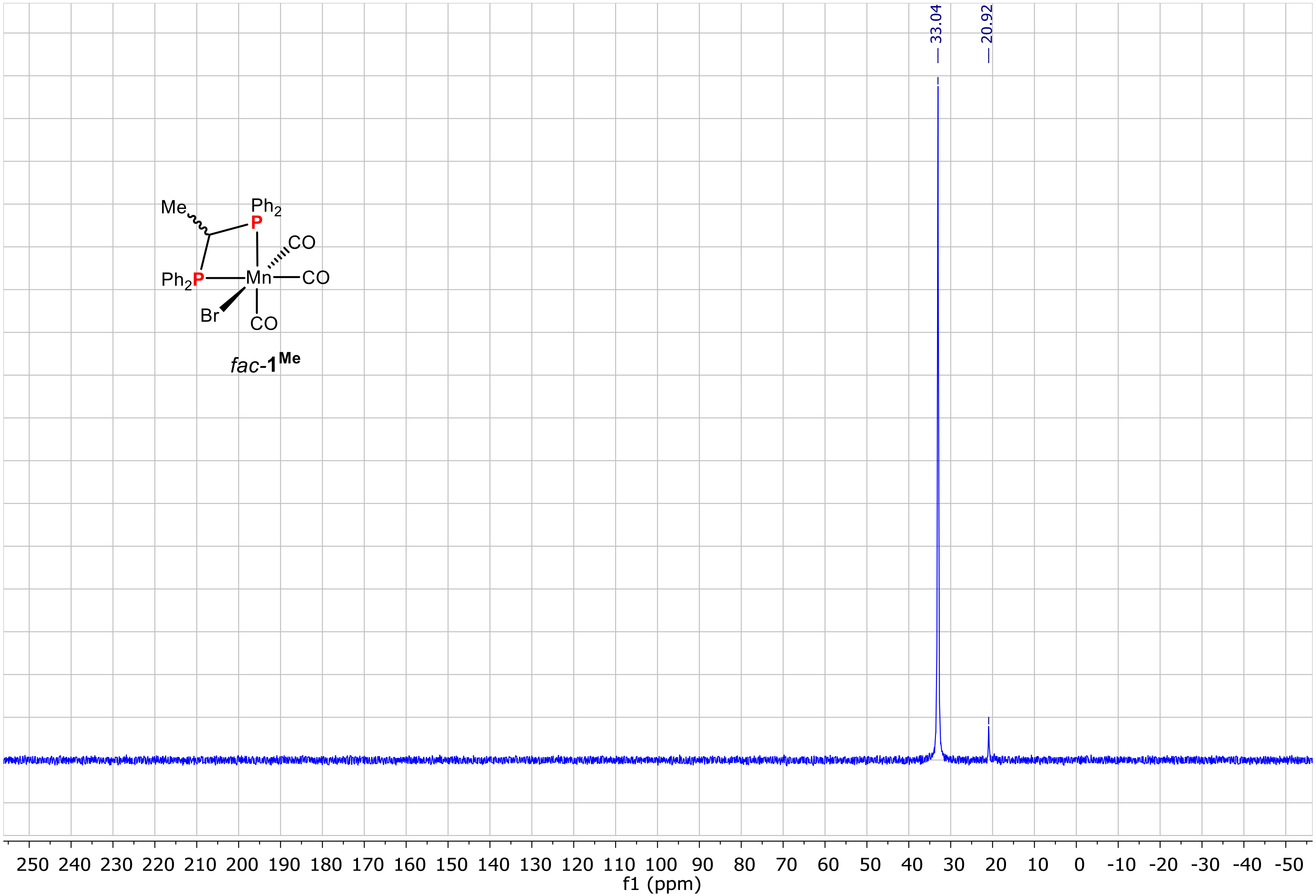


Figure S7. $^{13}C\{^1H\}$ NMR spectrum of complex *fac*-**1**$^{\mathbf{Me}}$ (100.6 MHz, C_6D_6, 25 °C)

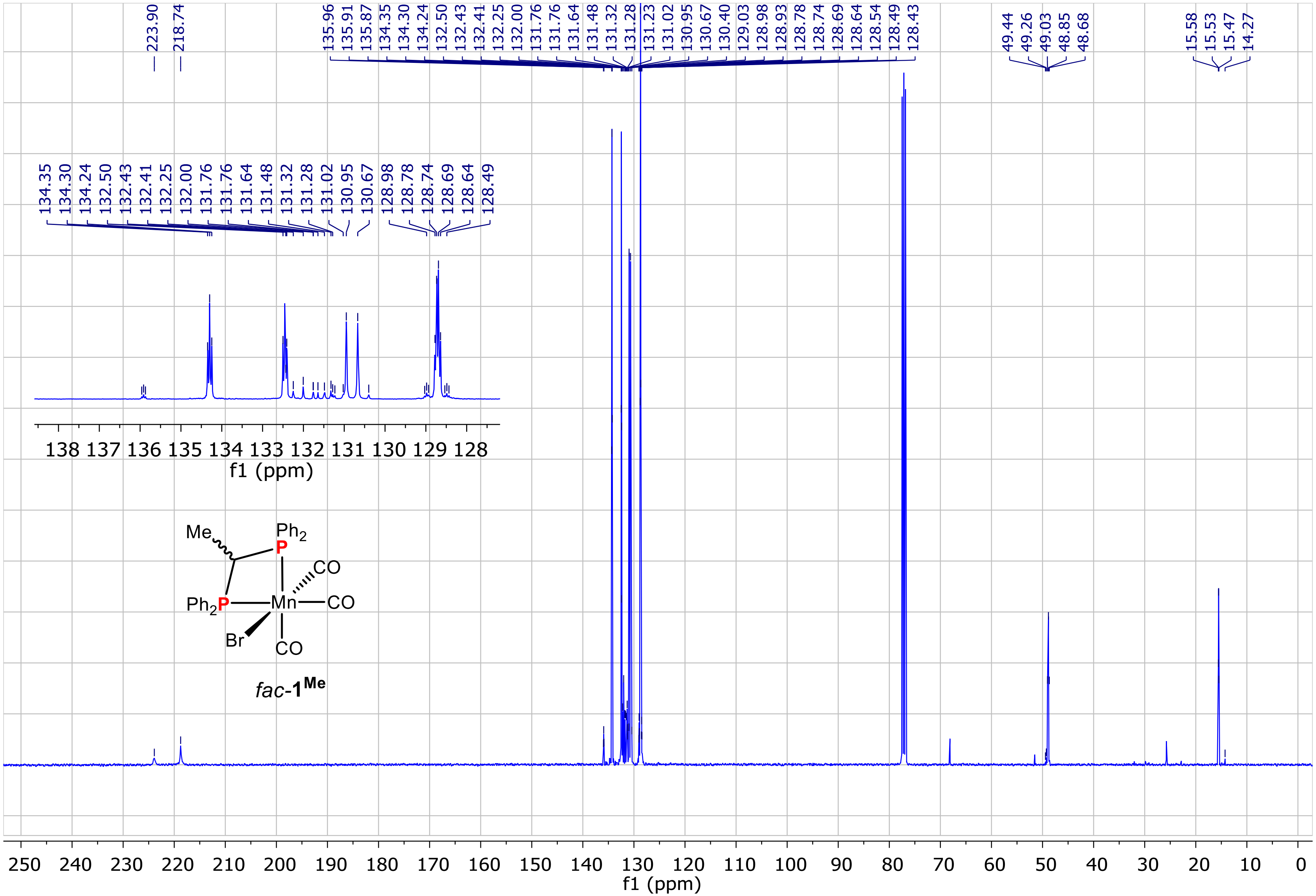


Figure S8. ^{1}H NMR spectrum of complex *fac*-**1**^{Ph} (400.1 MHz, C_6D_6, 25 °C)

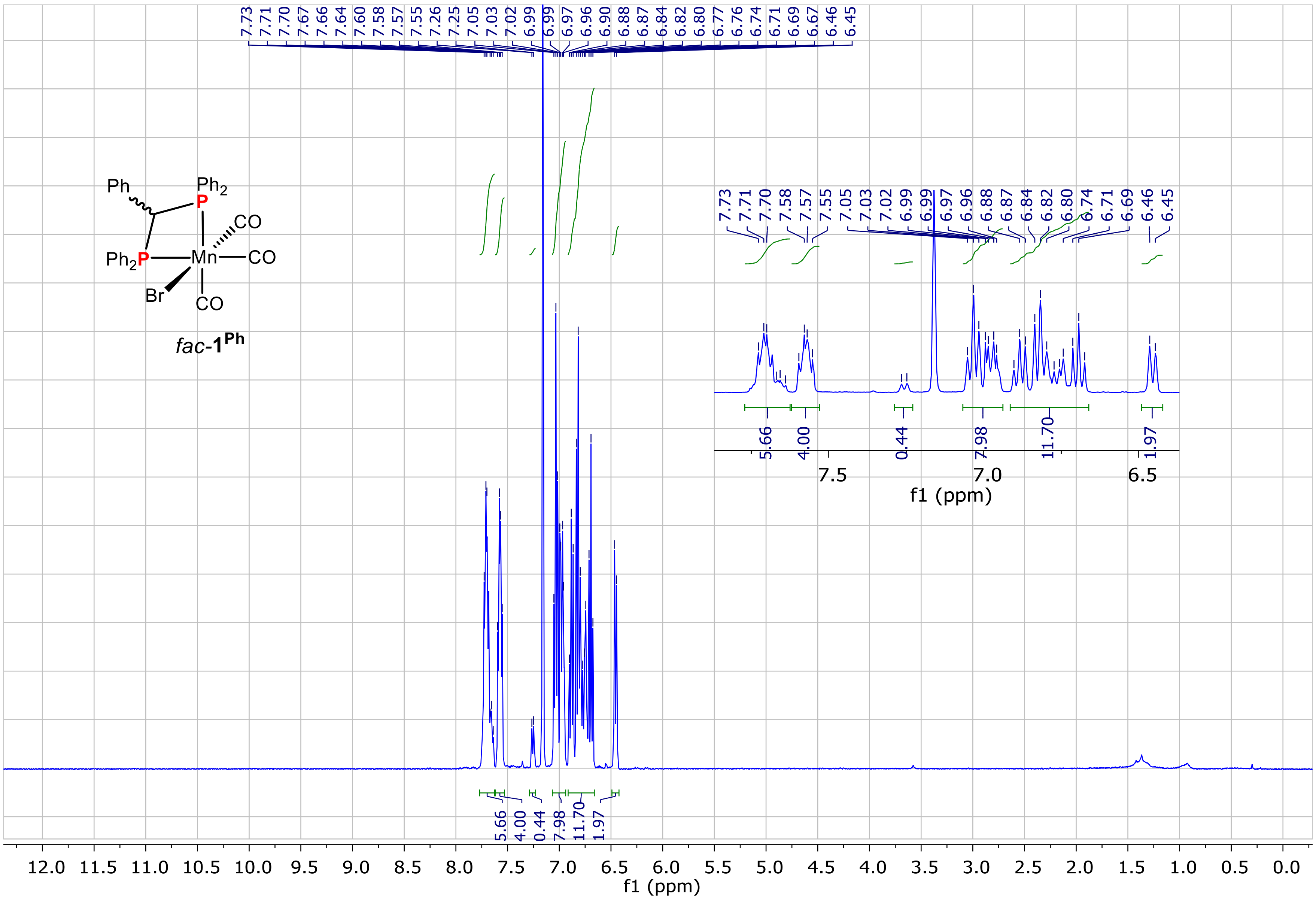


Figure S9. $^{31}P\{^{1}H\}$ NMR spectrum of complex *fac*-$\mathbf{1^{Ph}}$ (162.0 MHz, C_6D_6, 25 °C)

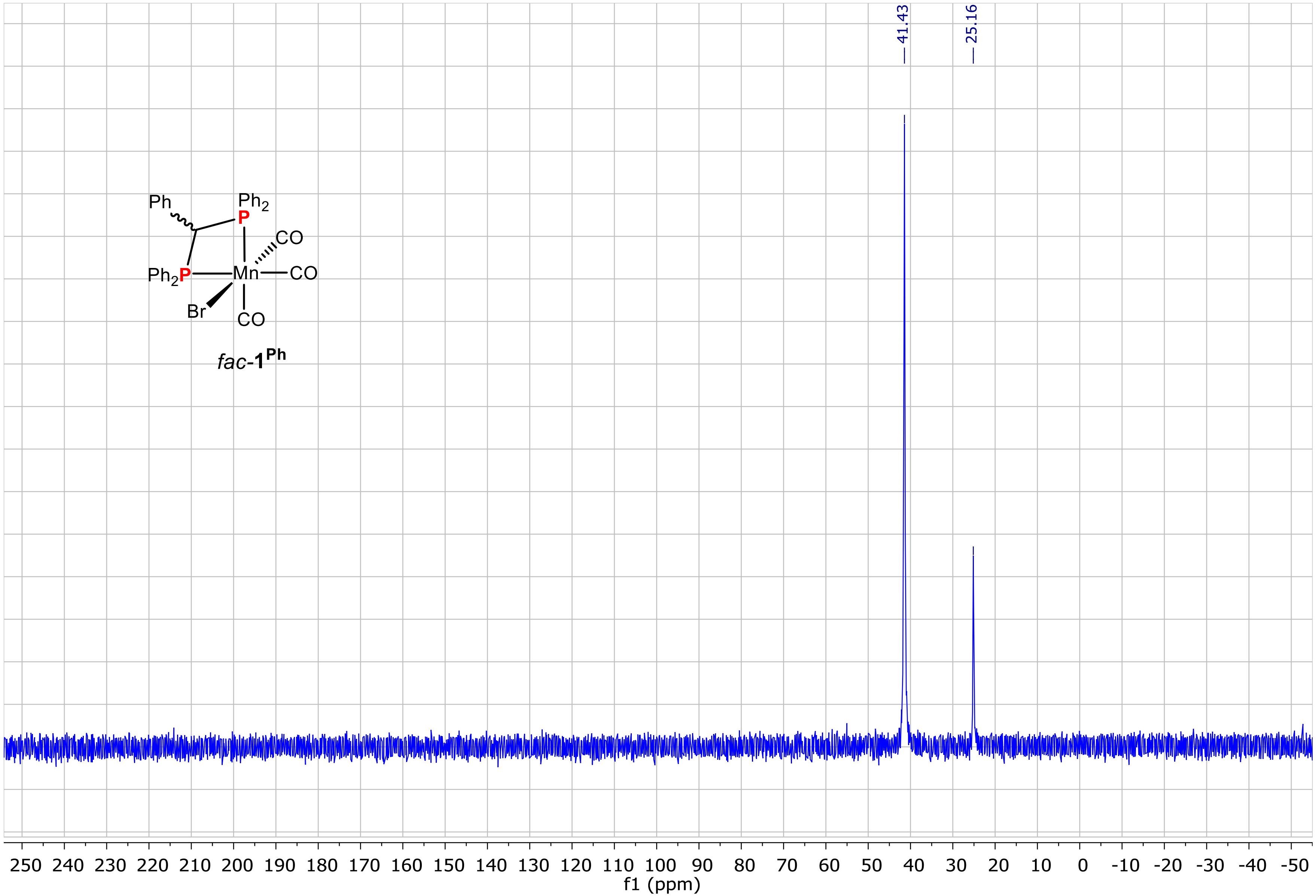


Figure S10. $^{13}C\{^1H\}$ NMR spectrum of complex *fac*-**1**^{Ph} (100.6 MHz, C_6D_6, 25 °C)

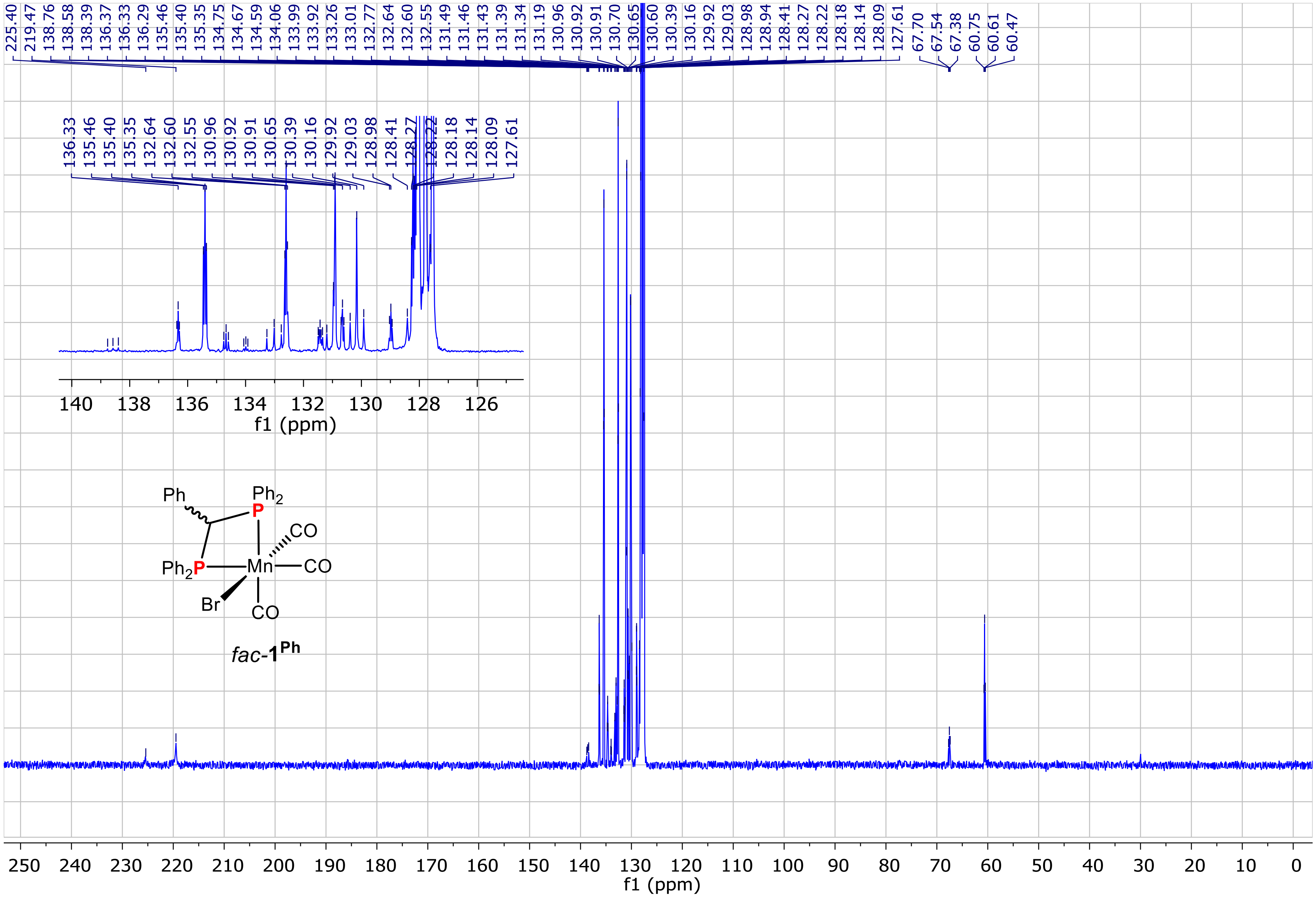


Figure S11. $^{13}C-^{1}H$ HMBC NMR spectrum of complex *fac*-**1**^{Ph} (100.6 MHz, C_6D_6, 25 °C)

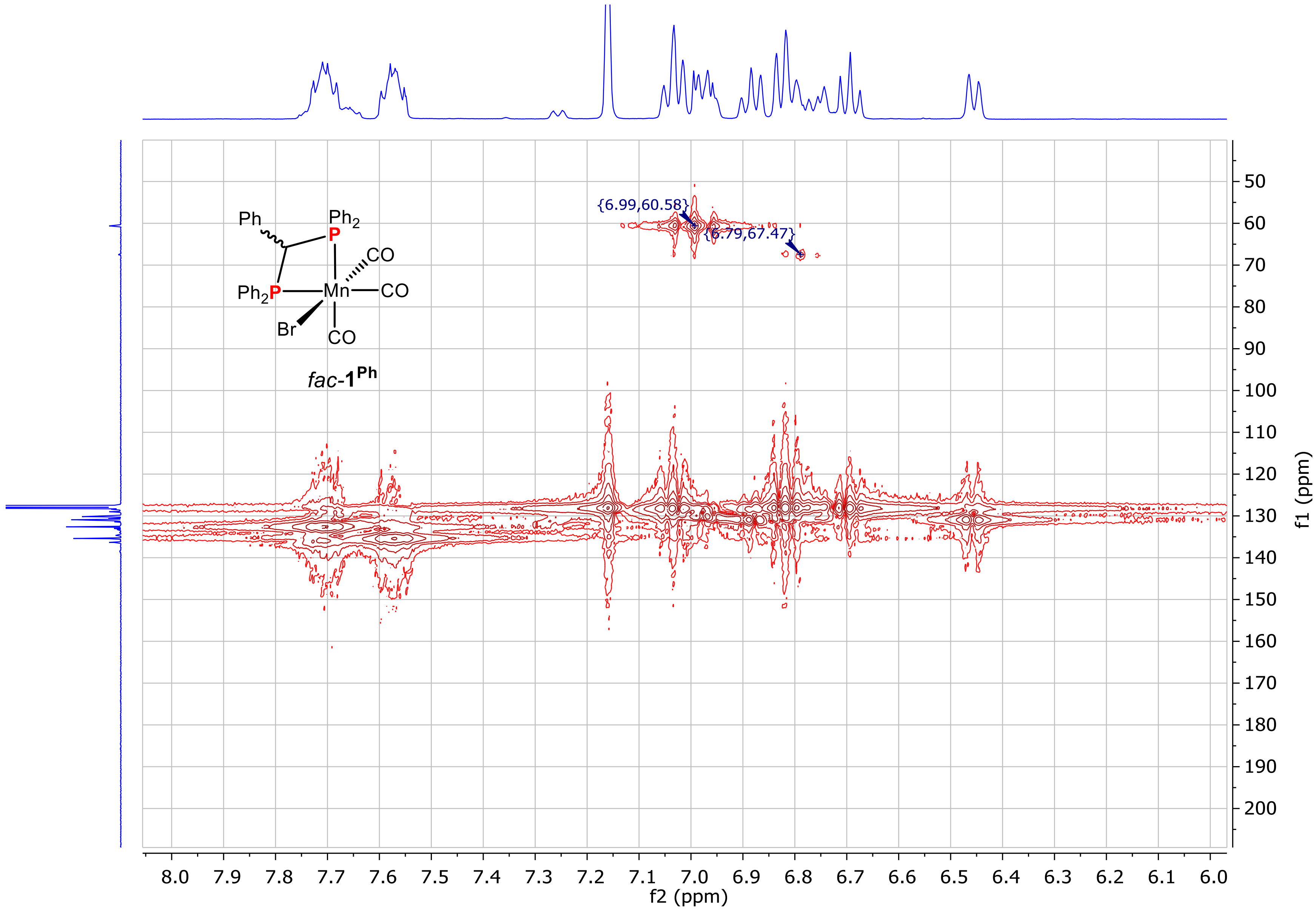


Figure S12. [1]H NMR spectrum of complex *fac*-**2^H** (400.1 MHz, C_6D_6, 25 °C), signals of residual toluene and HMDS are marked with asterisk

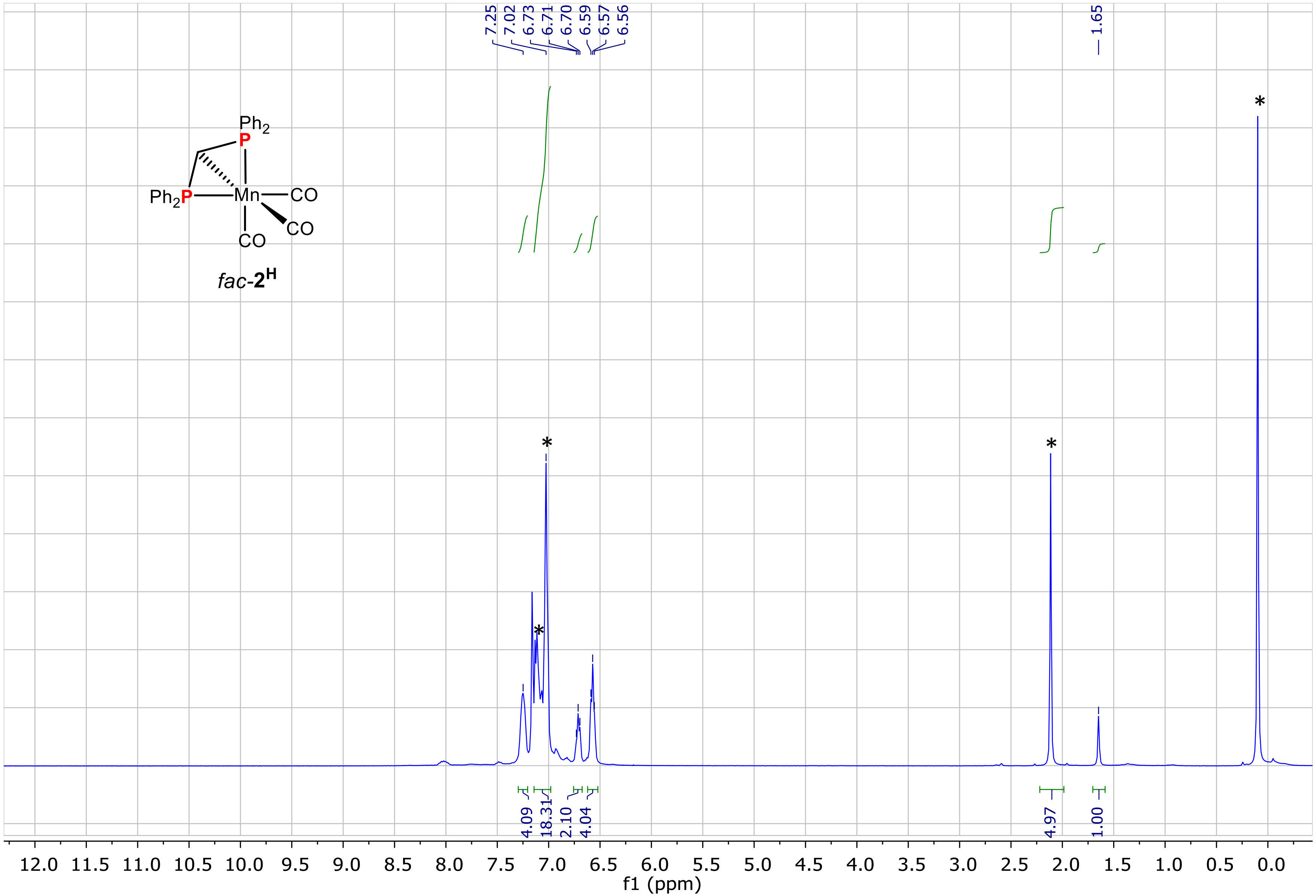


Figure S13. $^{31}P\{^{1}H\}$ NMR spectrum of complex *fac*-**2^{H}** (162.0 MHz, C_6D_6, 25 °C)

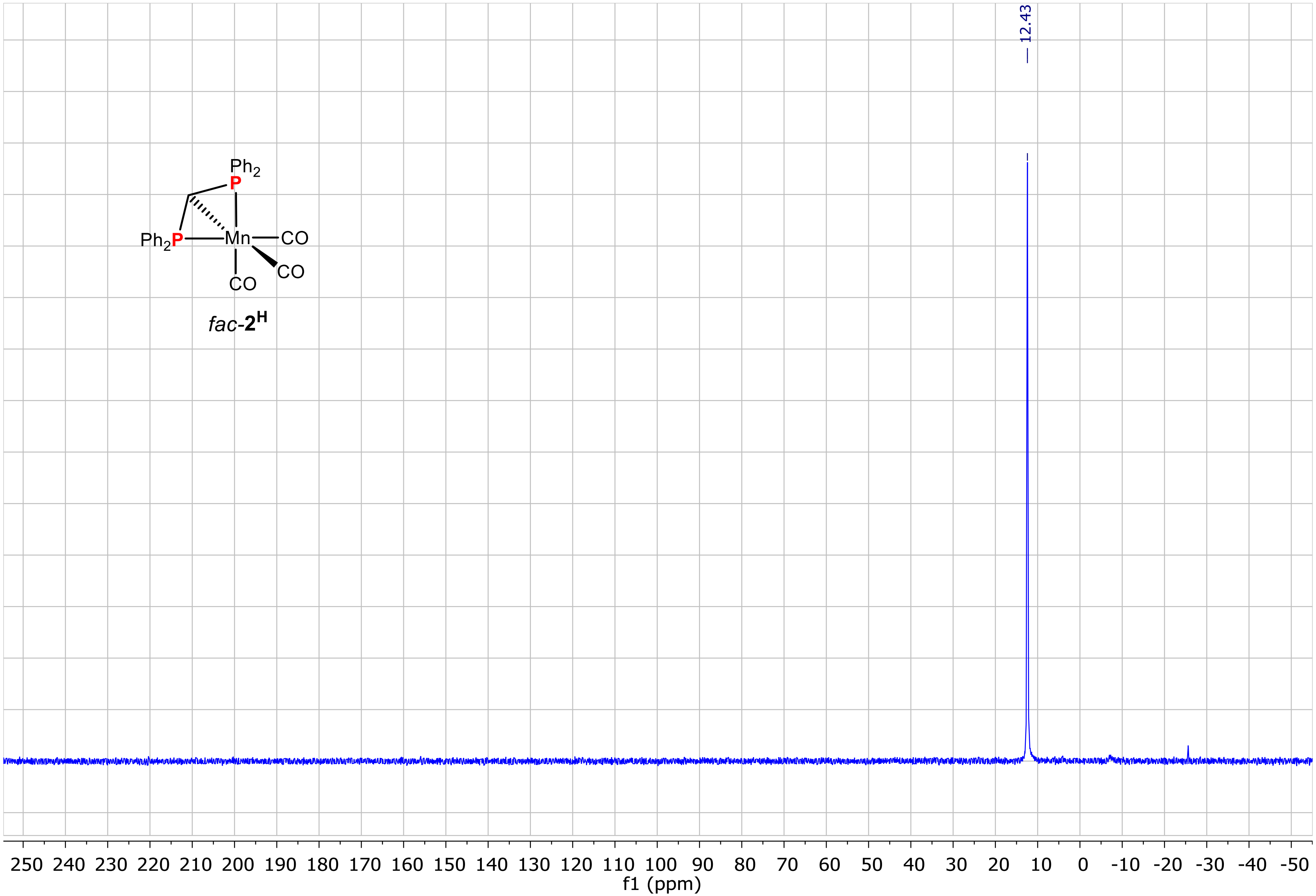


Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum of complex *fac*-**2^H** (100.6 MHz, C_6D_6, 25 °C), signals of residual toluene and HMDS are marked with asterisk

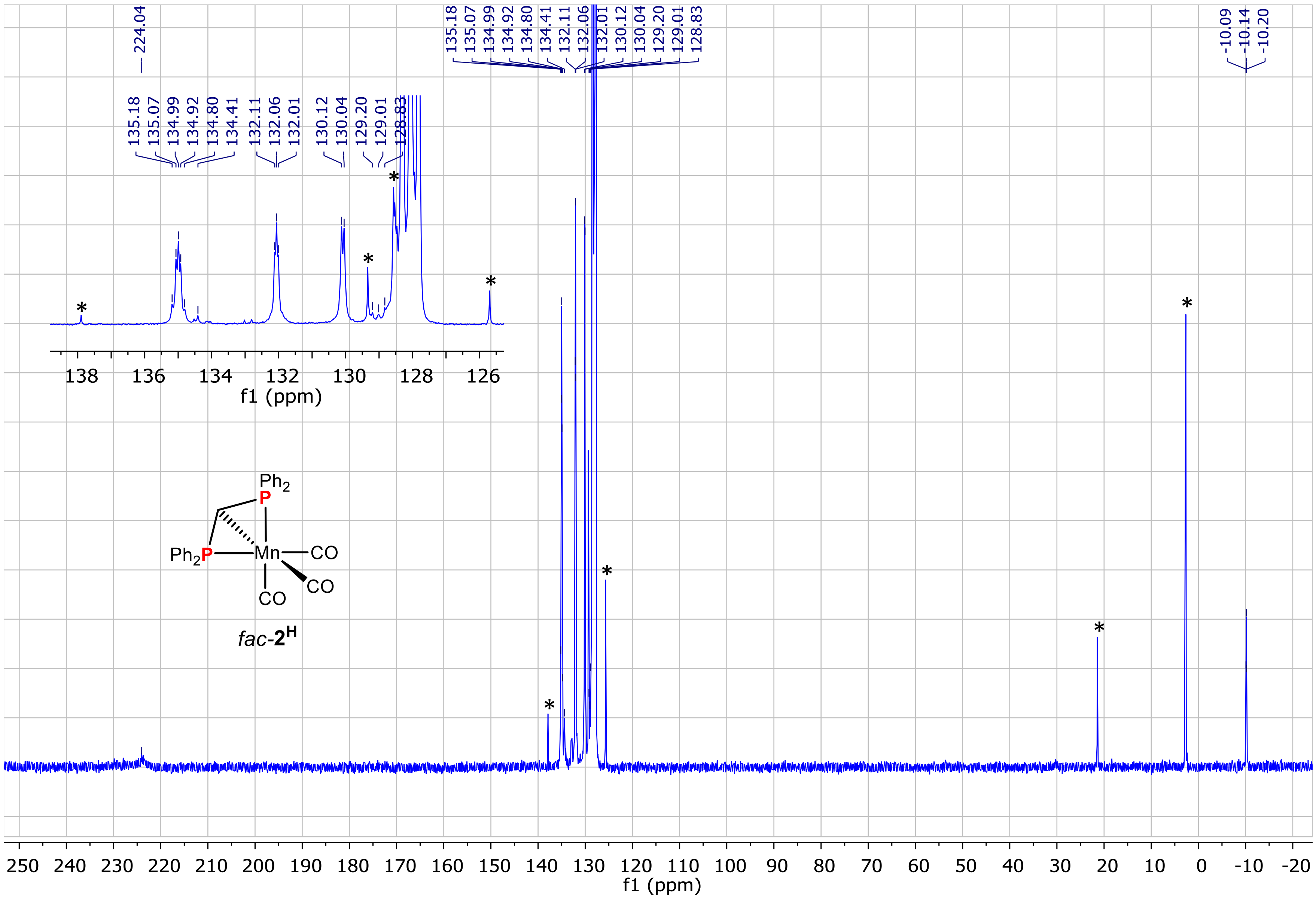


Figure S15. ^1H NMR spectrum (400.1 MHz, C_6D_6, 25 °C) of the crude product obtained by the reaction of complex *fac*-$\mathbf{2^H}$ with H_2 (1 atm. at 25 °C)

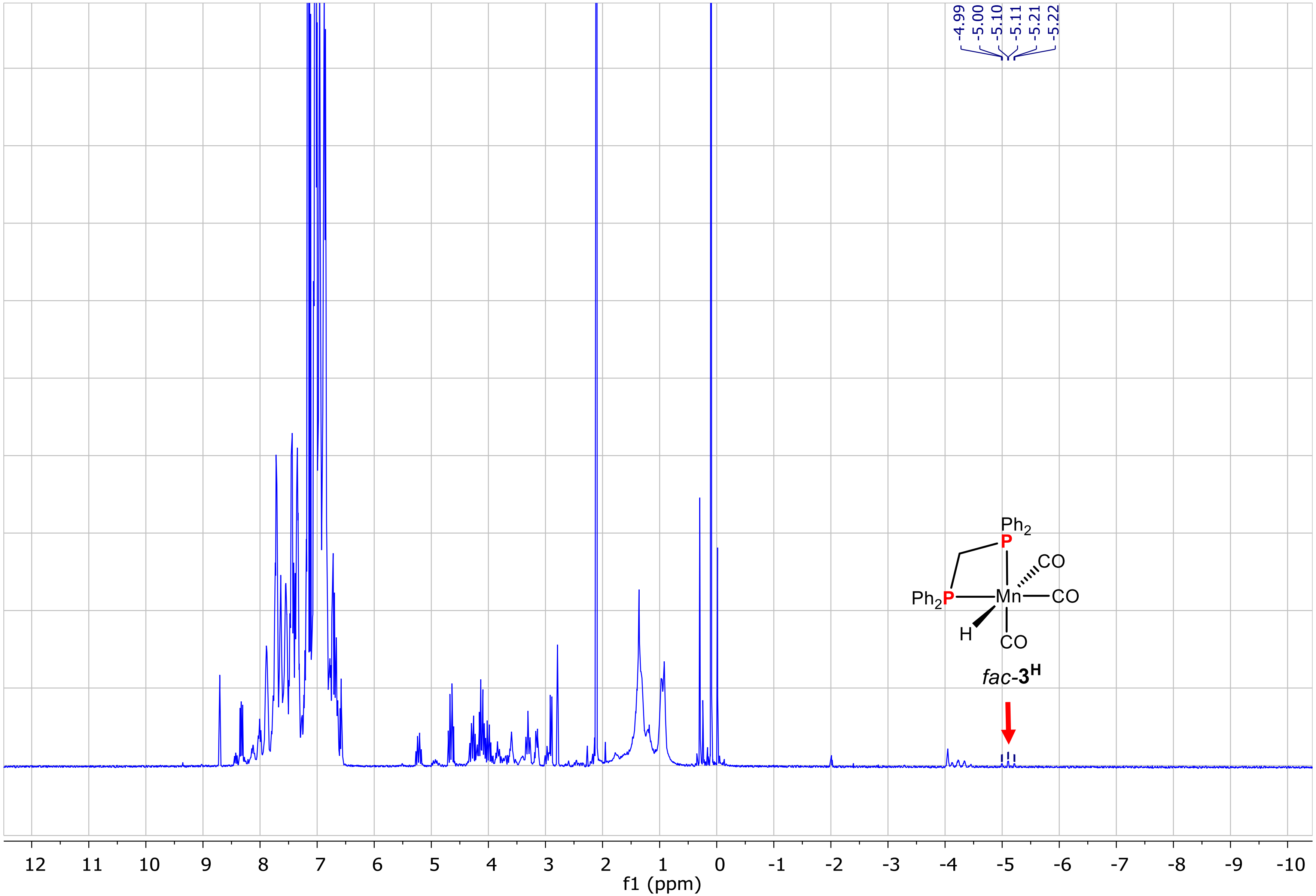


Figure S16. $^{31}P\{^{1}H\}$ NMR spectrum (162.0 MHz, C_6D_6, 25 °C) of the crude product obtained by the reaction of complex *fac*-$\mathbf{2^H}$ with H_2 (1 atm. at 25 °C)

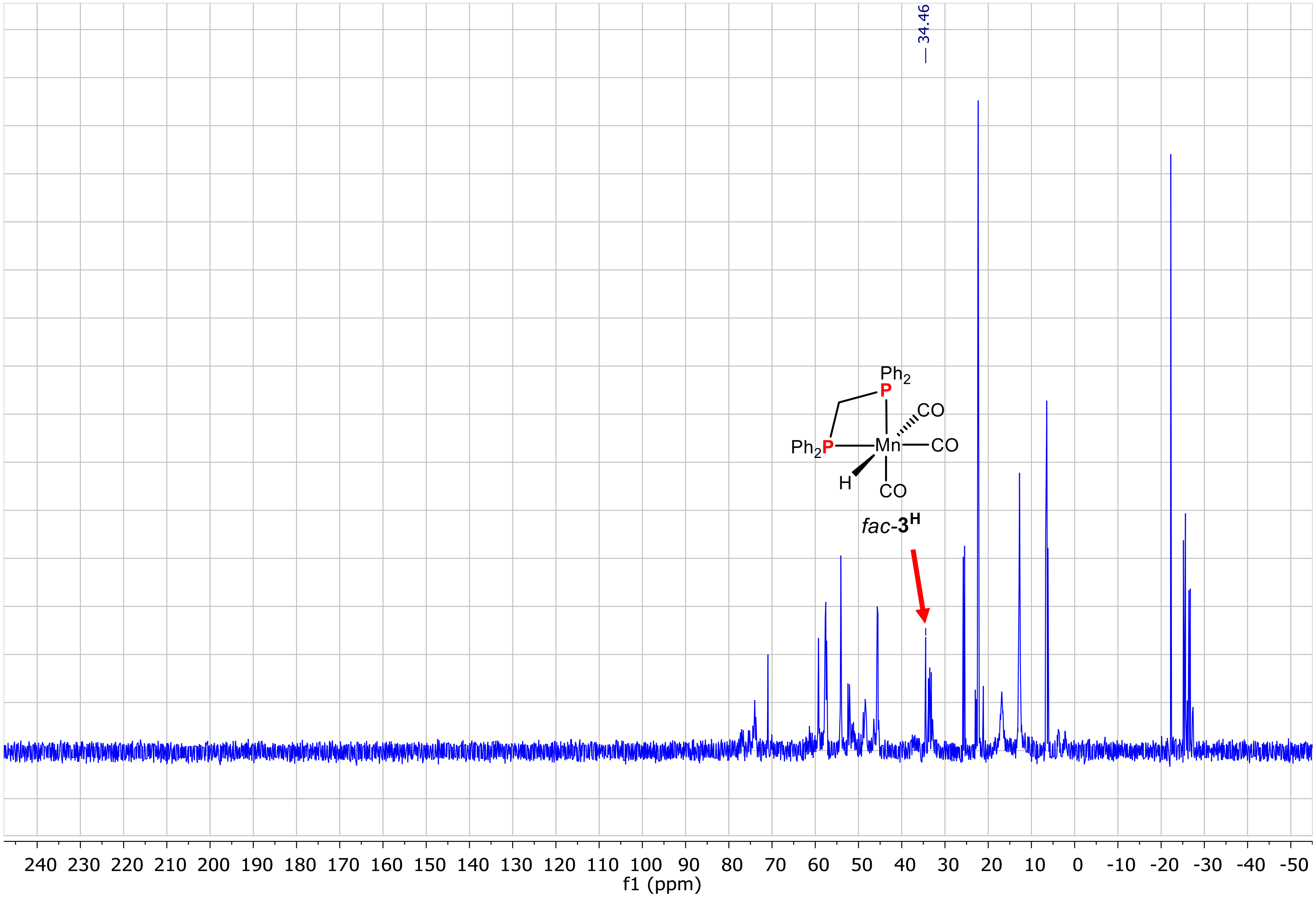


Figure S17. [1]H NMR spectrum (400.1 MHz, C_6D_6, 25 °C) of the crude product obtained by the reaction of complex *fac*-**2**$^{\mathbf{H}}$ with H_2 (50 atm. at 50 °C)

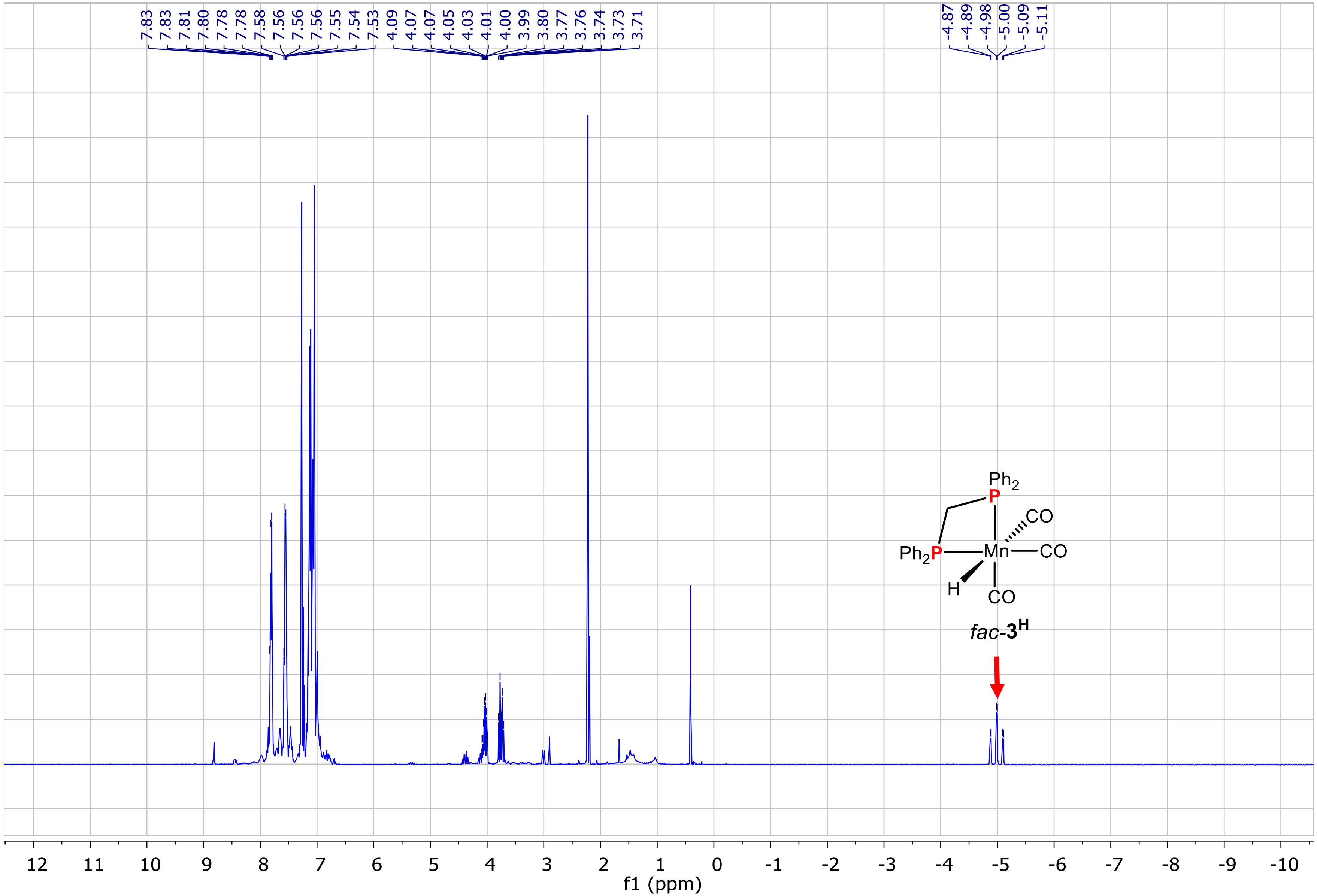


Figure S18. $^{31}P\{^{1}H\}$ NMR spectrum (162.0 MHz, C_6D_6, 25 °C) of the crude product obtained by the reaction of complex *fac*-**2^H** with H_2 (50 atm. at 50 °C)

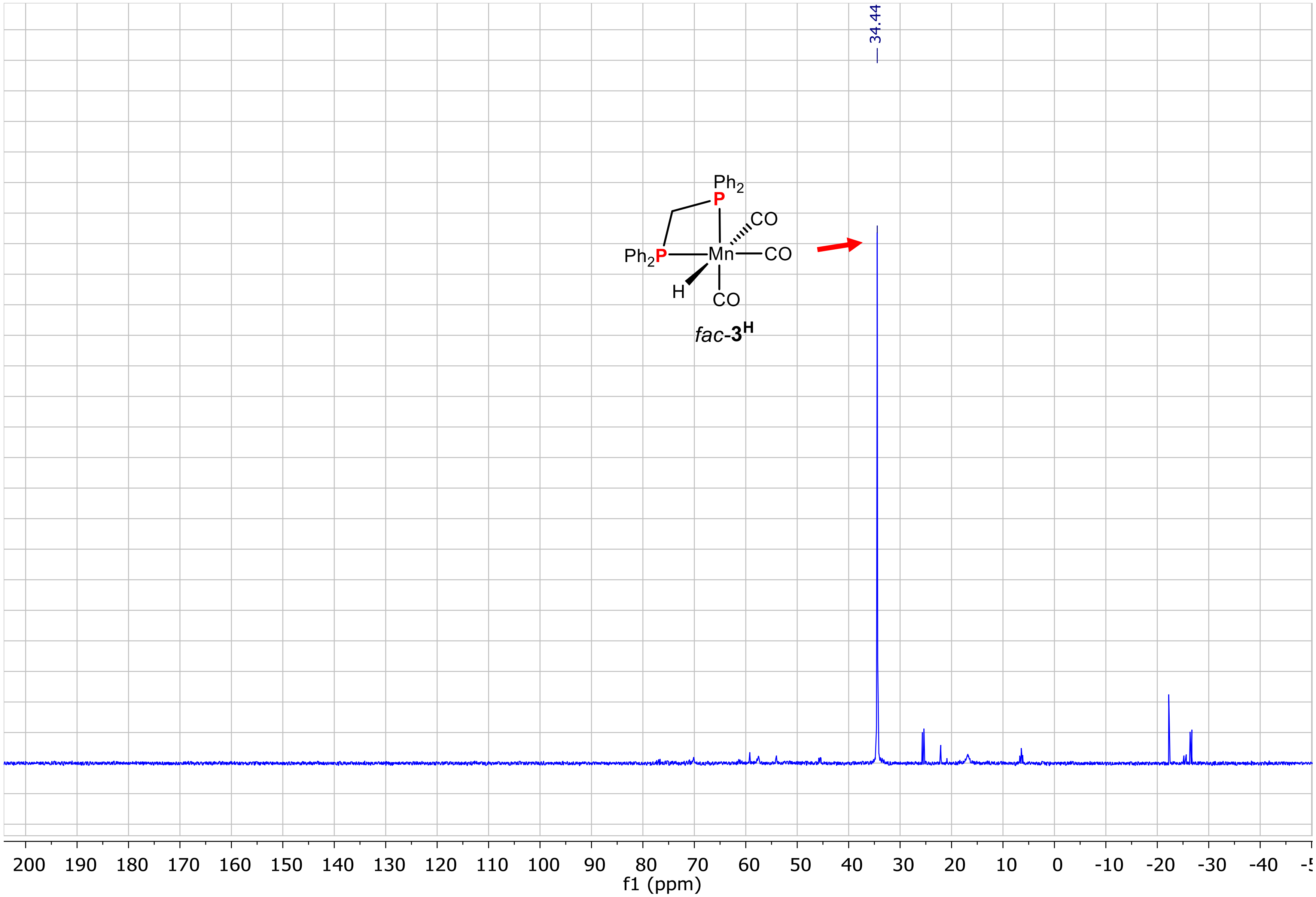


Figure S19. ^{1}H NMR spectrum of complex *fac*-$\mathbf{3^H}$ (400.1 MHz, C_6D_6, 25 °C)

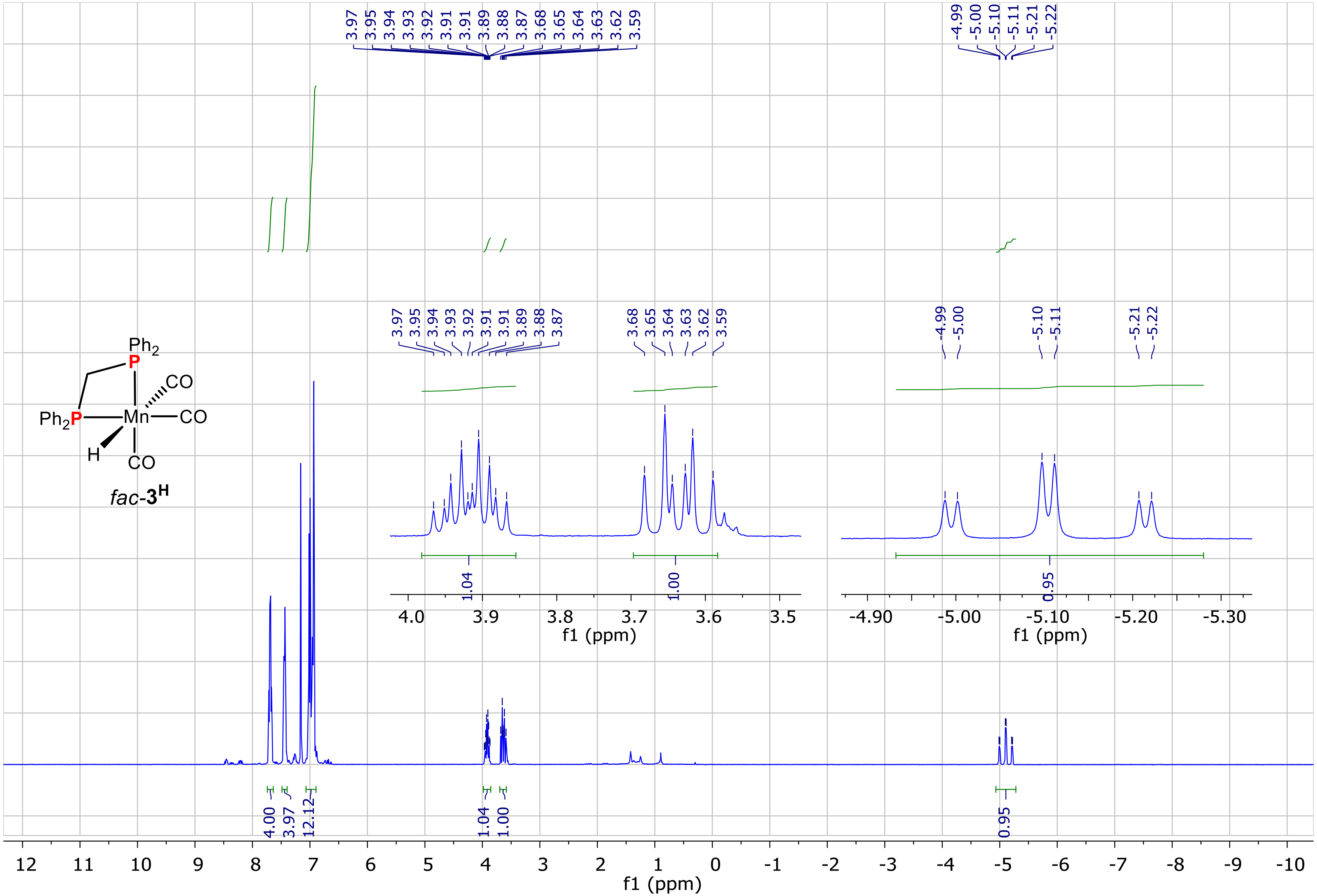


Figure S20. $^{31}P\{^{1}H\}$ NMR spectrum of complex *fac*-**3^{H}** (162.0 MHz, C_6D_6, 25 °C)

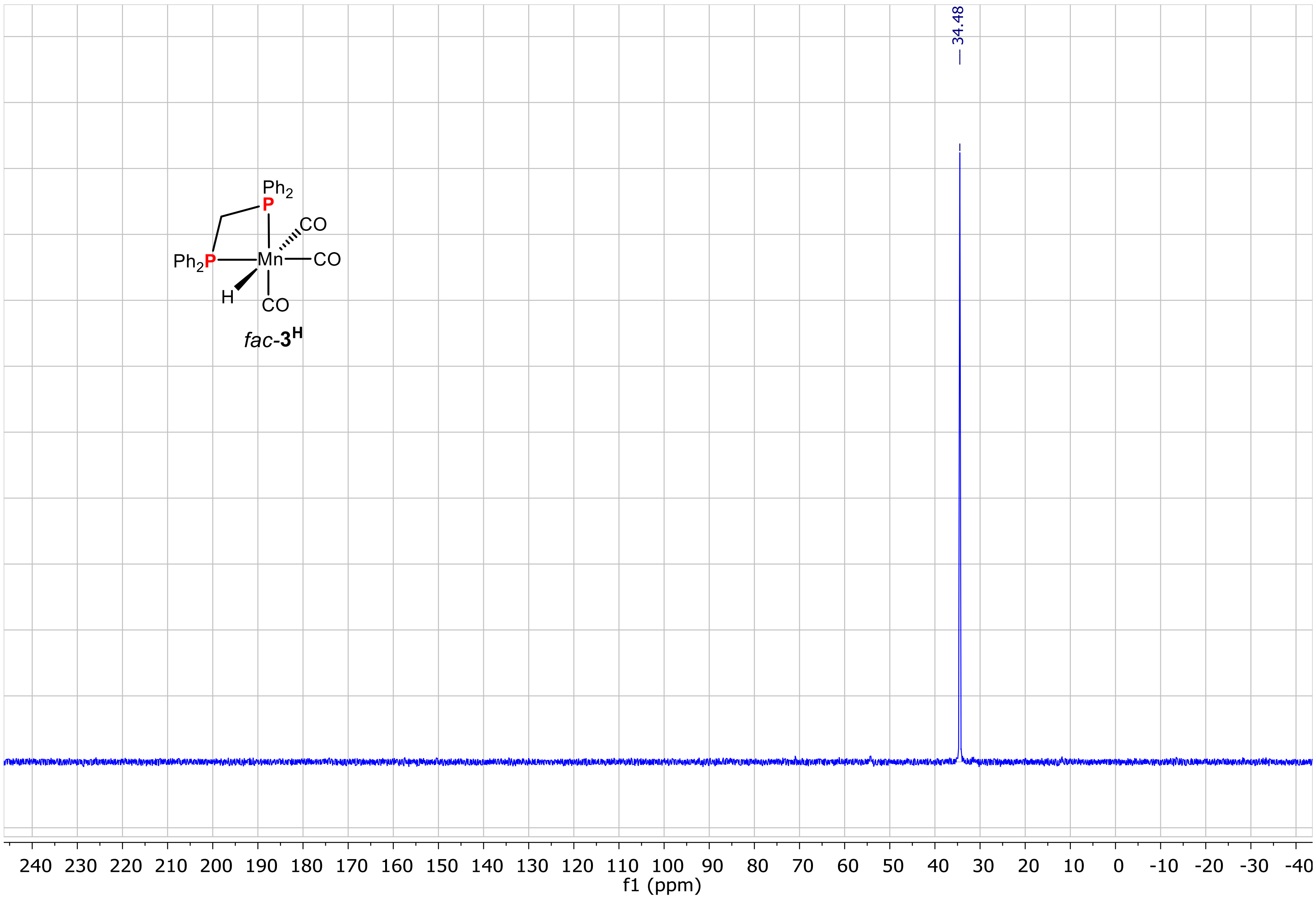


Figure S21. ^{1}H 1D NOESY spectrum of complex *fac*-**3^H^** (600.1 MHz, C_6D_6, 25 °C, irradiation at −5.10 ppm)

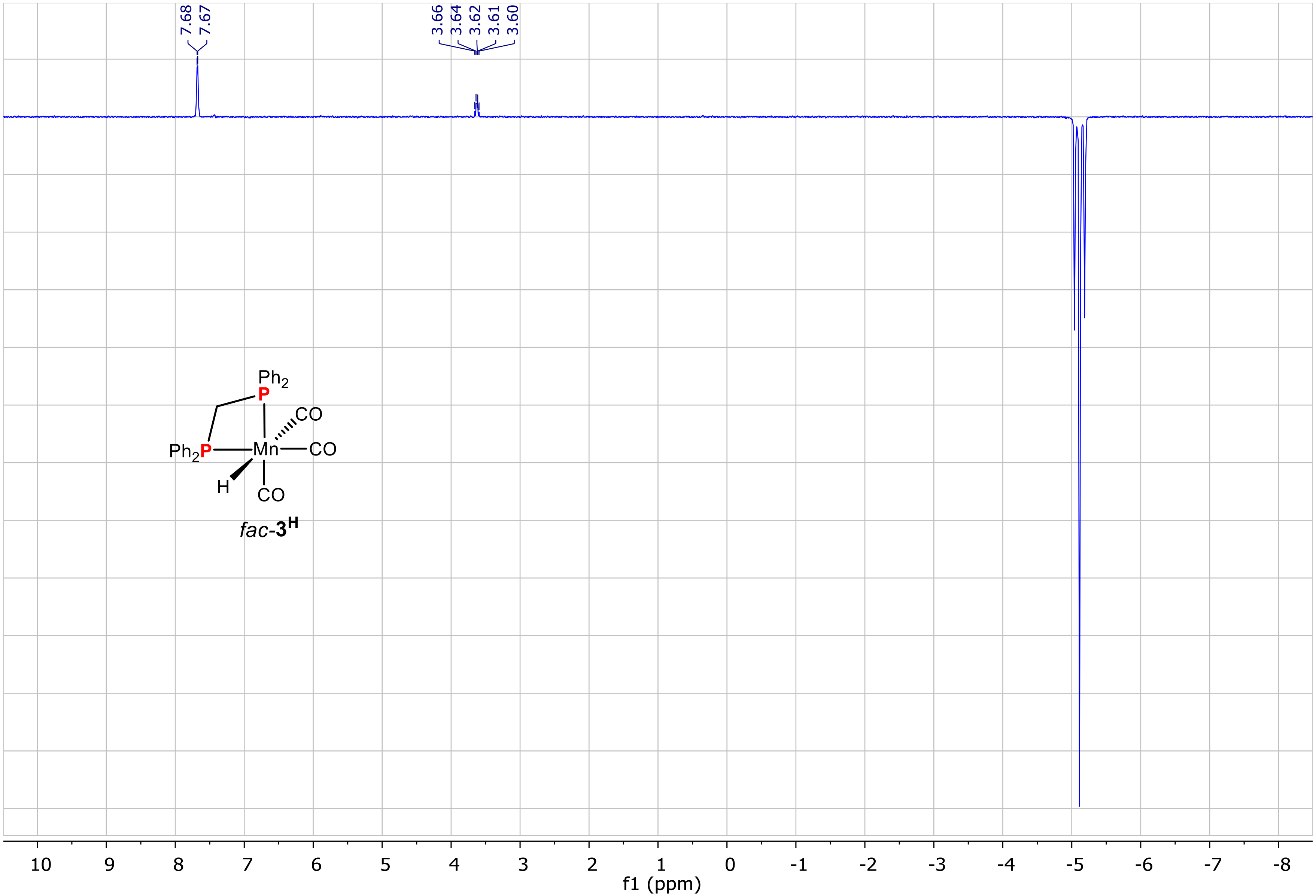


Figure S22. $^{13}C\{^{1}H\}$ NMR spectrum of complex *fac*-**3^H** (150.9 MHz, C_6D_6, 25 °C)

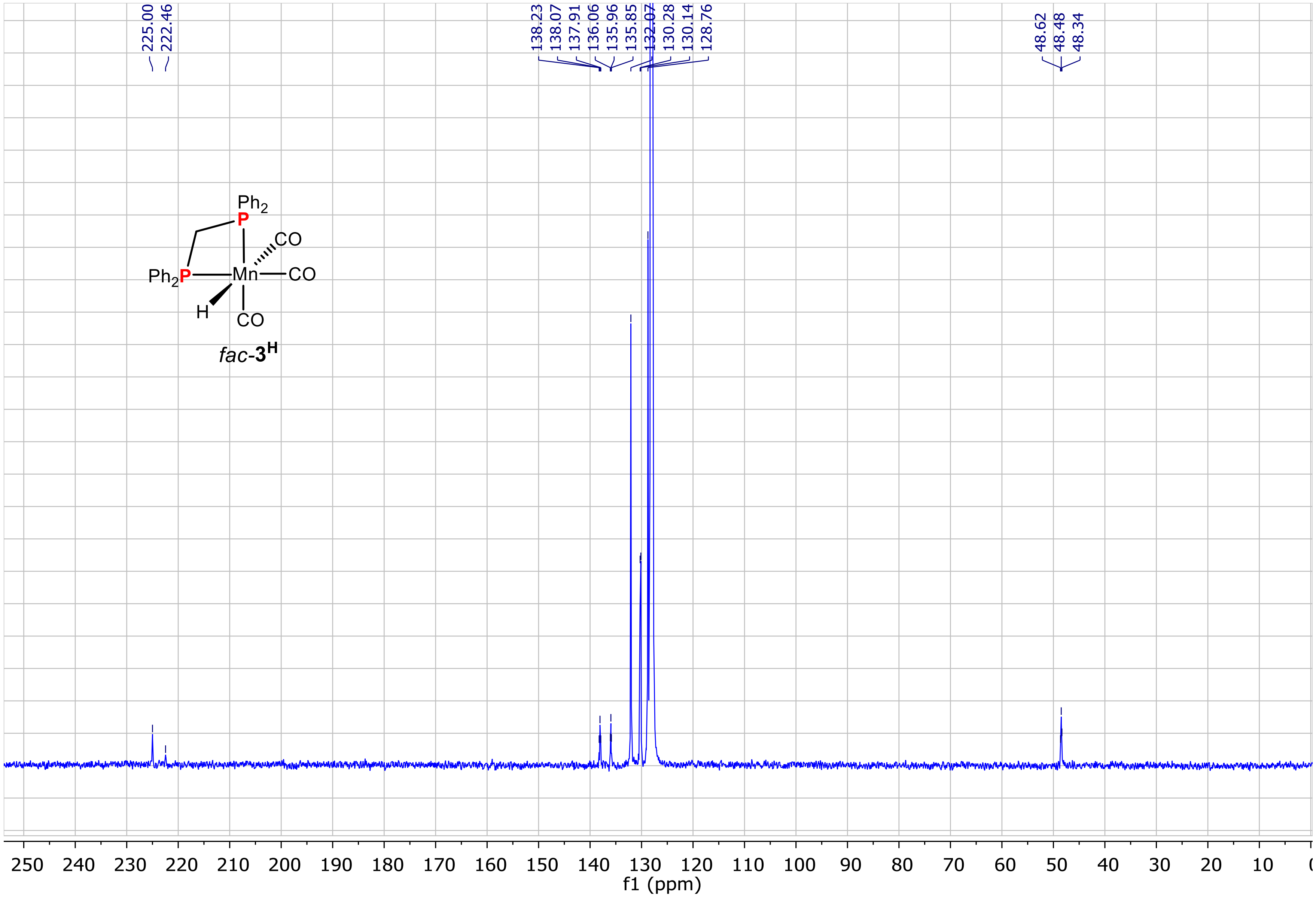


Figure S23. ^{1}H NMR spectrum of complex *fac*-$\mathbf{2^{Me}}$ (400.1 MHz, C_6D_6, 25 °C), the signals of residual toluene and HMDS are marked with asterisk

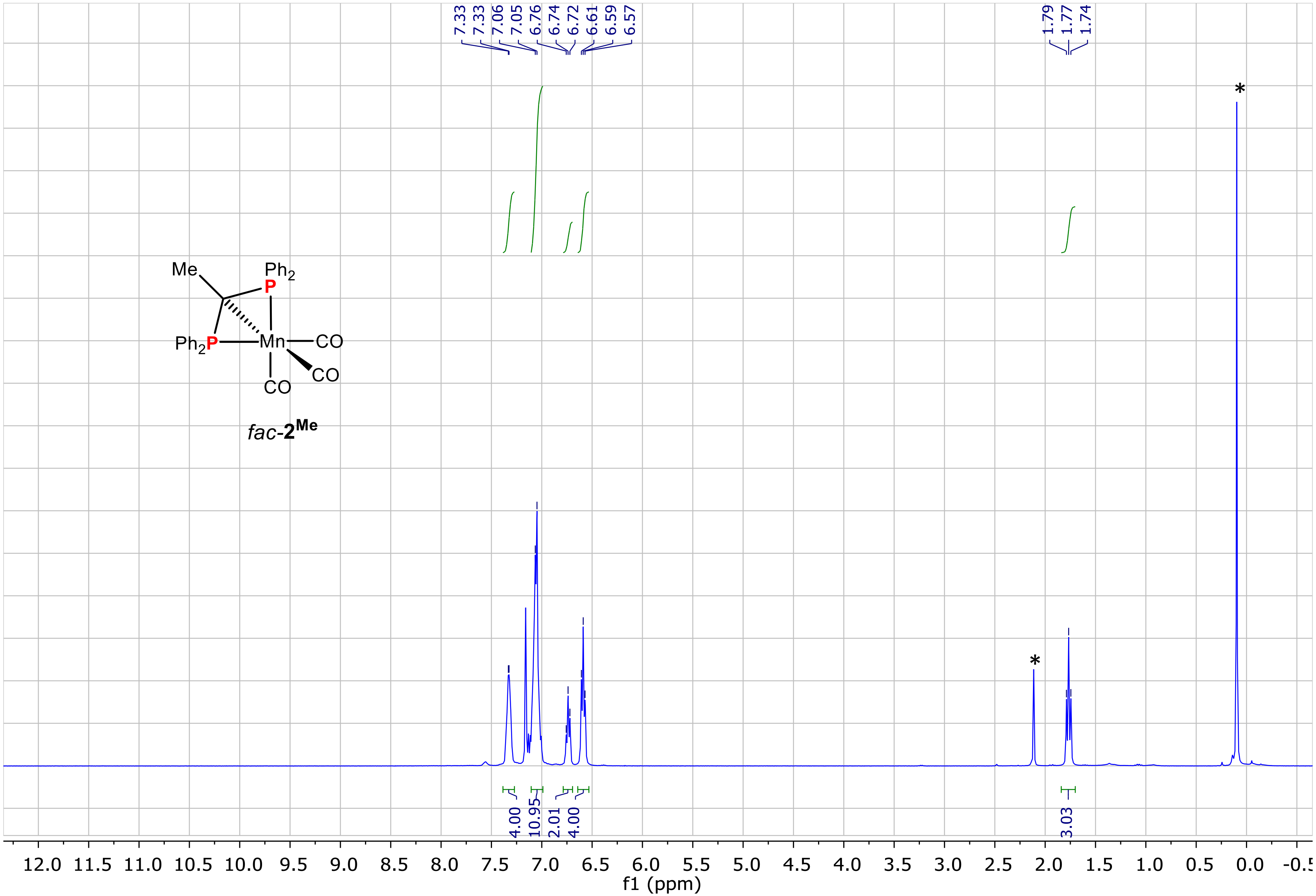


Figure S24. $^{31}P\{^{1}H\}$ NMR spectrum of complex *fac*-**2**$^{\mathbf{Me}}$ (162.0 MHz, C_6D_6, 25 °C)

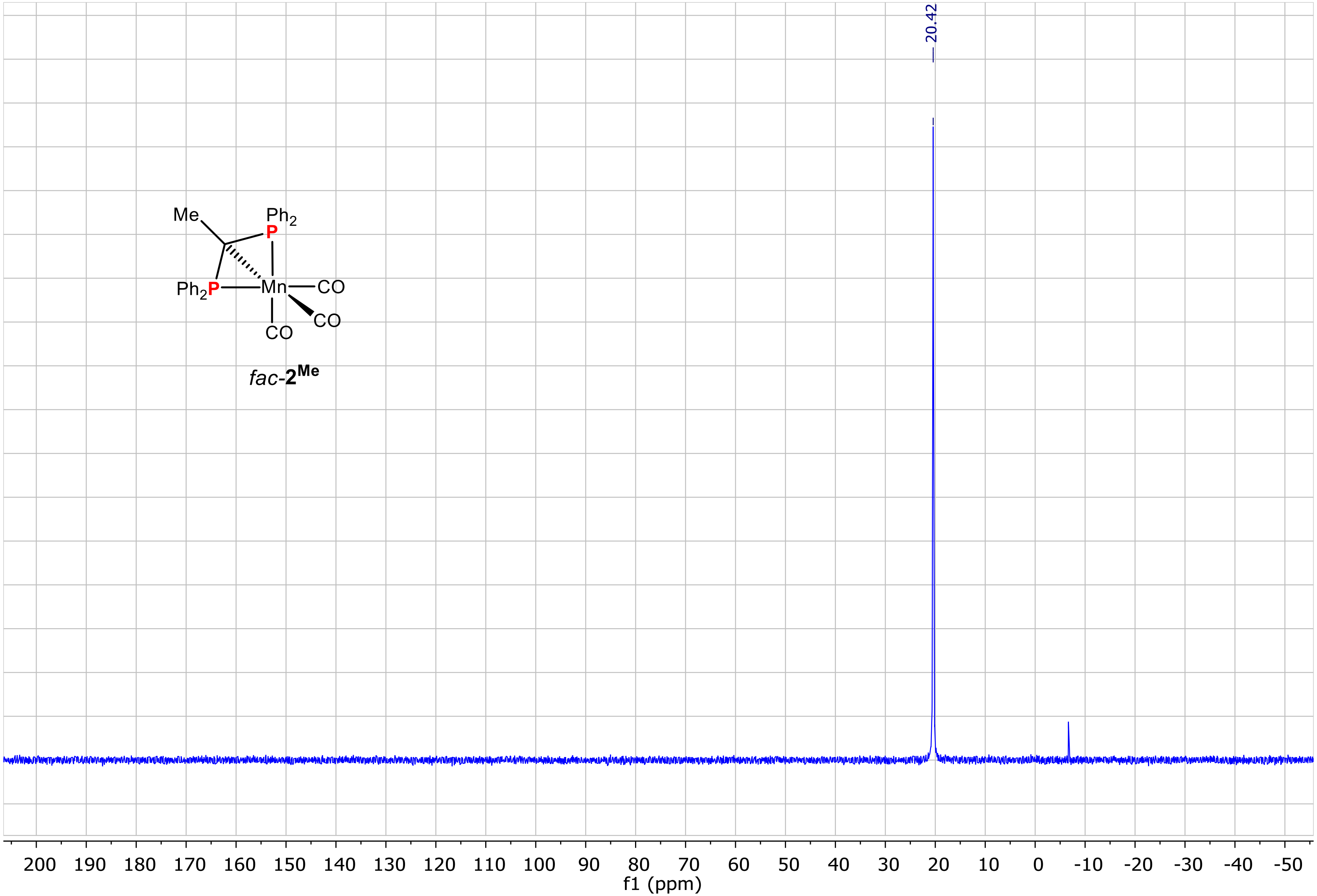


Figure S25. $^{13}C\{^{1}H\}$ NMR spectrum of complex *fac*-**2**$^{\mathbf{Me}}$ (100.6 MHz, C_6D_6, 25 °C), the signals of residual toluene and HMDS are marked with asterisk

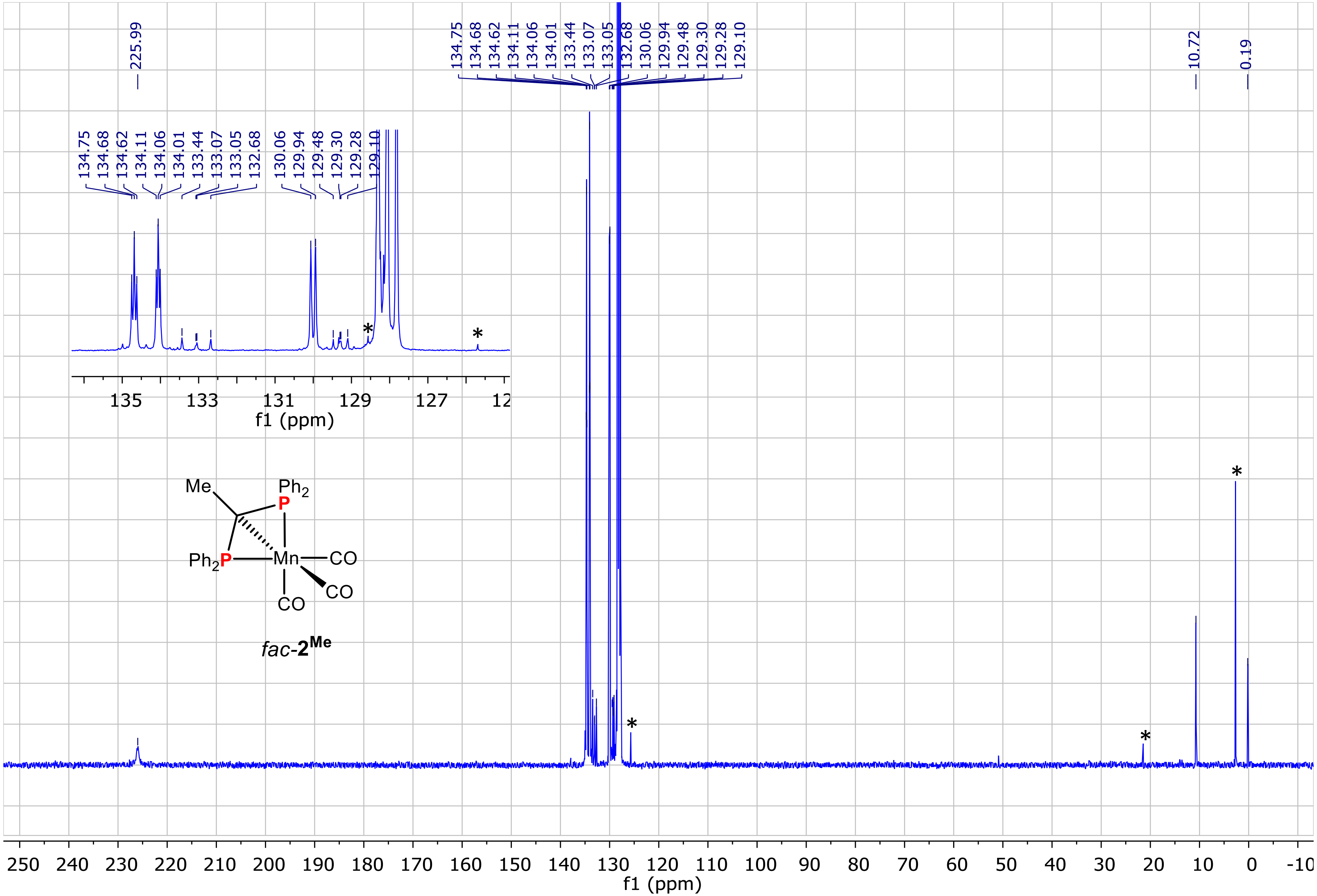


Figure S26. ^1H NMR spectrum (400.1 MHz, C_6D_6, 25 °C) of the crude product obtained by the reaction of complex *fac*-$\mathbf{2^{Me}}$ with H_2 (1 atm. at 25 °C)

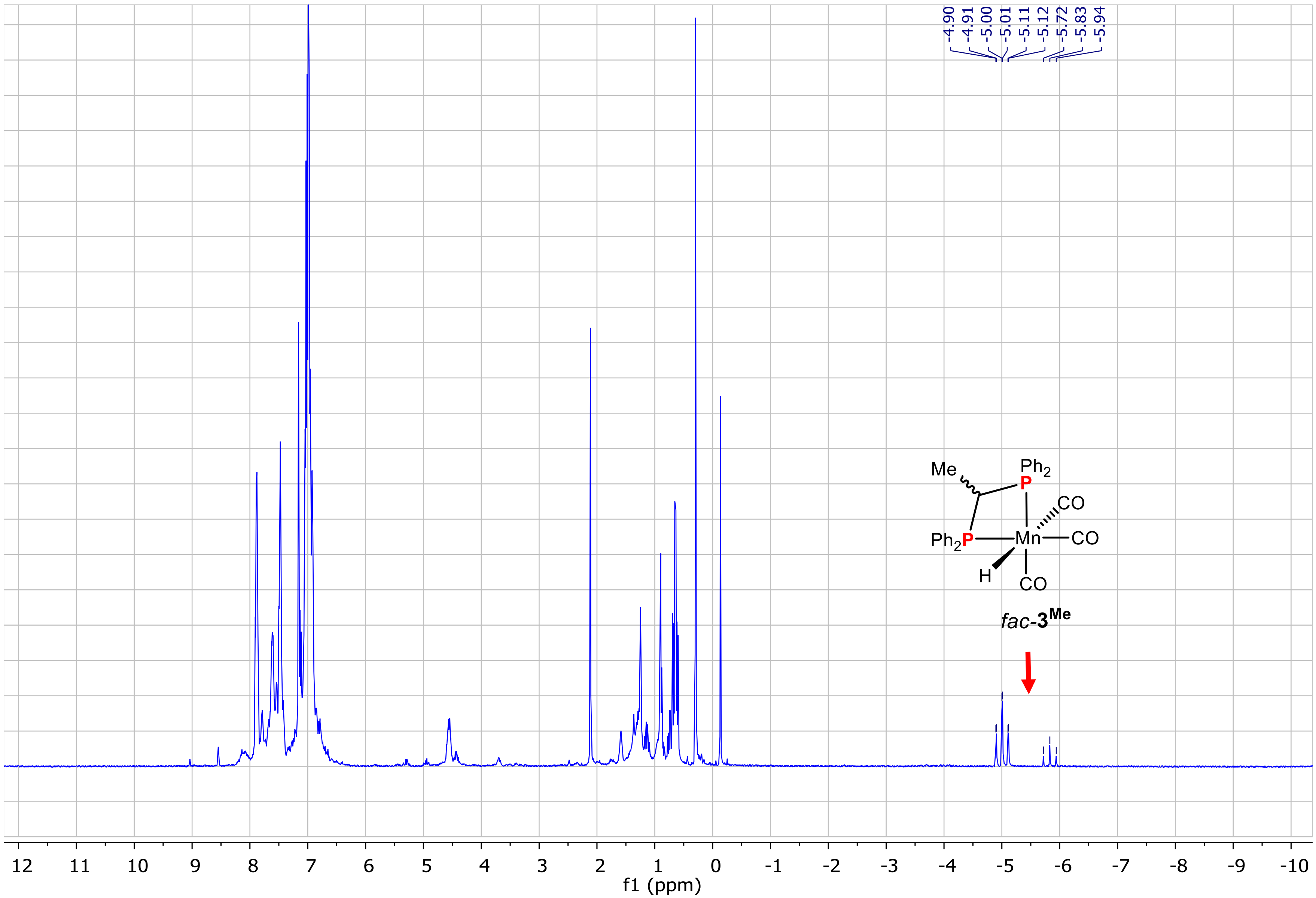


Figure S27. $^{31}P\{^{1}H\}$ NMR spectrum (400.1 MHz, C_6D_6, 25 °C) of the crude product obtained by the reaction of complex *fac*-**2**^{Me} with H_2 (1 atm. at 25 °C)

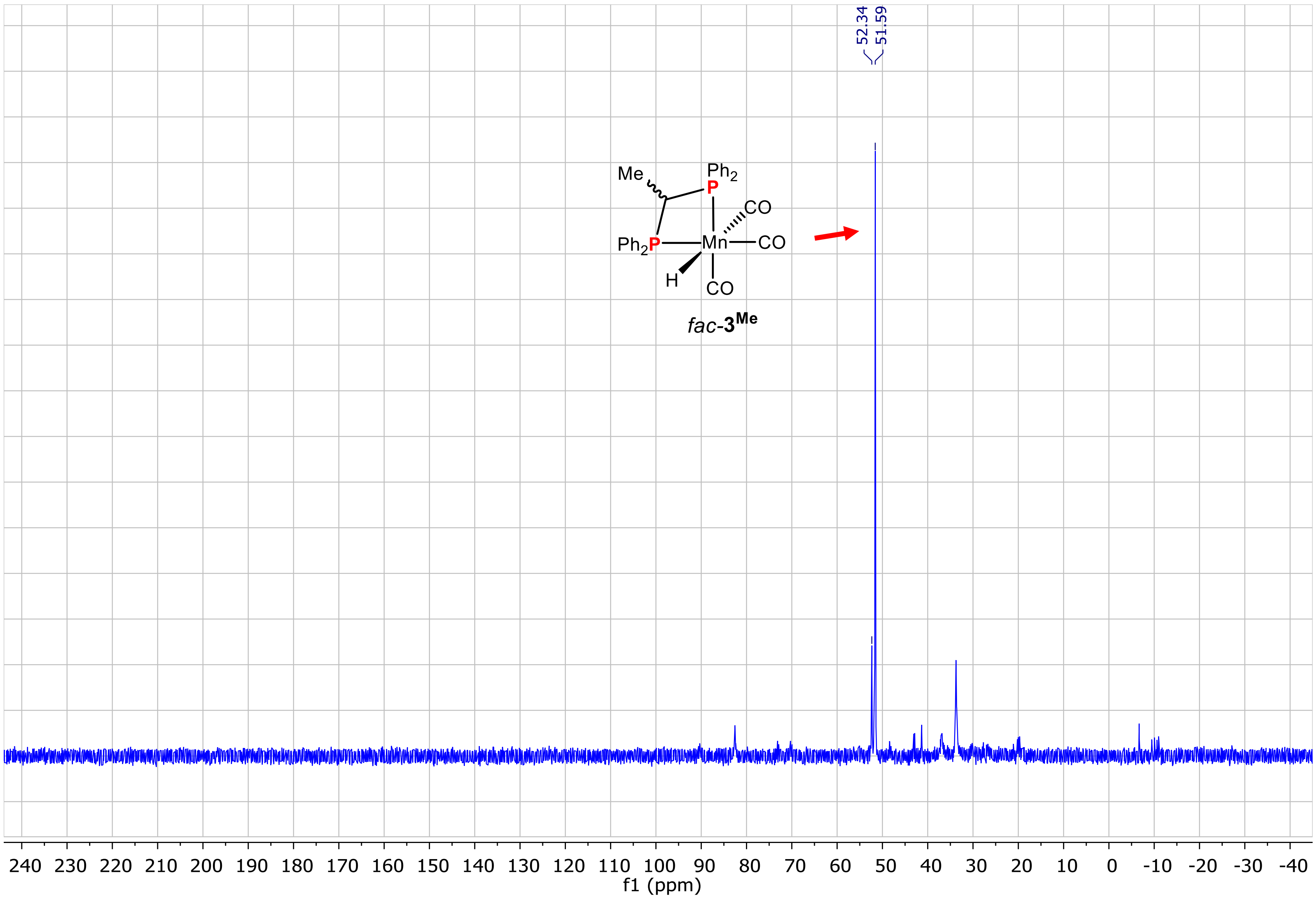


Figure S28. [1]H NMR spectrum (400.1 MHz, C_6D_6, 25 °C) of the crude product obtained by the reaction of complex *fac*-**2**$^{\mathbf{Me}}$ with H_2 (50 atm. at 25 °C)

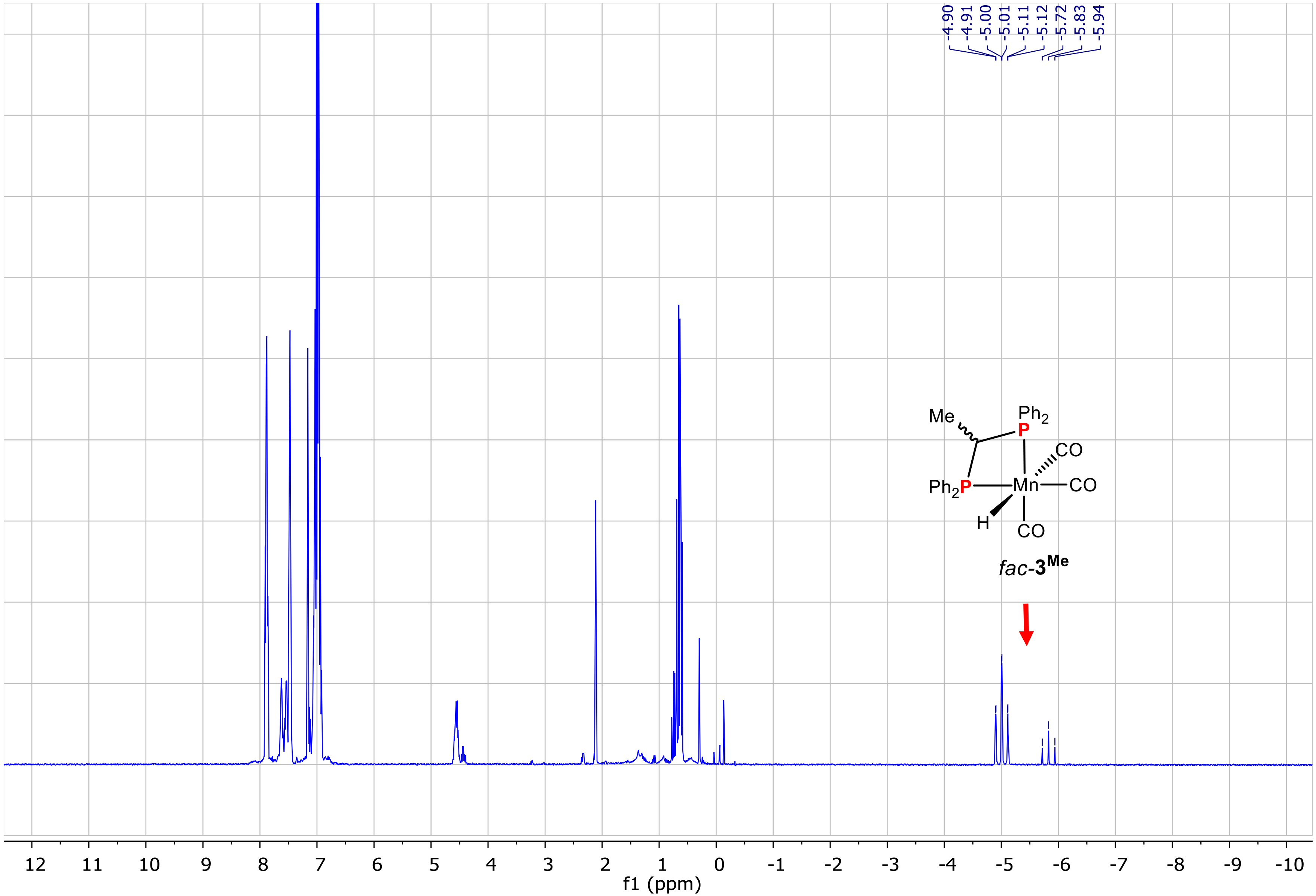


Figure S29. $^{31}P\{^1H\}$ NMR spectrum (400.1 MHz, C_6D_6, 25 °C) of the crude product obtained by the reaction of complex *fac*-**2**^{Me} with H_2 (50 atm. at 25 °C)

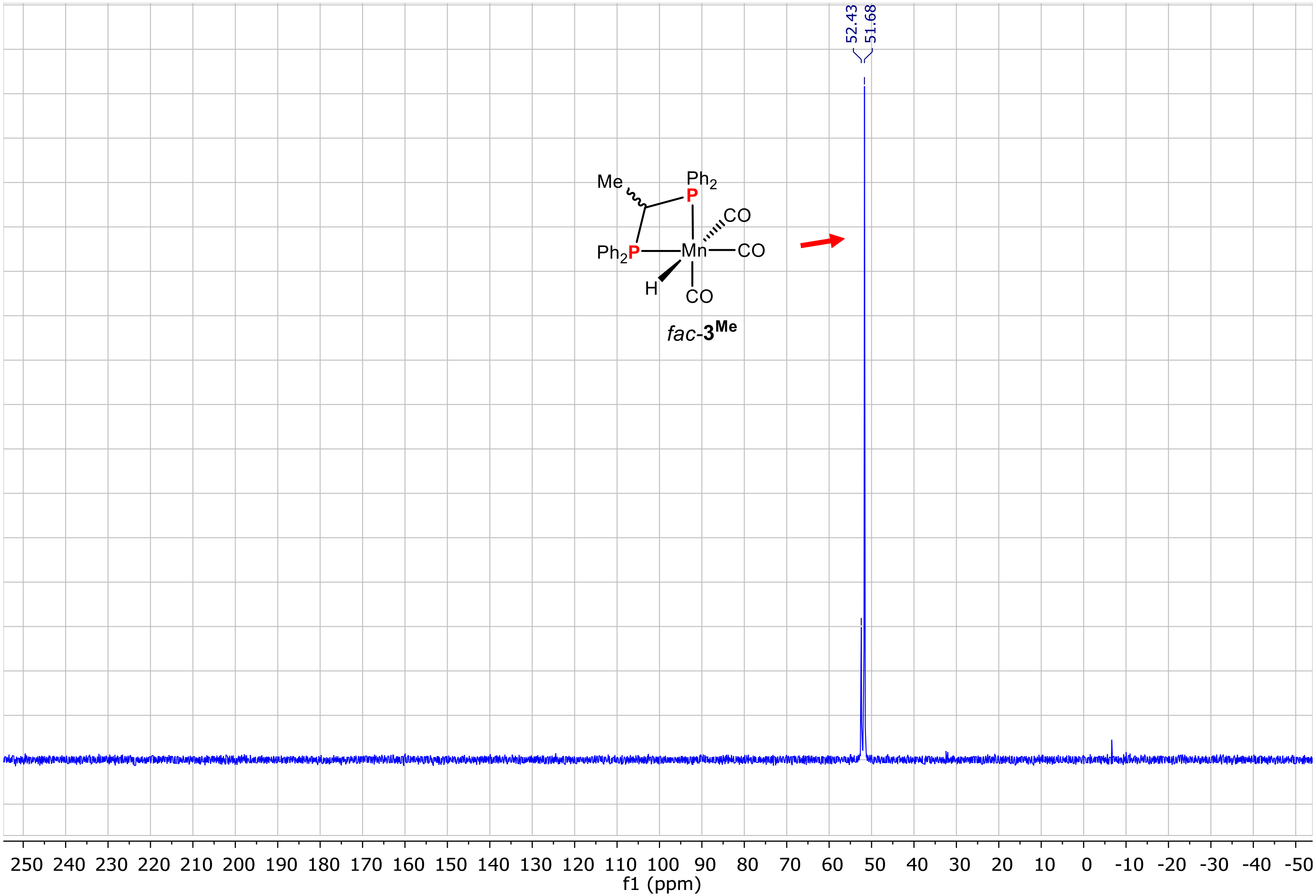


Figure S30. ^{1}H NMR spectrum of complex *fac*-**3**^{Me} (400.1 MHz, C_6D_6, 25 °C), the signals of residual toluene are marked with asterisk

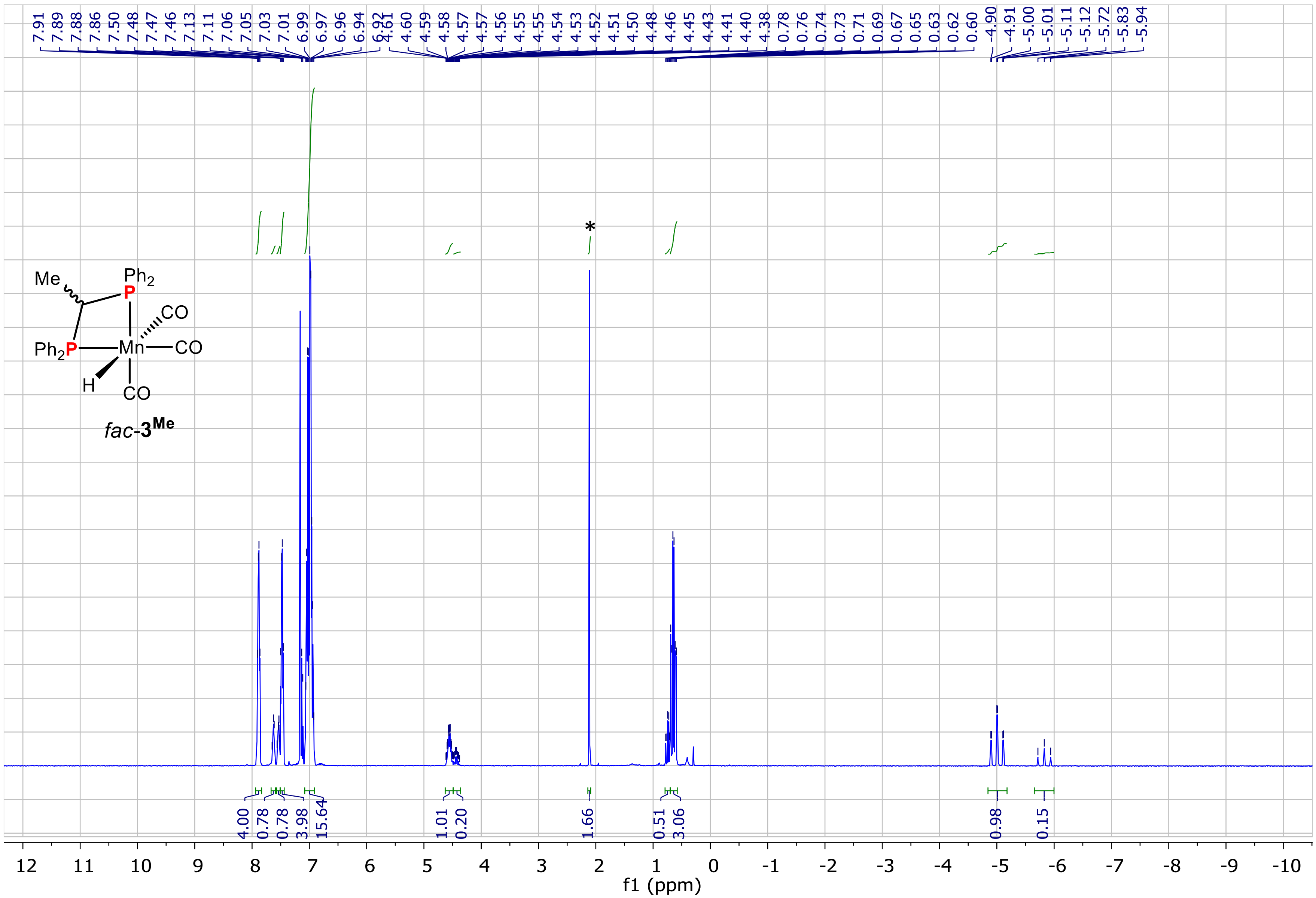


Figure S31. $^1H\{^{31}P\}$ NMR spectrum of complex *fac*-**3**^{Me} (400.1 MHz, C_6D_6, 25 °C), the signals of residual toluene are marked with asterisk

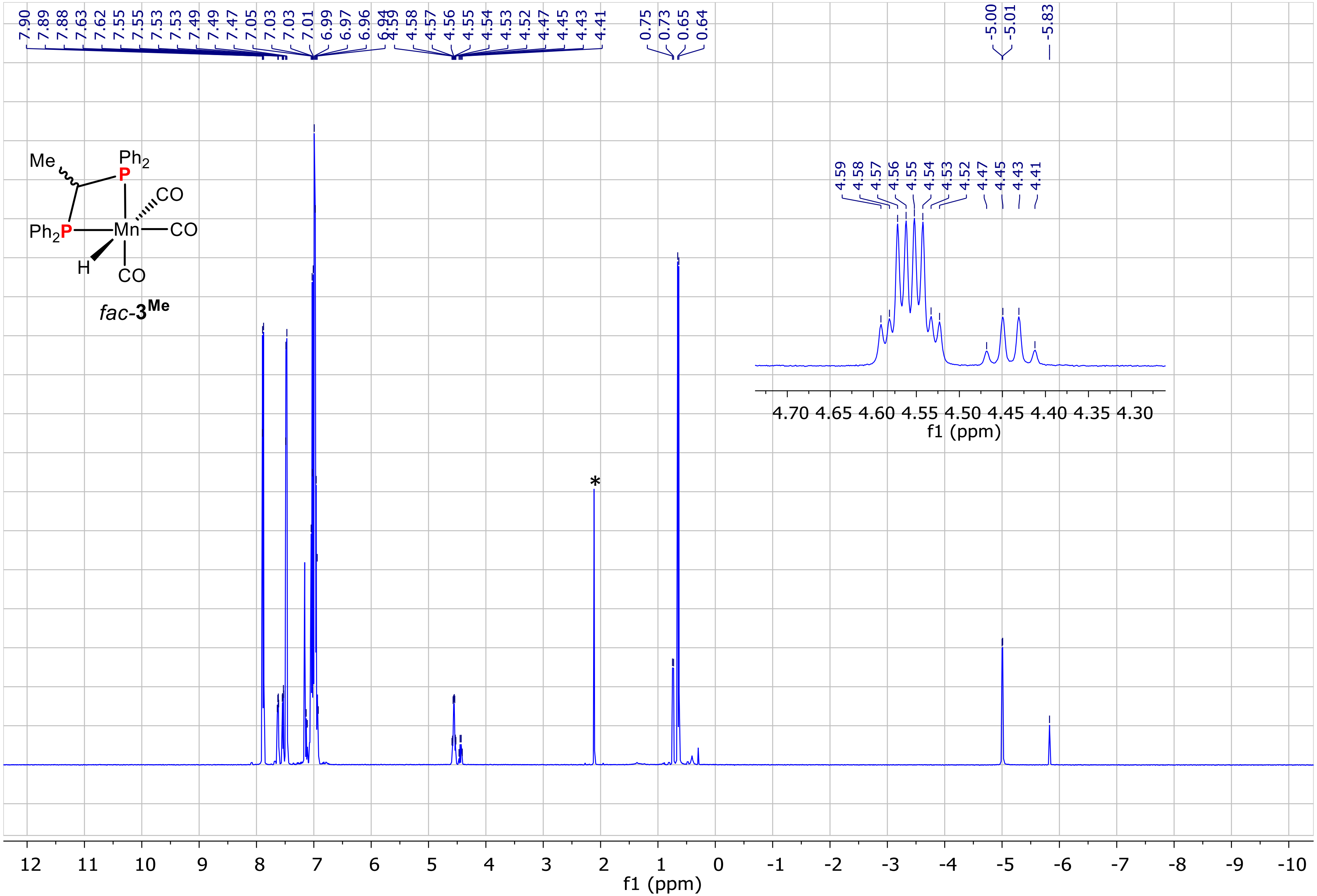


Figure S32. $^{31}P\{^{1}H\}$ NMR spectrum of complex *fac*-$\mathbf{3^{Me}}$ (162.0 MHz, C_6D_6, 25 °C)

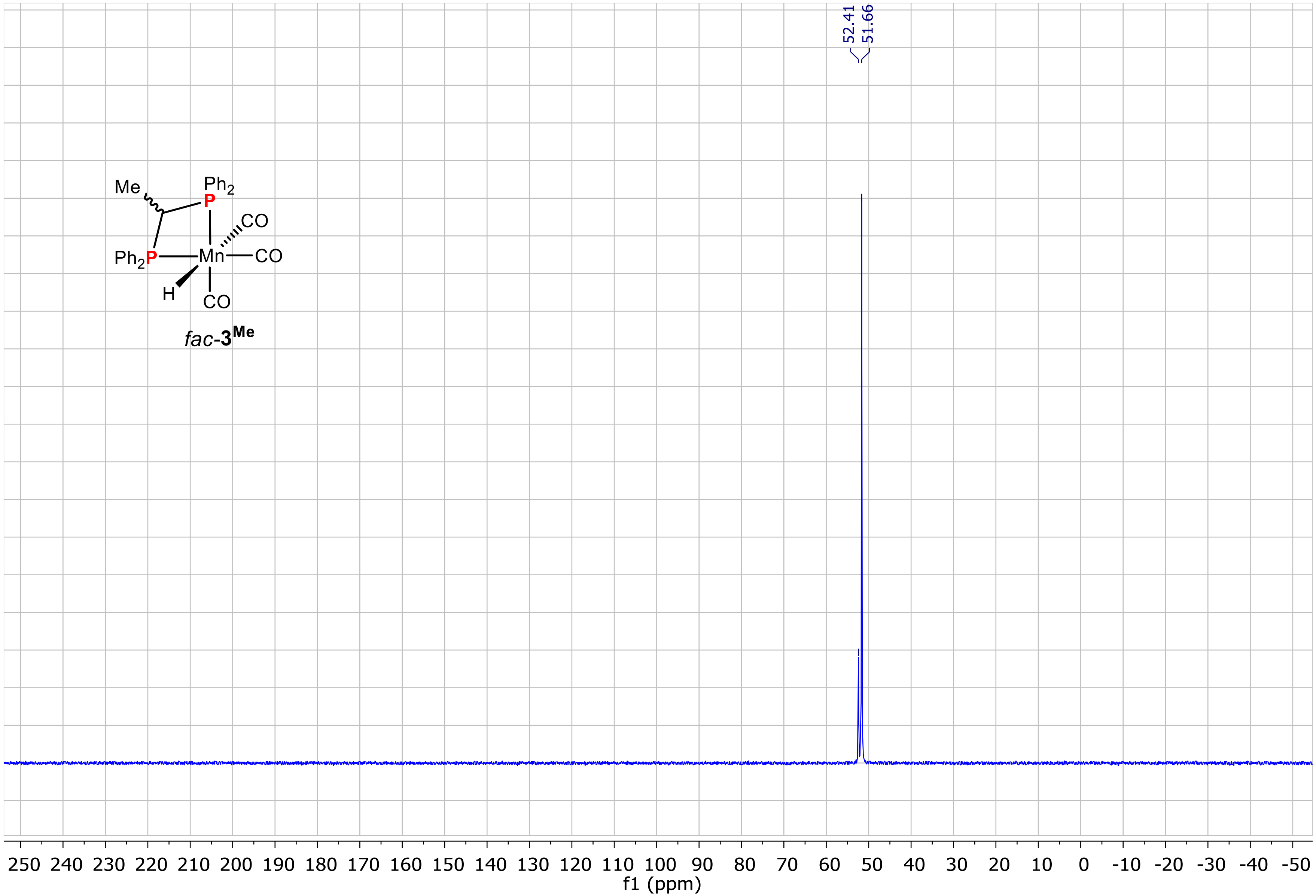


Figure S33. $^{13}C\{^1H\}$ NMR spectrum of complex *fac*-**3**$^{\mathbf{Me}}$ (100.6 MHz, C_6D_6, 25 °C), the signals of residual toluene are marked with asterisk

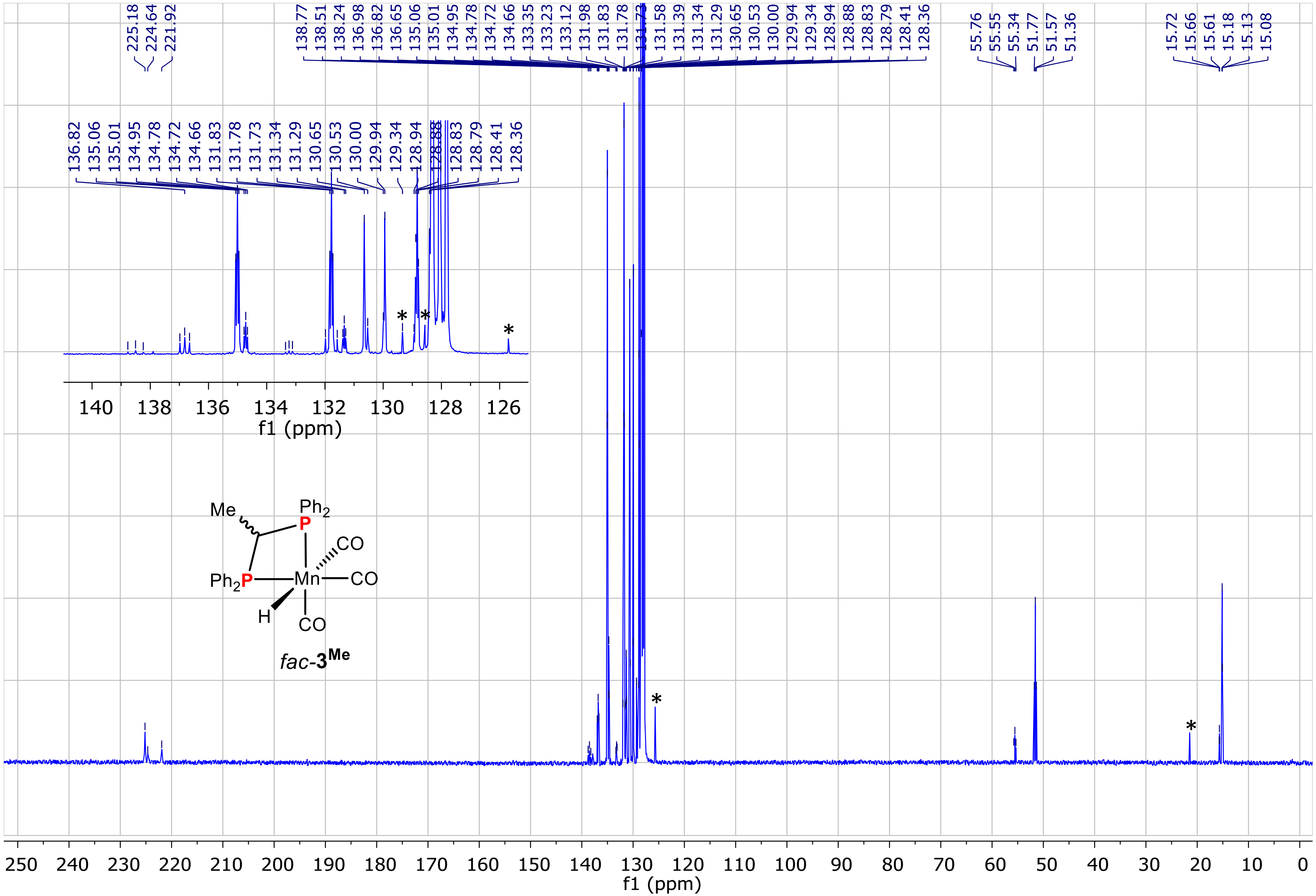


Figure S34. $^{1}H\{^{31}P\}$ 1D NOESY spectrum of complex *fac*-$\mathbf{3}^{\mathbf{Me}}$ (600.1 MHz, C_6D_6, 25 °C, irradiation at −5.02 ppm)

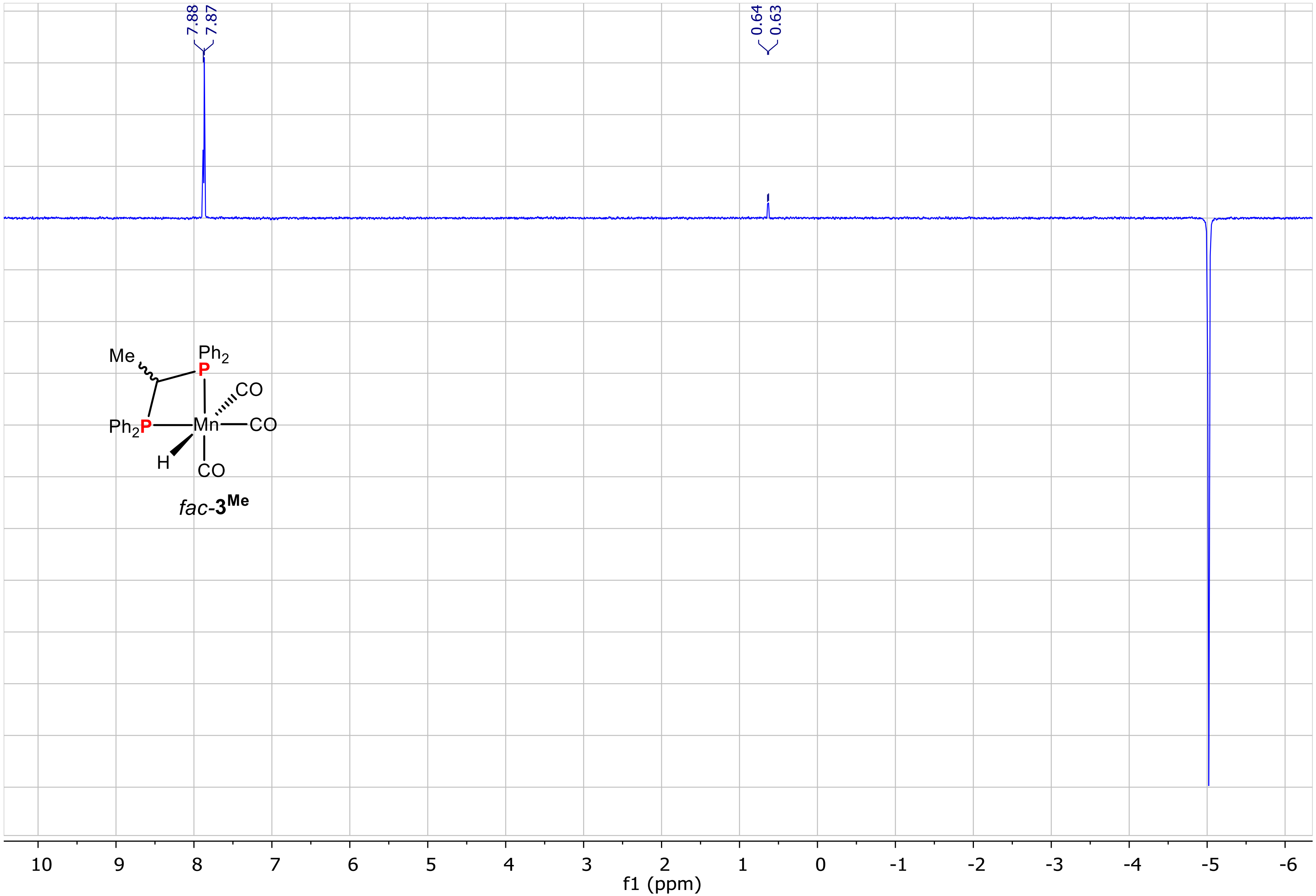


Figure S35. $^1H\{^{31}P\}$ 1D NOESY spectrum of complex *fac*-$\mathbf{3}^{\mathbf{Me}}$ (600.1 MHz, C_6D_6, 25 °C, irradiation at −5.84 ppm)

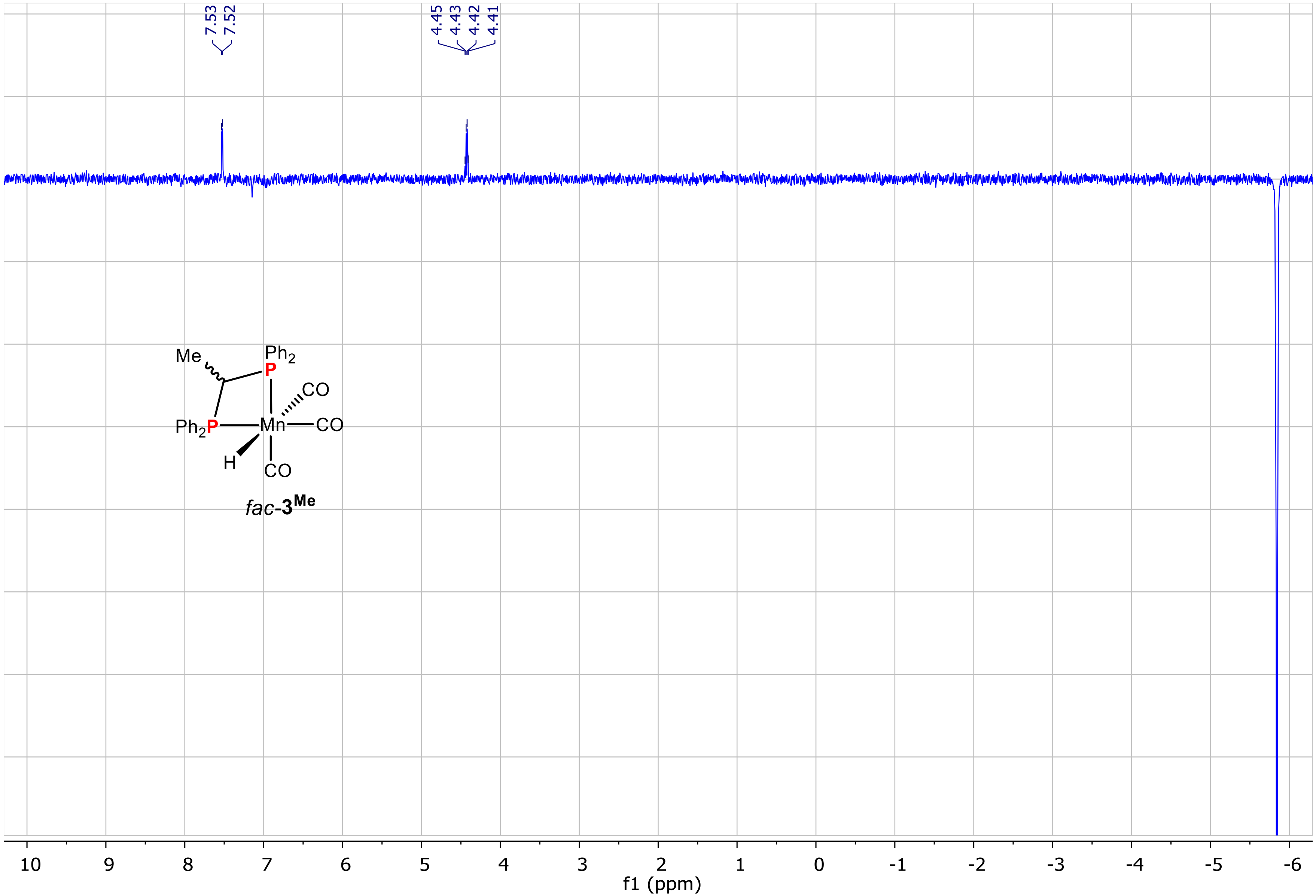


Figure S36. ^{1}H NMR spectrum of complex *fac*-**2^{Ph}** (400.1 MHz, C_6D_6, 25 °C), the signals of residual toluene is marked with asterisk

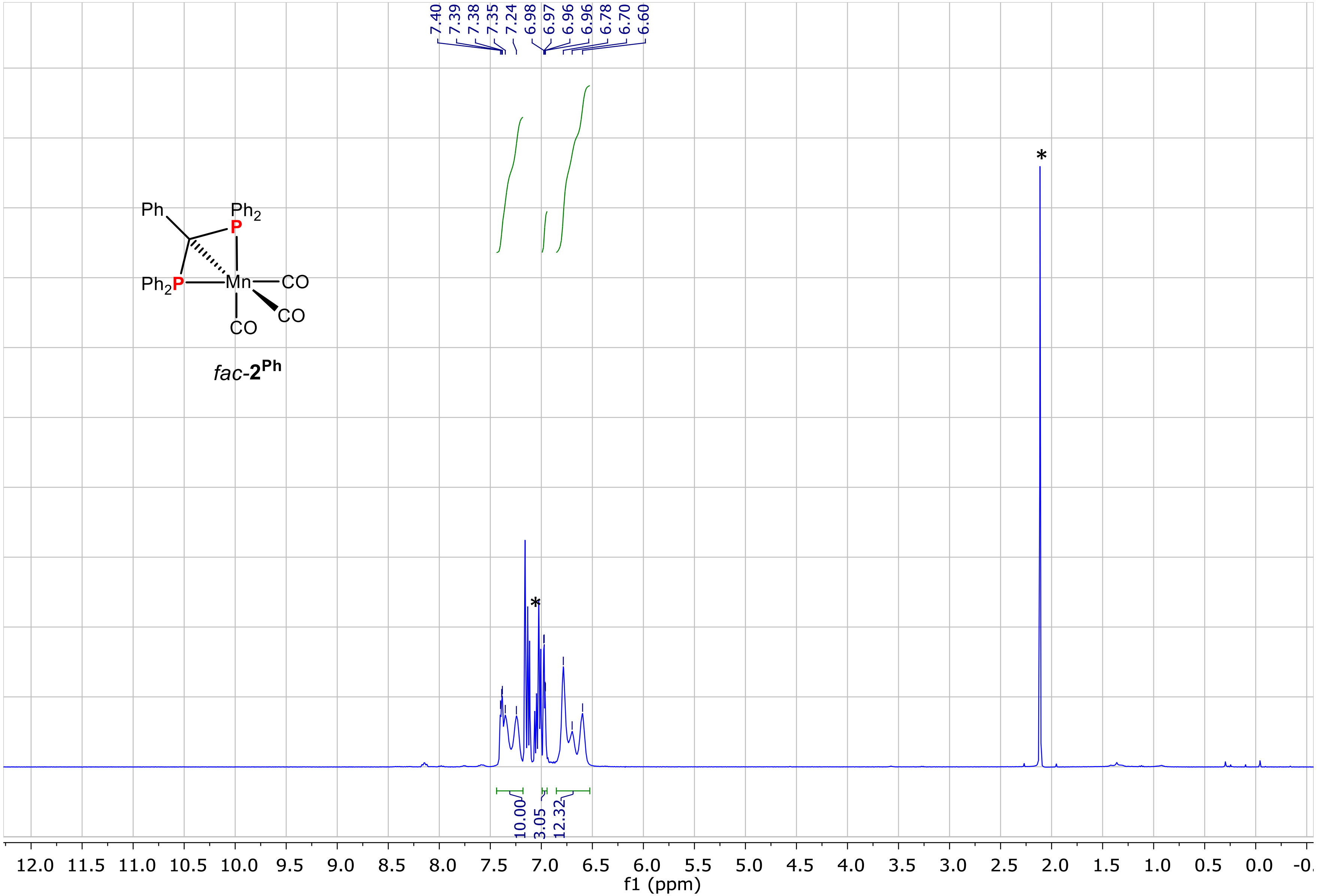


Figure S37. $^{31}P\{^{1}H\}$ NMR spectrum of complex *fac*-$\mathbf{2^{Ph}}$ (162.0 MHz, C_6D_6, 25 °C)

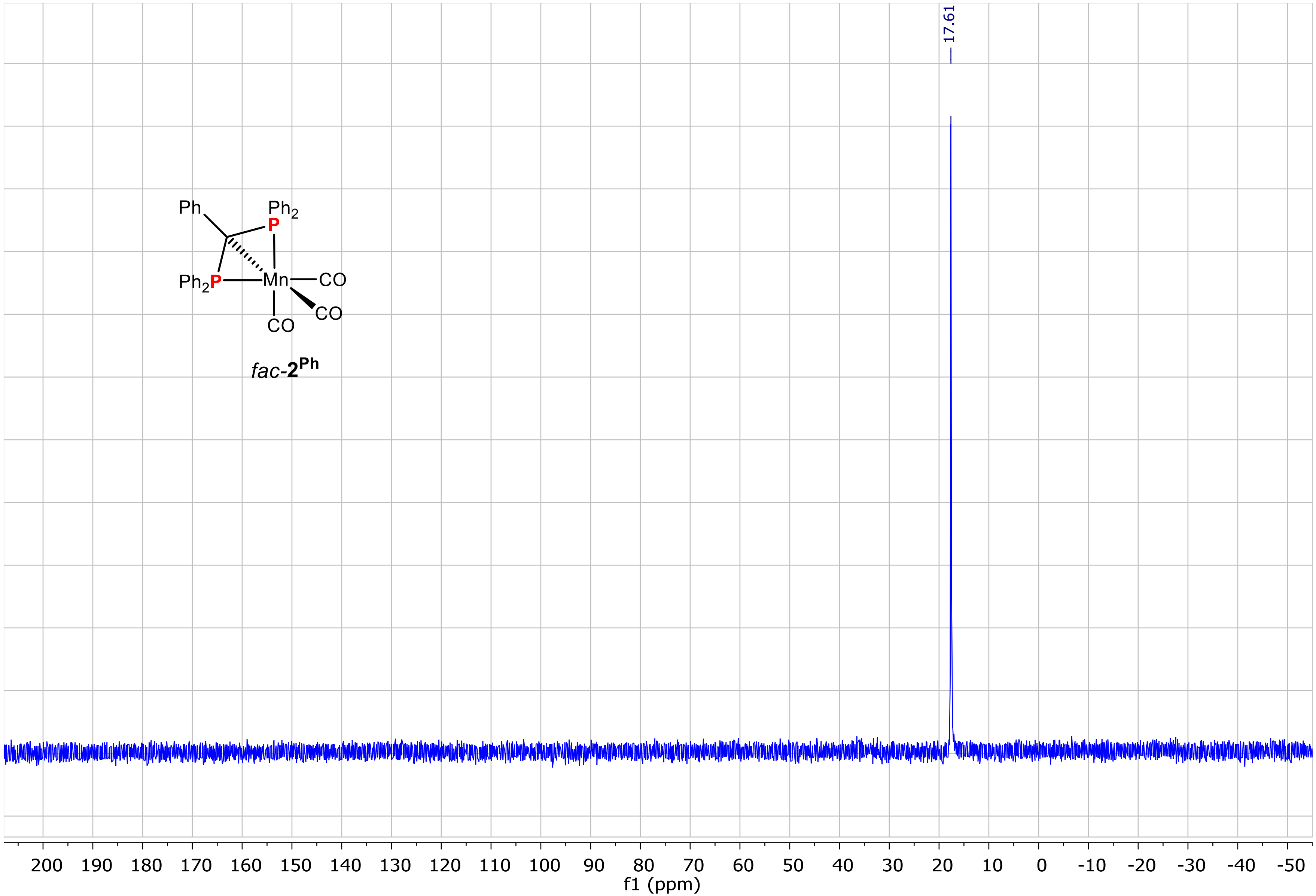


Figure S38. $^{13}C\{^1H\}$ NMR spectrum of complex *fac*-$\mathbf{2}^{\mathbf{Ph}}$ (100.6 MHz, C_6D_6, 25 °C), the signals of residual toluene are marked with asterisk

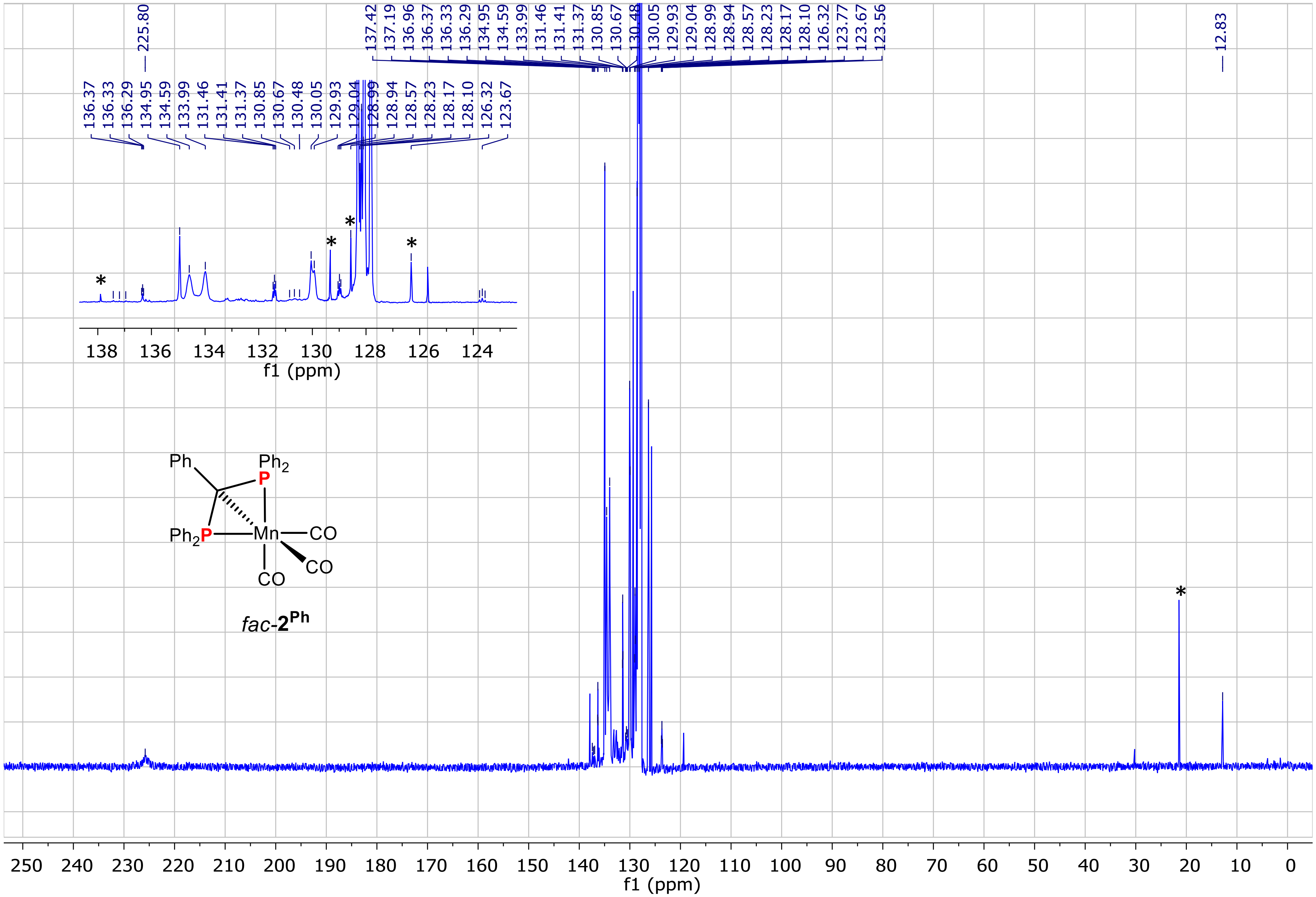


Figure S39. $^{13}C\{^{1}H\}$ NMR spectrum of complex *fac*-**2**$^{\mathbf{Ph}}$ (100.6 MHz, toluene-d$_8$, −40 °C)

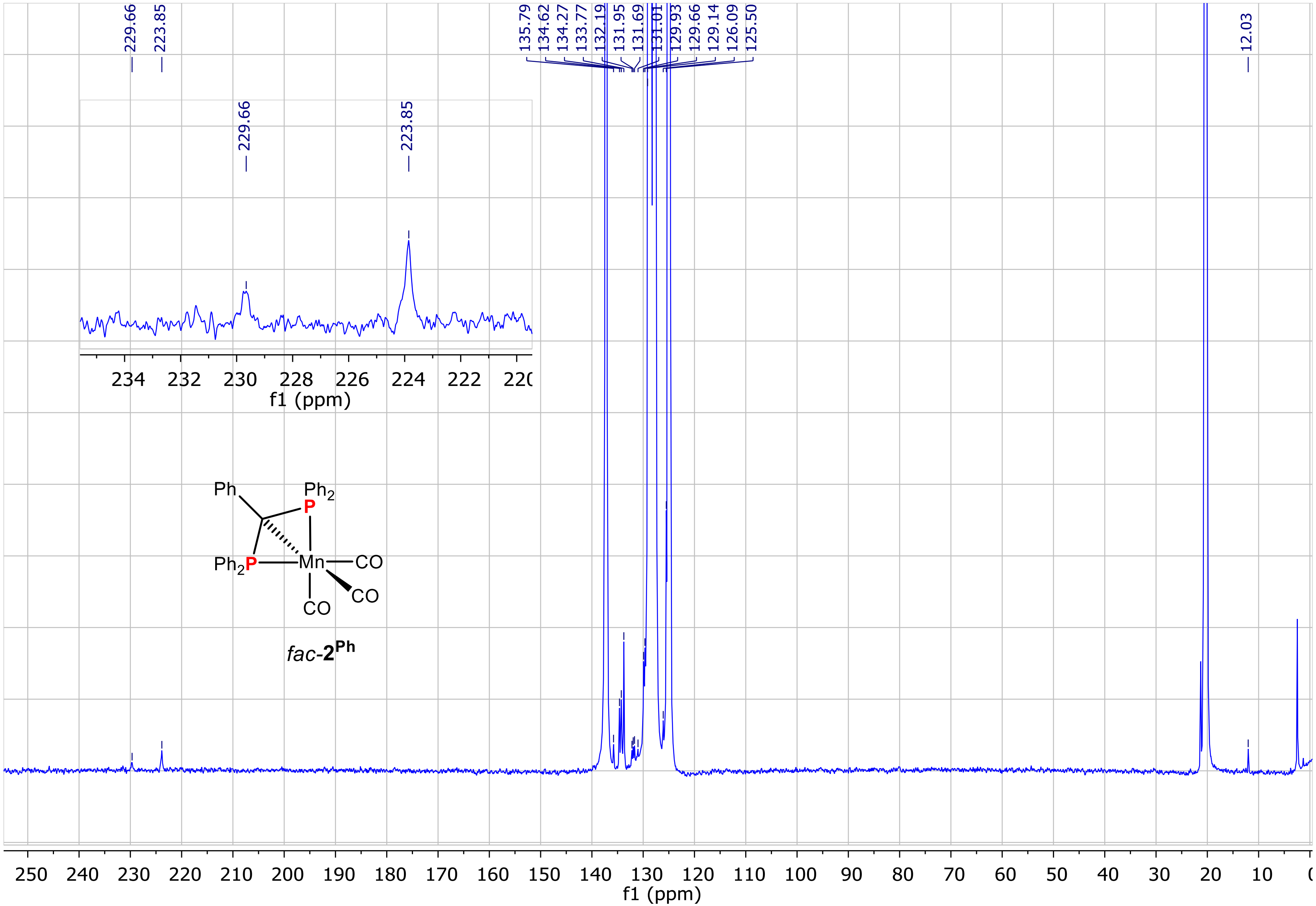


Figure S40. ^{1}H NMR spectrum (400.1 MHz, C_6D_6, 25 °C) of the crude product obtained by the reaction of complex *fac*-**2**^{Ph} with H_2 (1 atm. at 25 °C)

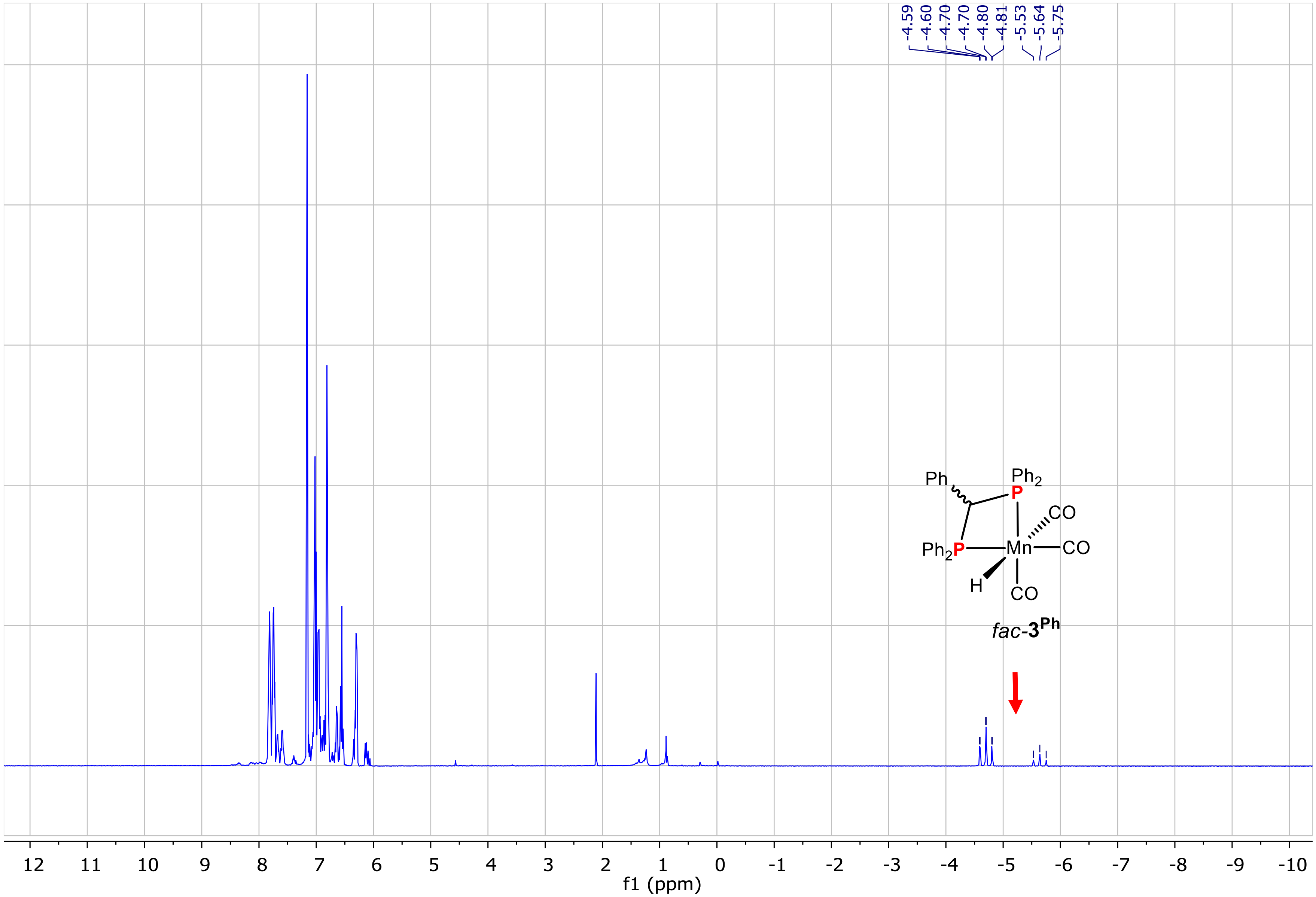


Figure S41. $^{31}P\{^1H\}$ NMR spectrum (400.1 MHz, C_6D_6, 25 °C) of the crude product obtained by the reaction of complex *fac*-$\mathbf{2}^{\mathbf{Ph}}$ with H_2 (1 atm. at 25 °C)

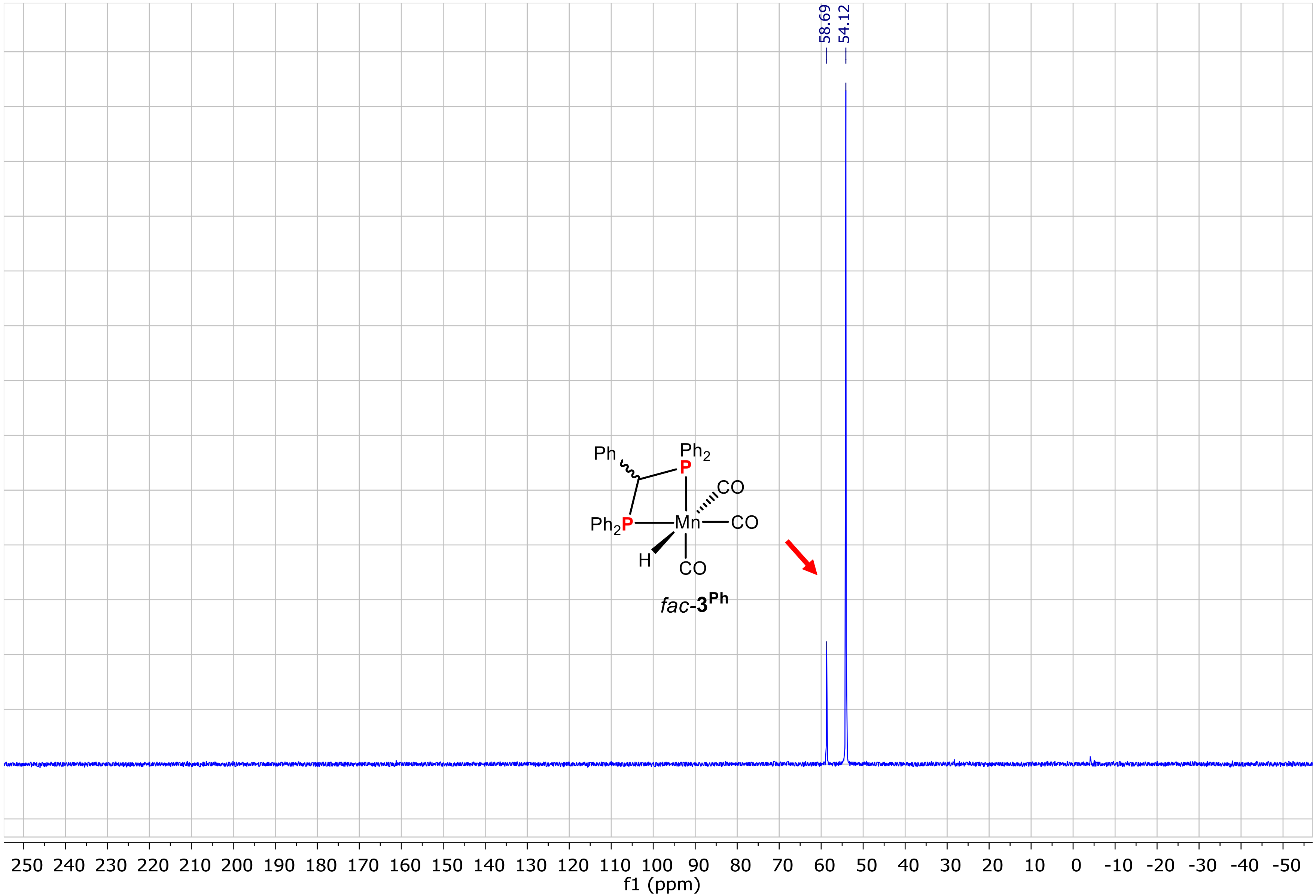


Figure S42. ^{1}H NMR spectrum of complex *fac*-$\mathbf{3^{Ph}}$ (400.1 MHz, C_6D_6, 25 °C), overlapping PC*H*(Ph)P signals are marked with red arrows

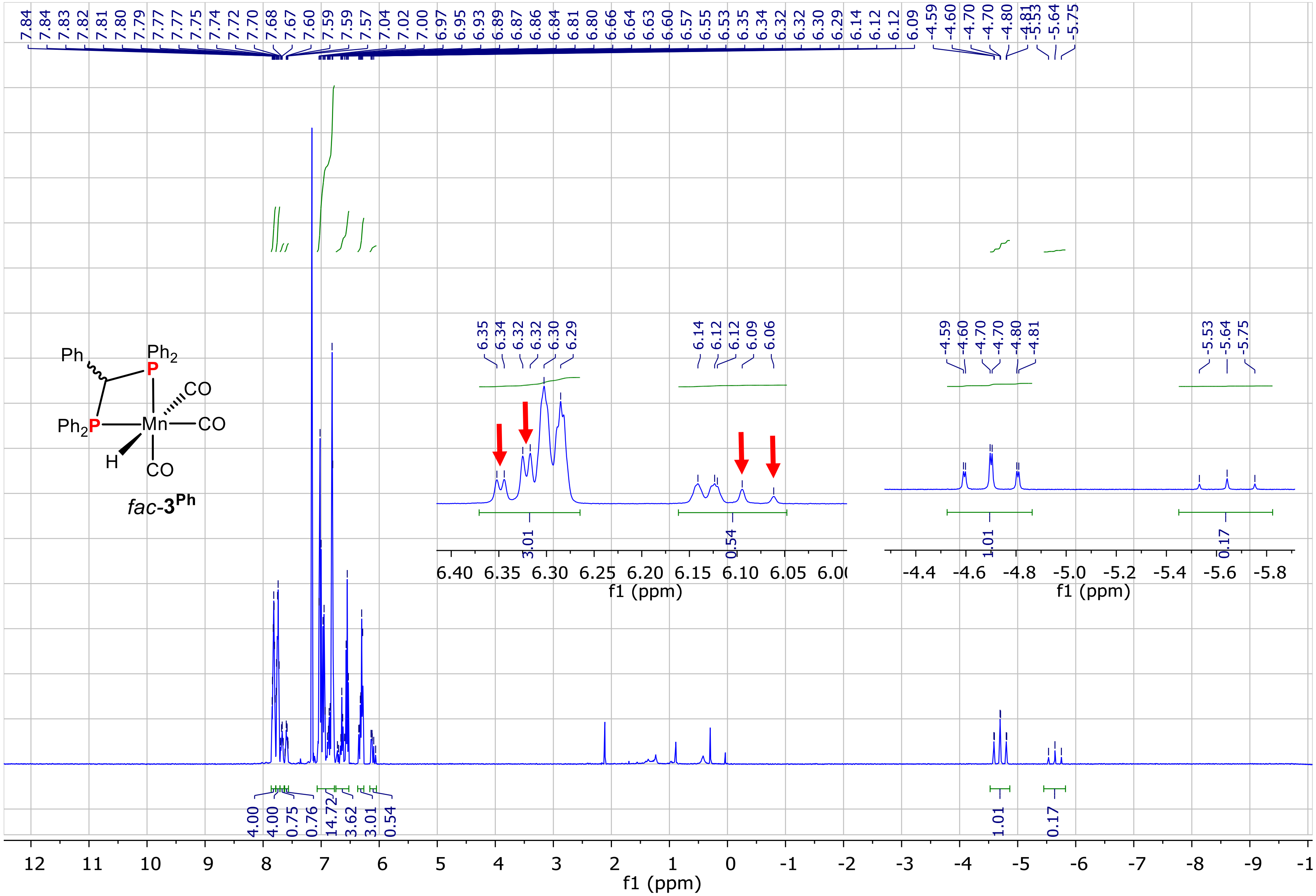


Figure S43. $^{1}H\{^{31}P\}$ NMR spectrum of complex *fac*-**3**^{Ph} (400.1 MHz, C_6D_6, 25 °C), overlapping PC*H*(Ph)P signals are marked with red arrows

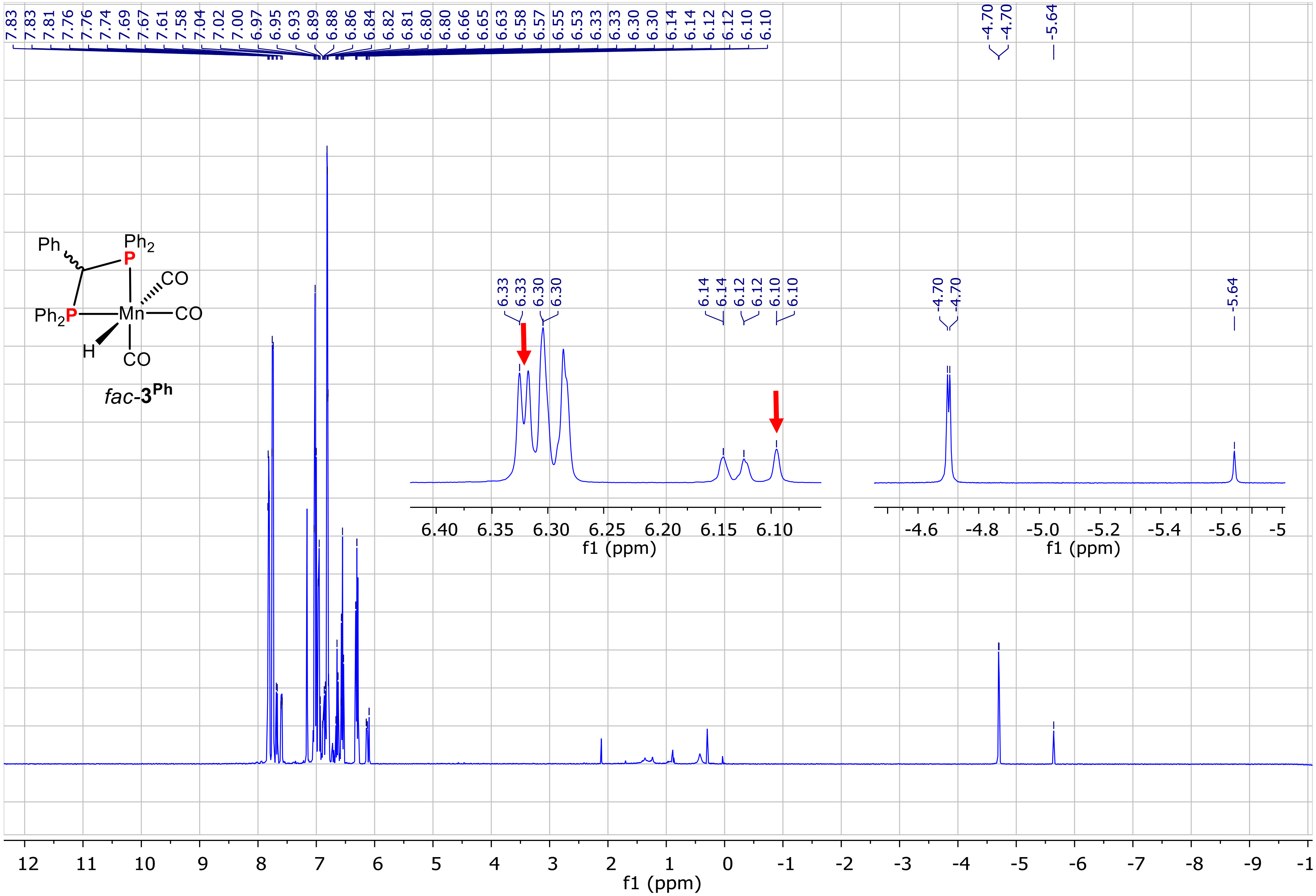


Figure S44. $^{31}P\{^{1}H\}$ NMR spectrum of complex *fac*-$\mathbf{3}^{\mathbf{Ph}}$ (162.0 MHz, C_6D_6, 25 °C)

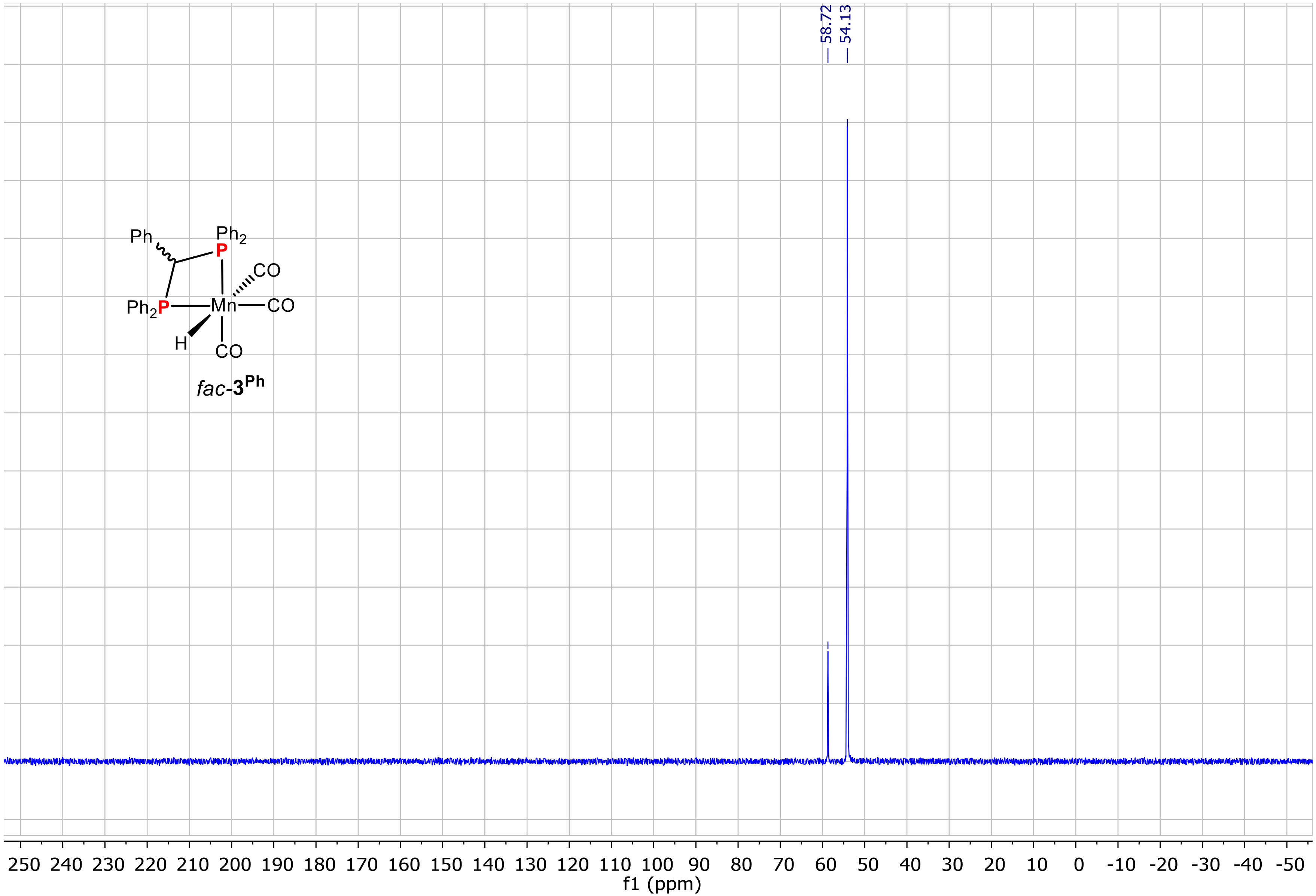


Figure S45. $^{13}C\{^{1}H\}$ NMR spectrum of complex *fac*-$\mathbf{3^{Ph}}$ (100.6 MHz, C_6D_6, 25 °C)

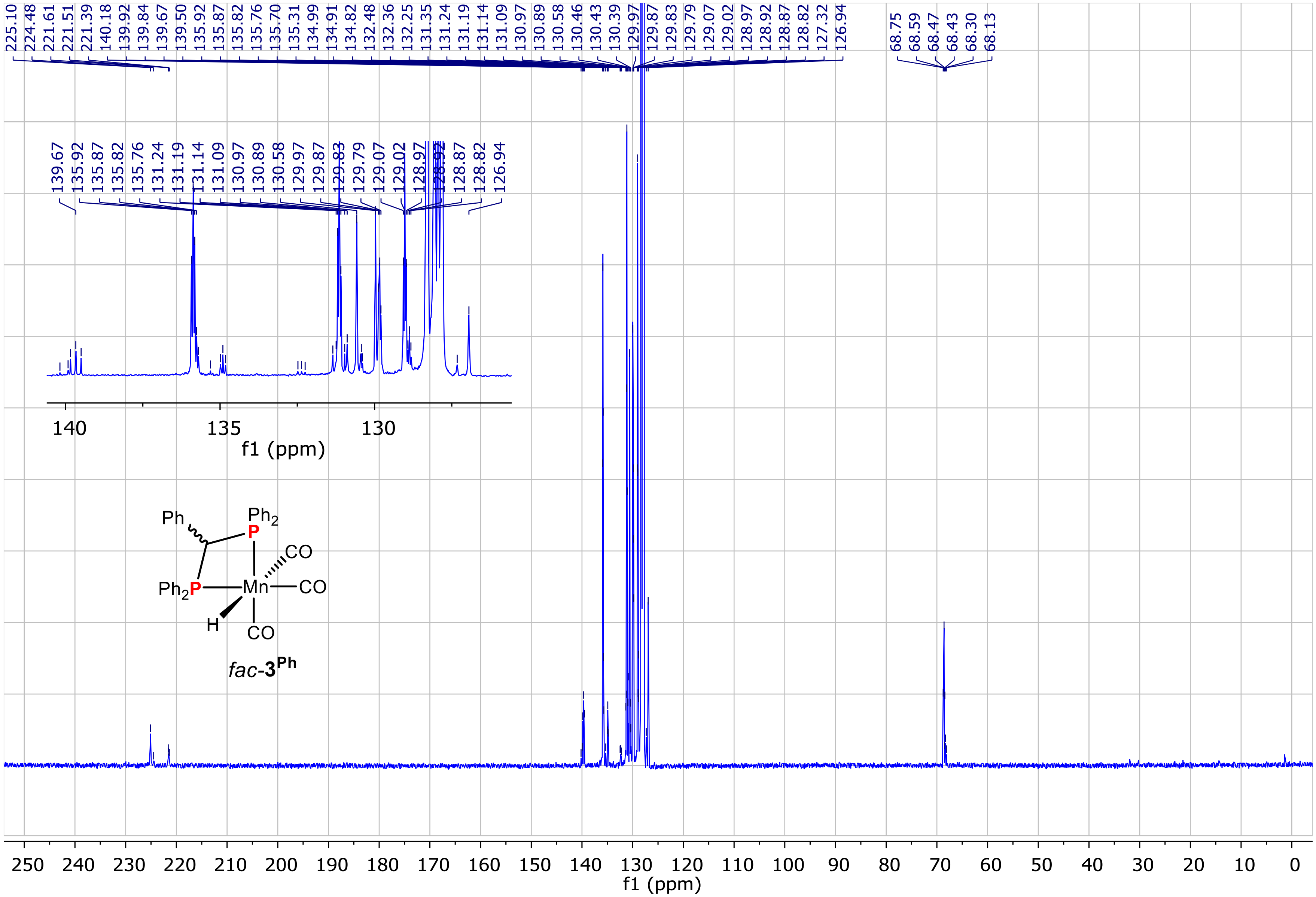


Figure S46. ^{1}H 1D NOESY spectrum of complex *fac*-$\mathbf{3}^{\mathbf{Ph}}$ (600.1 MHz, C_6D_6, 25 °C, irradiation at −4.70 ppm)

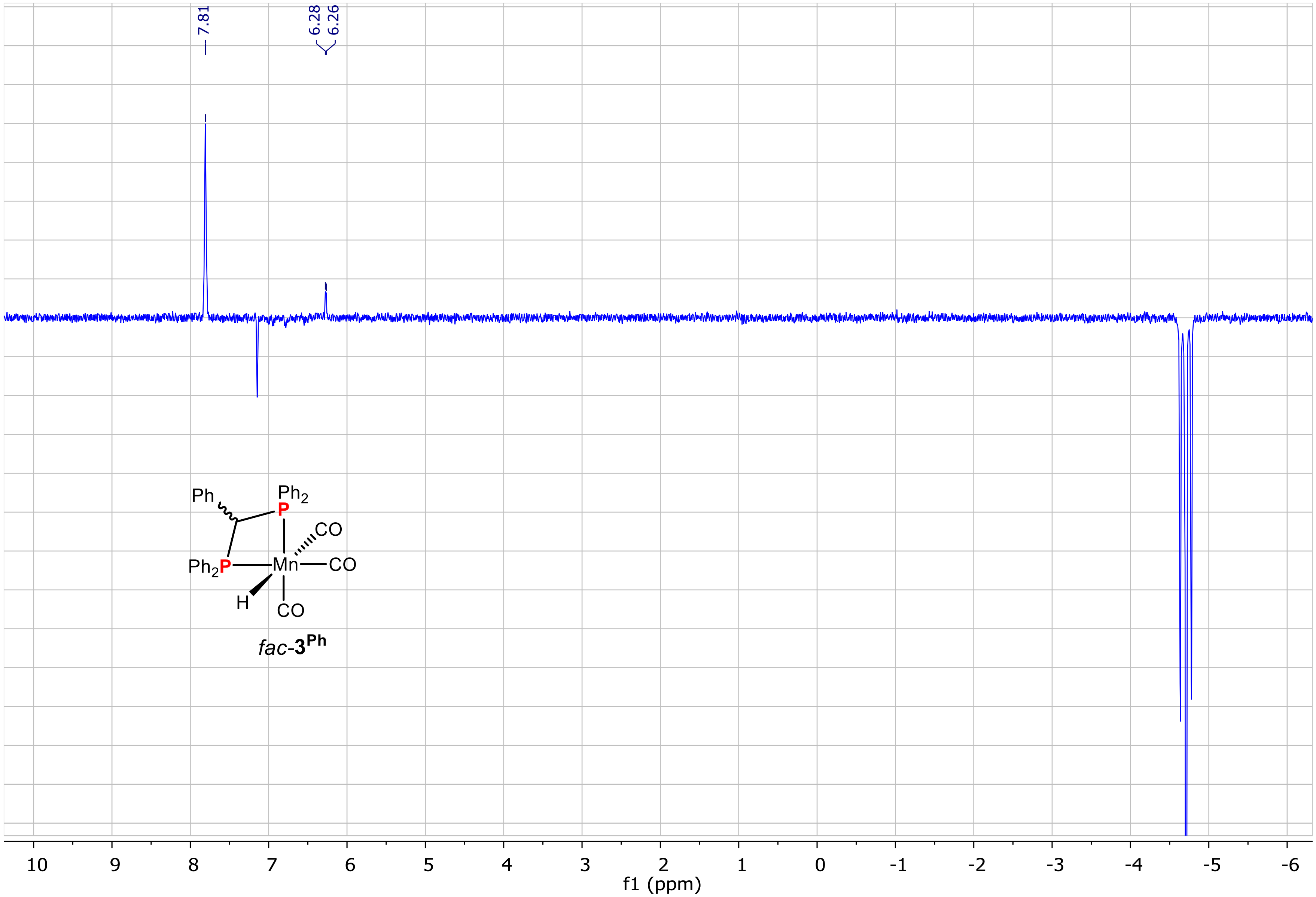
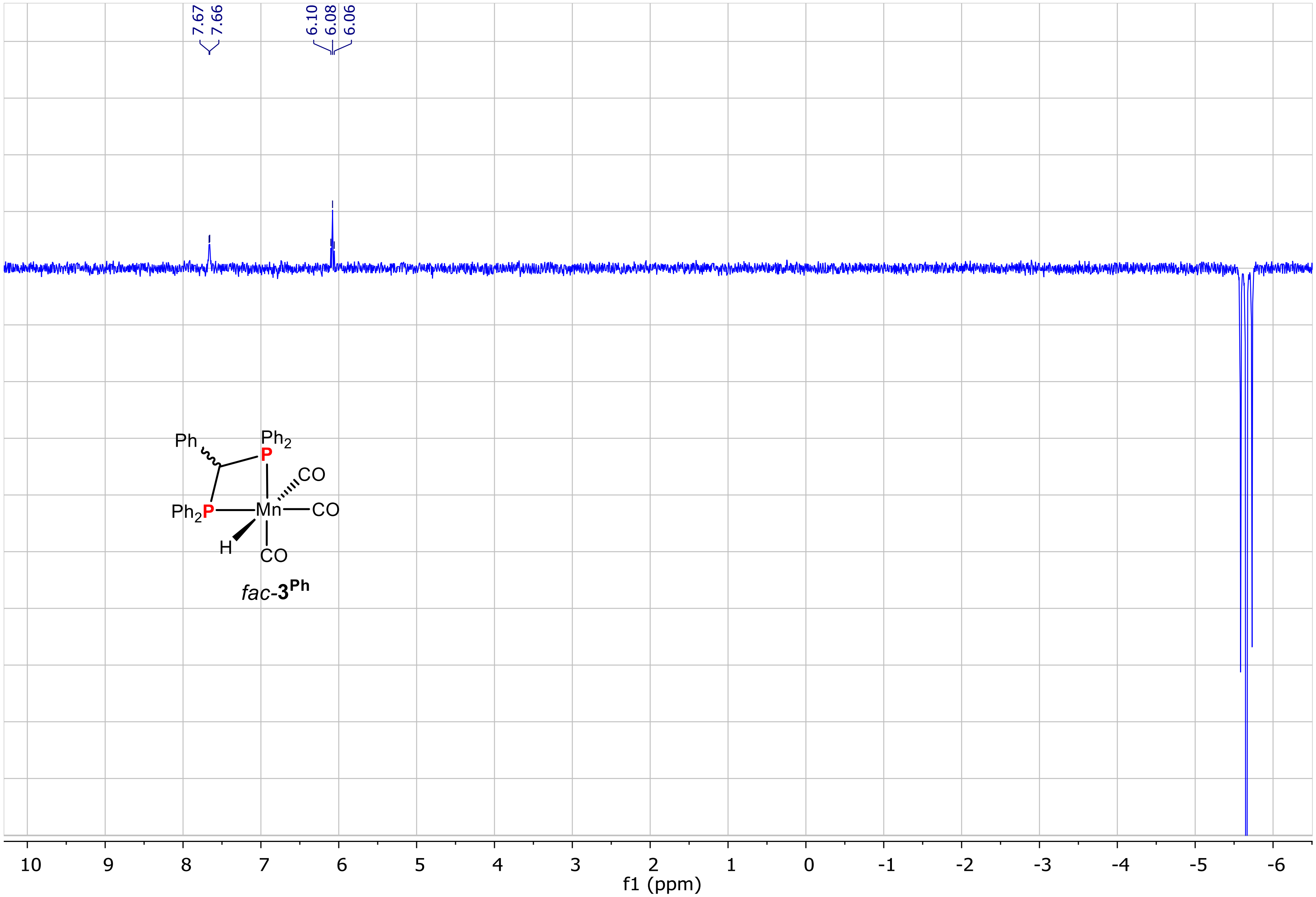


Figure S47. ^{1}H 1D NOESY spectrum of complex *fac*-**3**^{Ph} (600.1 MHz, C_6D_6, 25 °C, irradiation at −5.64 ppm)



IR monitoring of reactions *fac*-1^R → *fac*-2^R → *fac*-3^R

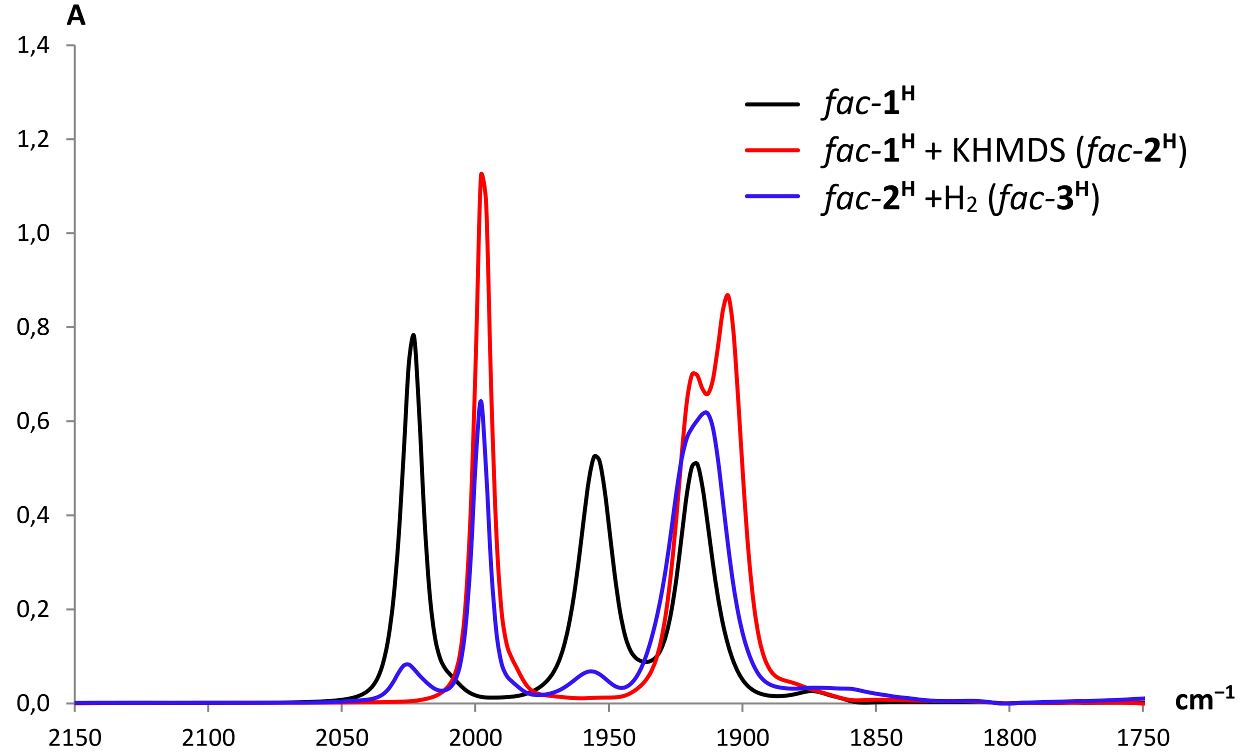


Figure S48. IR spectra of complex *fac*-**1**^{H} in toluene (black), intermediate *fac*-**2**^{H} obtained upon addition of KHMDS (red), and after treatment of *fac*-**2**^{H} with 50 atm. of H_2 at 50°C for 16h (blue).

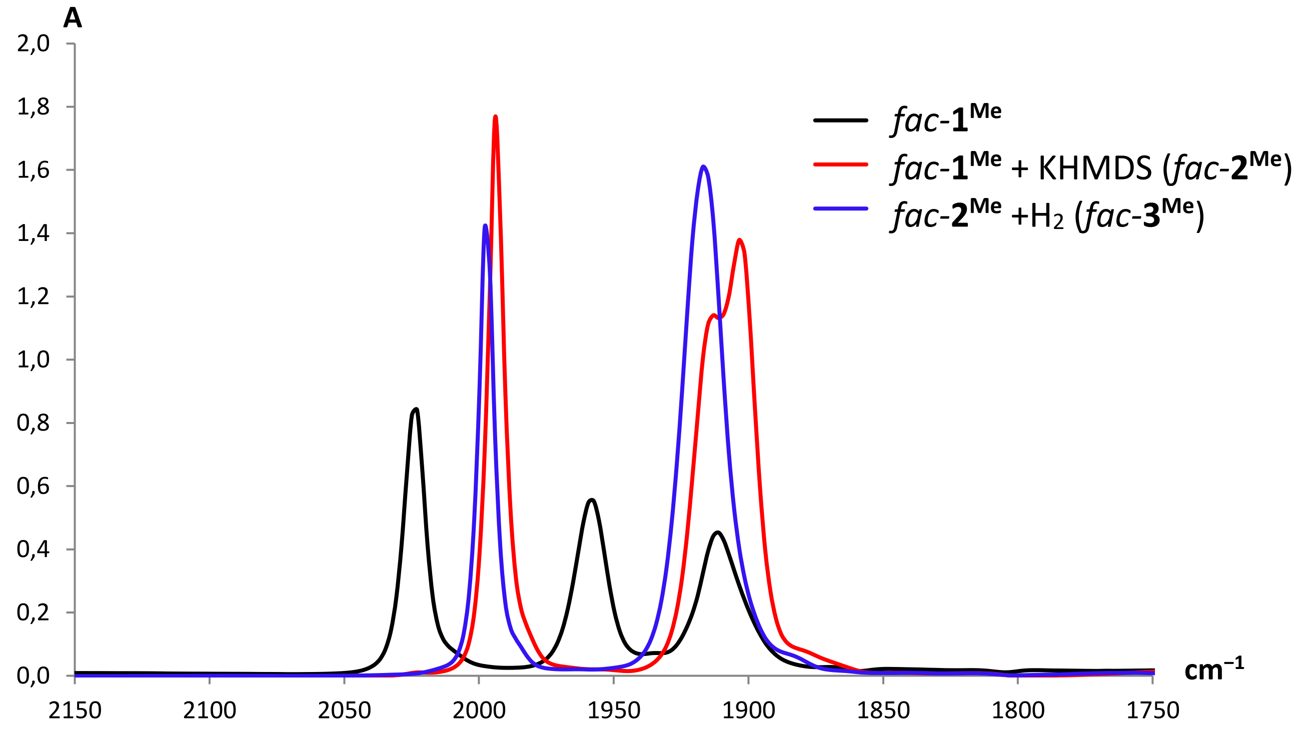


Figure S49. IR spectra of complex *fac*-**1**^{Me} in toluene (black, lower peak intensity due to limited solubility), intermediate *fac*-**2**^{Me} obtained upon addition of KHMDS (red), and after treatment of the latter complex with 50 atm. of H_2 at room temperature for 1h (blue).

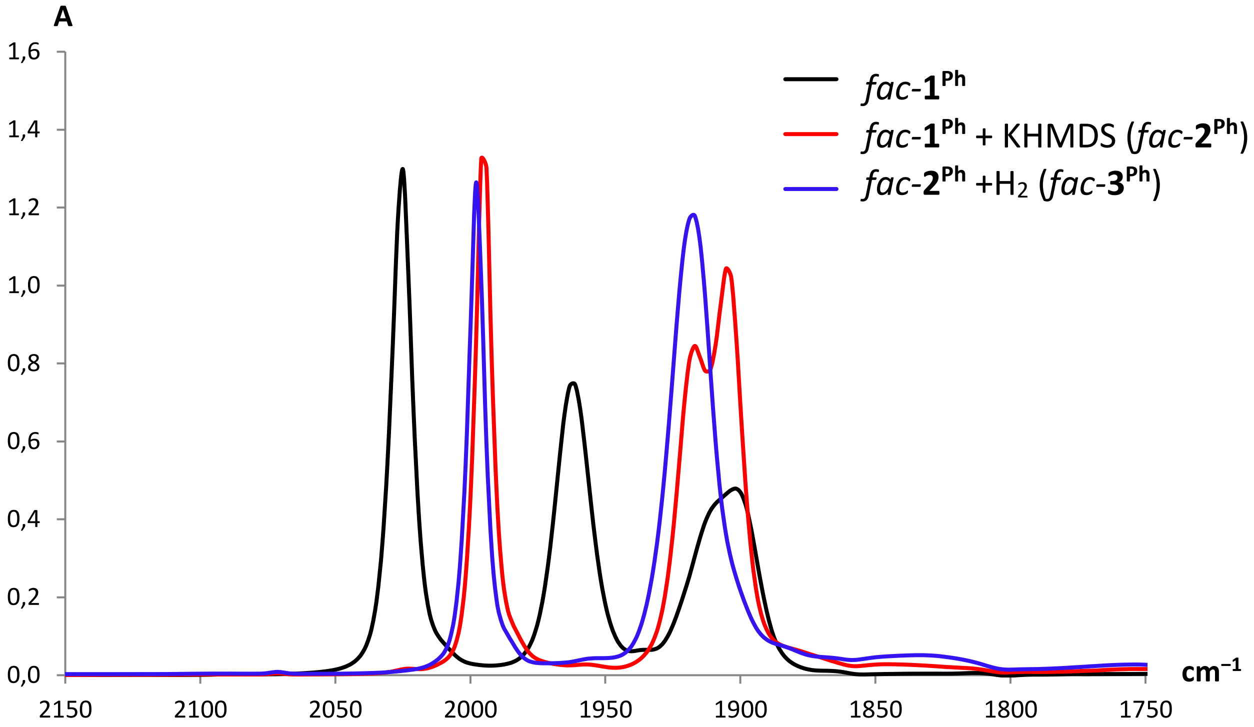


Figure S50. IR spectra of complex *fac*-**1**^{Ph} in toluene (black), intermediate *fac*-**2**^{Ph} obtained upon addition of KHMDS (red), and after treatment of the latter complex with 1 atm. of H_2 at room temperature for 5 min (blue).

X-ray diffraction studies

Single crystals of complexes *fac*-$\mathbf{2}^{Ph}$ and *fac,anti*-$\mathbf{3}^{Ph}$ suitable for X-ray diffraction experiments were obtained by the crystallization from concentrated toluene solution at −20° C and room temperature, respectively. The single-crystal X-ray diffraction data for complexes *fac*-$\mathbf{2}^{Ph}$ and *fac,anti*-$\mathbf{3}^{Ph}$ were collected at −173 °C on a Bruker D8/APEX II/Incoatec Mo IµS Microsource diffractometer and Nonius Mach 3/APEX II/sealed Mo X-ray tube diffractometer, respectively. All calculations were performed on a PC compatible computer using the WinGX system.[7] The structure was solved using the SIR92 program[8] which revealed in each instance the position of most of the non-hydrogen atoms. All the remaining non-hydrogen atoms were located by the usual combination of full matrix least-squares refinement on F^2 and difference electron density syntheses using the SHELXTL program.[9] Atomic scattering factors were taken from the usual tabulations. Anomalous dispersion terms for the Mn was included in Fc. All non-hydrogen atoms were allowed to vibrate anisotropically. The hydrogen atoms were set in idealized positions (R_2CH_2, C–H = 0.99 Å, $U_{iso}(H) = 1.2U_{eq}(C)$; C(sp^2)–H = 0.95 Å; $U_{iso}(H) = 1.2U_{eq}(C)$) and their positions refined as “riding” atoms, besides H1 hydride atom in *fac,anti*-$\mathbf{3}^{Ph}$, which position was located from Fourier differences map and refined with the restrained isotropic thermal parameter ($U_{iso}(H) = 0.05$). After completing the initial structure solution for complex *fac*-$\mathbf{2}^{Ph}$, it was found that 30% of the total cell volume was filled with disordered toluene molecules, which, however, could not be precisely modeled in terms of discrete molecules. The disordered solvent contribution was then subtracted from the observed data using the SQUEEZE procedure.[10] CCDC 1954917-1954918 contain the supplementary crystallographic data for the structures unveiled in this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

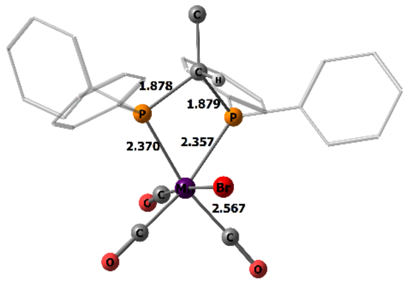
Computational results

All structures of complexes and transition states were optimized by Gaussian 09[11] utilizing BP86 functional[12] with def2-TZVP basis set[13] without any symmetry restrictions. Optimizations were performed in the toluene introduced with the SMD continuum solvation model.[14] This approach was previously successfully applied for Mn(I) complexes [(κ^2*P,Ĉ*-Ph_2PCH_2NHC)$Mn(CO)_3X$].[15] The overall geometry of complexes *fac*-**2**$^{\mathbf{Ph}}$ and *fac,anti*-**3**$^{\mathbf{Ph}}$ is well described by the chosen approach (Table S1) except Mn−H distance being 0.058 Å longer than experimentally observed value. This difference can be explained by a systematic shortening of X−H bond determined by X-ray diffraction due to the localization of hydrogen atom electron between X and H nuclei and libration phenomenon.[16] All minima on the PES were confirmed to have no negative values in their diagonalized force constants matrix. The transition state structures showed only one negative eigenvalue in their diagonalized force constant matrices, and their associated eigenvectors were confirmed to correspond to the motion along the reaction coordinate under consideration using the intrinsic reaction coordinate (IRC) method.[17] Wiberg bond indexes (WBI)[18] and charges were calculated using NBO6 method.[19]

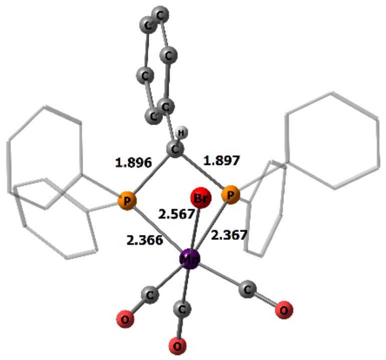
Table S1. Calculated and experimental bond distances (Å) and valent angles (°) for Mn(I) complexes *fac*-**2**$^{\mathbf{Ph}}$ and *fac,anti*-**3**$^{\mathbf{Ph}}$.

	fac-**2**$^{\mathbf{Ph}}$			*fac,anti*-**3**$^{\mathbf{Ph}}$ (X=H)		
	X-ray	DFT	Δ	X-ray	DFT	Δ
Mn–X	-	-		1.528	1.586	-0.058
Mn–P^1	2.222	2.252	-0.030	2.283	2.289	-0.006
Mn–P^2	2.225	2.258	-0.033	2.255	2.289	-0.034
Mn–C$_{br}$	2.214	2.246	-0.032	3.123	3.150	-0.027
Mn–CO^1	1.795	1.787	0.008	1.813	1.810	0.003
Mn–CO^2	1.798	1.797	0.001	1.794	1.797	-0.003
Mn–CO^3	1.804	1.798	0.006	1.820	1.797	0.023
P^1–C$_{br}$	1.775	1.791	-0.016	1.888	1.903	-0.015
P^2–C$_{br}$	1.772	1.786	-0.014	1.874	1.903	-0.029
C^1–O^1	1.164	1.168	-0.004	1.150	1.167	-0.017
C^2–O^2	1.159	1.167	-0.008	1.147	1.166	-0.019
C^3–O^3	1.156	1.166	-0.010	1.153	1.166	-0.013
P^1–C$_{br}$–P^2	103.6	104.7	-1.1	91.4	92.2	-0.8
X–Mn–P^1				79.2	80.0	-0.8
X–Mn–P^1				79.8	80.0	-0.2
X–Mn–CO^1				175.0	177.2	-2.2
X–Mn–CO^2				89.1	86.2	2.9
X–Mn–CO^3				89.3	86.3	3.0
Mn–C^1–O^1	177.7	179.6	-1.9	177.5	178.2	-0.7
Mn–C^2–O^2	175.5	175.9	-0.4	178.2	177.8	0.4
Mn–C^3–O^3	178.2	176.0	2.2	178.3	177.8	0.5

For octahedral Mn(I) [(κ^2-$Ph_2PCH(R)PPh_2$)$Mn(CO)_3X$] bromide complexes *fac*-**1**$^{\mathbf{R}}$ (R = Me, Ph) three isomers were located on PES: two facial *fac,syn*-**1**$^{\mathbf{R}}$ and *fac,anti*-**1**$^{\mathbf{R}}$ differing by the relative position of the hydrogen atom in dppm bridge to bromide ligand and one meridional *mer*-**1**$^{\mathbf{R}}$ (Figure S51). As expected *mer*-**1**$^{\mathbf{R}}$ are less stable than *fac*-**1**$^{\mathbf{R}}$ isomers. The latter are rather close in energy being consistent with their coexistence in solution observed by NMR spectroscopy. Similar situation was also found in calculated Mn(I) [(κ^2-$Ph_2PCH(R)PPh_2$)$Mn(CO)_3H$] hydride complexes *fac*-**3**$^{\mathbf{Me}}$ and *fac*-**3**$^{\mathbf{Ph}}$ (R = Me, Ph) (Figure S52), with only notable stronger destabilization of *fac,syn*-**3**$^{\mathbf{R}}$ *vs. fac,anti*-**3**$^{\mathbf{R}}$ isomers than calculated for the corresponding bromide derivatives *fac*-**1**$^{\mathbf{R}}$.

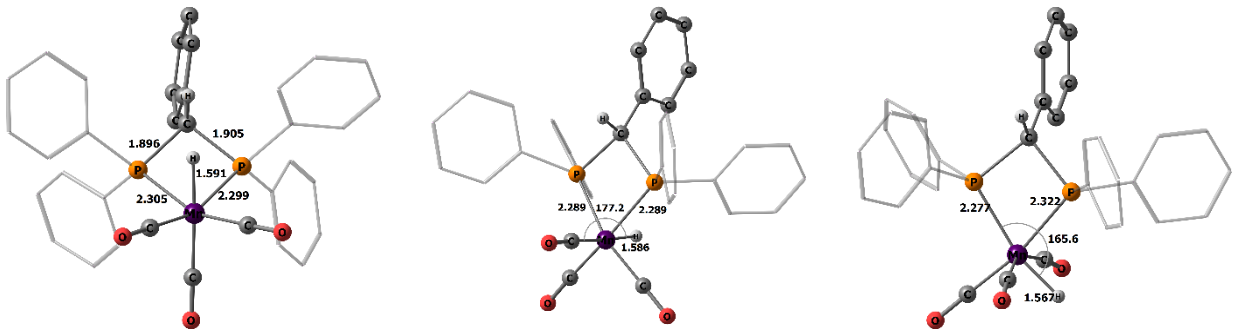


fac,syn-**1**$^{\mathbf{Me}}$ 0.0 (0.0) *fac,anti*-**1**$^{\mathbf{Me}}$ 0.3 (0.8) *mer*-**1**$^{\mathbf{Me}}$ 5.9 (5.3)

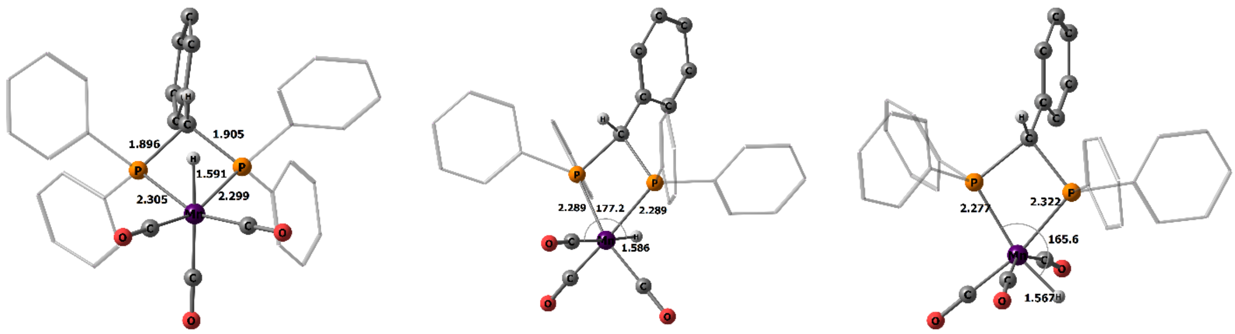


fac,syn-**1**$^{\mathbf{Ph}}$ 0.0 (0.0) *fac,anti*-**1**$^{\mathbf{Ph}}$ **−**0.2 (0.3) *mer*-**1**$^{\mathbf{Ph}}$ 3.9 (4.6)

Figure S51. Optimized structures and thermodynamic data for Mn(I) complexes [($Ph_2PCH(R)PPh_2$)Mn(CO)$_3$Br] (*fac*-**1**$^{\mathbf{Me}}$, R = Me, upper line; *fac*-**2**$^{\mathbf{Ph}}$, R = Ph, bottom line). Related ΔG^{298} and ΔE (in parenthesis) are given in kcal.mol^{-1} and referred to *fac,syn*-**1**$^{\mathbf{R}}$.



fac,syn-**3**$^{\mathbf{Ph}}$ 0.0 (0.0) *fac,anti*-**3**$^{\mathbf{Ph}}$ −3.2 (−2.6) *mer*-**3**$^{\mathbf{Ph}}$ 2.4 (3.0)



fac,syn-**3**$^{\mathbf{Ph}}$ 0.0 (0.0) *fac,anti*-**3**$^{\mathbf{Ph}}$ −2.5 (−1.8) *mer*-**3**$^{\mathbf{Ph}}$ 4.0 (5.1)

Figure S52. Optimized structures and thermodynamic data for Mn(I) complexes [($Ph_2PCH(R)PPh_2$)Mn(CO)$_3$H] (*fac*-**3**$^{\mathbf{Me}}$, R = Me, upper line; *fac*-**3**$^{\mathbf{Ph}}$, R = Ph, bottom line). Related ΔG^{298} and ΔE (in parenthesis) are given in kcal.mol^{-1} and referred to *fac,syn*-**3**$^{\mathbf{R}}$.

The optimized geometries and thermodynamic data for diphosphinomethanide complexes *fac*-**2**^{R} and **4**^{R} and for the corresponding transition states **TS1**^{R} (*fac*-**2**^{R} → **4**^{R}) and **TS2**^{R} (**4**^{R} → *fac,syn*-**3**^{R}) are shown in Figure S53.

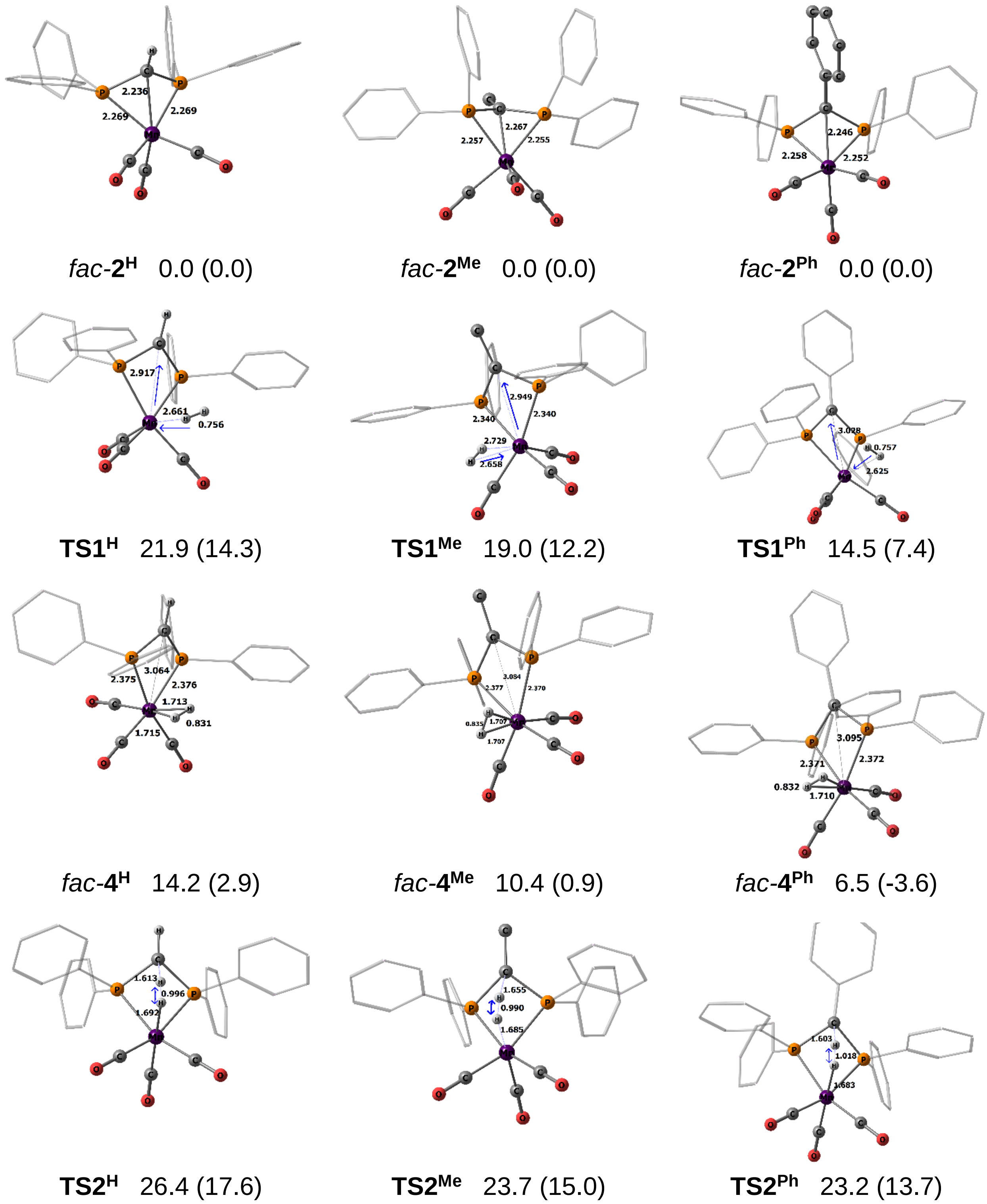
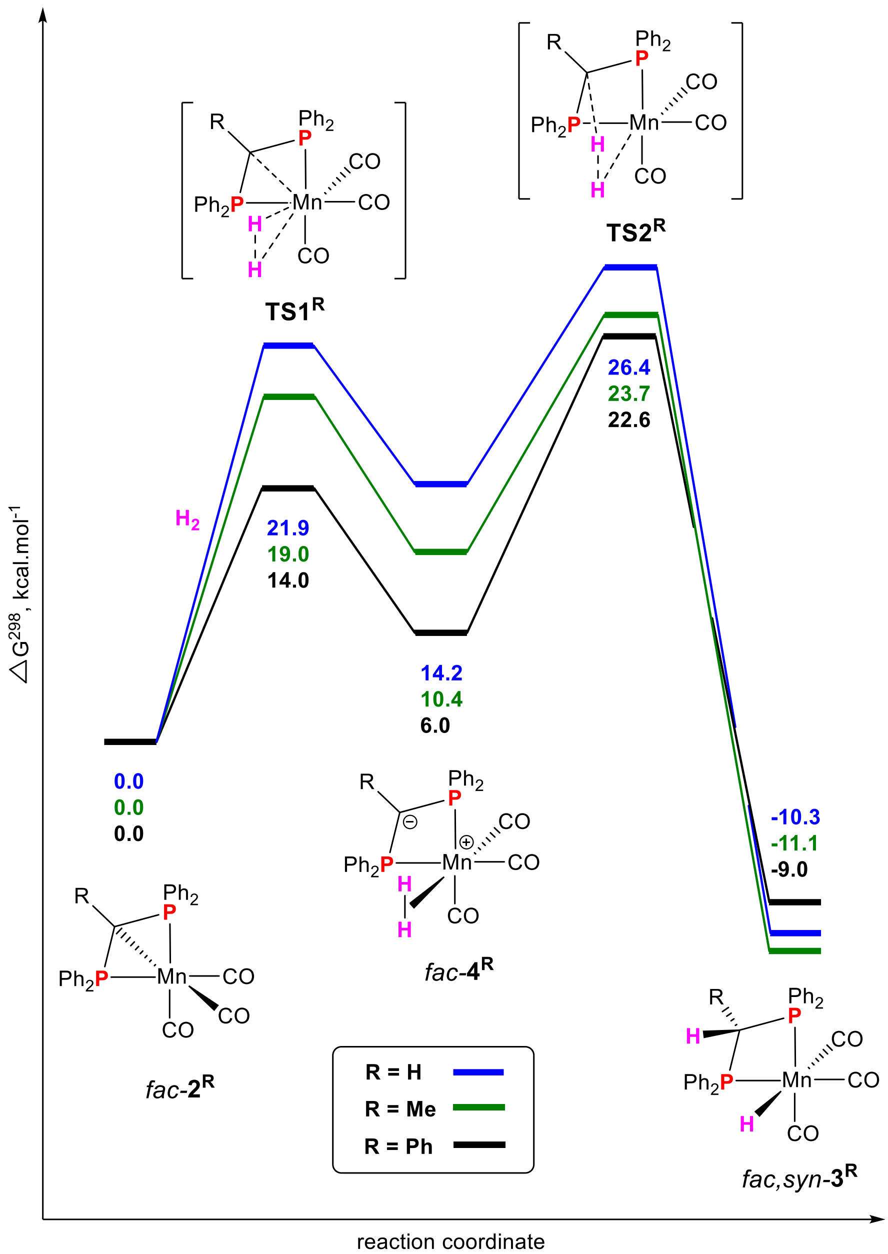


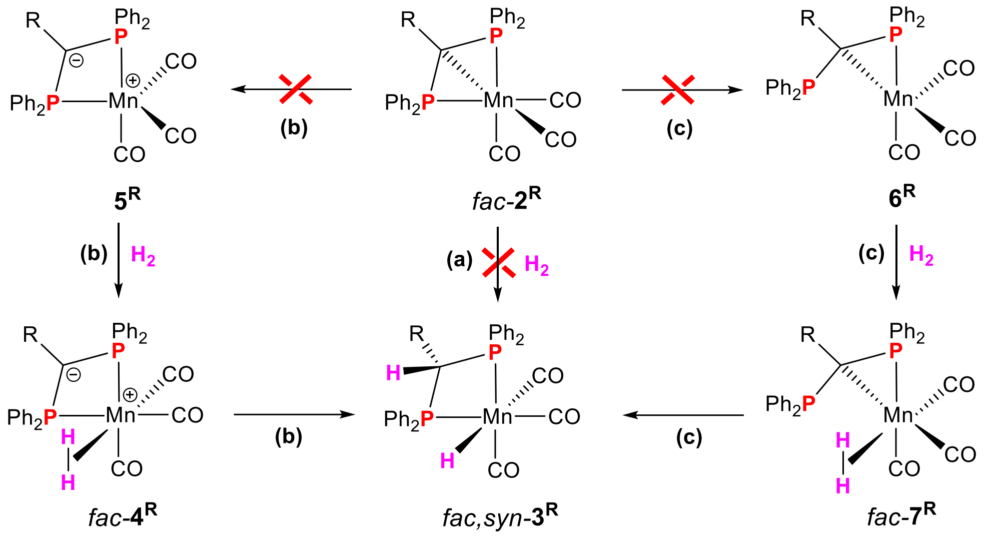
Figure S53. Optimized structures and thermodynamic data for Mn(I) complexes *fac*-[(κ^{3}*P,C,P*-$Ph_2PC(R)PPh_2$)$Mn(CO)_3$] (*fac*-**2**^{R}), *fac*-[(κ^{2}*P,P*-$Ph_2PC(R)PPh_2$)$Mn(CO)_3$(η^{2}-H_2)] (*fac*-**4**^{R}) and transition states **TS1**^{R} and **TS2**^{R} (R = H, left column; R = Me, central column; R = Ph, right column). Related ΔG^{298} and ΔE (in parenthesis) are given in kcal.mol^{-1} and referred to the reactants (*fac*-**2**^{R} + H_2).

The additional ΔH^{298} profile for the mechanism of cooperative H_2 activation by complexes *fac*-**2^{R}** is shown in Scheme S1, all energies summarized in Table S2. Calculated WBI and charges for *fac*-**2^{R}**-**4^{R}** are given in Table S2.



Scheme S1. DFT mechanism of cooperative H_2 activation with complexes *fac*-**2^{R}** (BP86/def2-TZVP, toluene SMD model, ΔH^{298} are given in kcal.mol^{-1} and referred to the reactants (*fac*-**2^{R}** + H_2).

Besides this established reaction pathway, we have explored several alternative mechanisms presented in Scheme S2. In particular, it was shown that a concerted H_2 molecule addition across Mn−C bond in complexes *fac*-**2^{R}** to form directly the hydride products *fac,syn*-**3^{R}** (path (a)) is not possible, as no transition state was located for this process. The stepwise formation of η^2-H_2 complexes *fac*-**4^{R}** from *fac*-**2^{R}** *via* the 16-electron intermediates **5^{R}** (path (b)) obtained though the heterolytic cleavage of the Mn−C bond is also not feasible due to the absence of minima on the PESs for the structures **5^{R}**. Finally, we considered the dissociation of one of the phosphine moieties in *fac*-**2**^{R} to form unsaturated species **6**^{R}, followed by H_2 coordination to form another η^2-H_2 complexes **7**^{R} and cooperative activation (path (c)), but here again we failed to optimize any compounds **6**^{R}.



Scheme S2. Alternative mechanistic possibilities for cooperative H_2 activation with complexes *fac*-**2**^{R} investigated by DFT methods.

Table S2. Energies (in kcal.mol^{-1}, referred to the reactants (*fac*-**2**^{R} + H_2) of transition states, intermediates and products for cooperative H_2 activation with complexes *fac*-**2**^{R}

		TS1^{R}	*fac*-**4**^{R}	**TS2**^{R}	*fac,syn*-**3**^{R}
R = Ph	ΔE	7.4	-3.6	13.7	-21.7
	$\Delta H^{\circ 298}$	8.1	-1.2	13.9	-17.8
	$\Delta G^{\circ 298}$	14.5	6.5	23.2	-8.5
R = Me	ΔE	12.2	0.9	15.0	-23.4
	$\Delta H^{\circ 298}$	12.5	3.1	15.0	-19.6
	$\Delta G^{\circ 298}$	19.0	10.4	23.7	-11.1
R = H	ΔE	14.3	2.9	17.6	-24.6
	$\Delta H^{\circ 298}$	14.8	5.4	17.9	-21.4
	$\Delta G^{\circ 298}$	21.9	14.2	26.4	-10.3

Table S3. NBO6 charges and Wiberg bond indexes (WBI)

charges	*fac*-**2**$^{\mathrm{H}}$	*fac*-**2**$^{\mathrm{Ph}}$	*fac*-**2**$^{\mathrm{Me}}$	*fac*-**4**$^{\mathrm{H}}$	*fac*-**4**$^{\mathrm{Ph}}$	*fac*-**4**$^{\mathrm{Me}}$	*fac*-**3**$^{\mathrm{H}}$	*fac,syn*-**3**$^{\mathrm{Ph}}$	*fac,syn*-**3**$^{\mathrm{Me}}$	*fac,anti*-**3**$^{\mathrm{Ph}}$	*fac,anti*-**3**$^{\mathrm{Me}}$
P^1	1.128	1.153	1.137	1.181	1.194	1.183	1.155	1.157	1.148	1.175	1.160
P^2	1.128	1.145	1.137	1.191	1.200	1.208	1.155	1.157	1.150	1.175	1.160
Mn	-0.935	-0.960	-0.933	-1.133	-1.135	-1.136	-1.240	-1.229	-1.230	-1.266	-1.251
C_{br}	-1.038	-0.776	-0.765	-1.280	-0.958	-0.997	-1.038	-0.804	-0.782	-0.812	-0.788
H(C)	0.261			0.256			0.284	0.284	0.271	0.284	0.259
H(Mn)							-0.050	-0.007	-0.026	-0.029	-0.047
$C^1(O^1)$	0.602	0.610	0.606	0.704	0.715	0.707	0.600	0.565	0.578	0.603	0.603
$C^2(O^2)$	0.611	0.619	0.607	0.645	0.651	0.649	0.661	0.668	0.670	0.658	0.661
$C^3(O^3)$	0.611	0.609	0.607	0.642	0.647	0.643	0.661	0.671	0.665	0.658	0.661
WBI											
Mn–P^1	0.391	0.387	0.392	0.391	0.384	0.389	0.398	0.397	0.393	0.400	0.399
Mn–P^2	0.391	0.400	0.392	0.386	0.381	0.384	0.398	0.396	0.395	0.400	0.399
Mn–C_{br}	0.307	0.298	0.282	0.013	0.015	0.015	0.017	0.020	0.020	0.018	0.017
Mn–CO^1	0.899	0.895	0.906	0.882	0.873	0.875	0.773	0.786	0.784	0.761	0.771
Mn–CO^2	0.852	0.847	0.848	0.818	0.813	0.817	0.836	0.825	0.827	0.828	0.832
Mn–CO^3	0.852	0.839	0.849	0.818	0.816	0.817	0.836	0.828	0.837	0.828	0.832
C^1–O^1	2.043	2.040	2.037	2.082	2.093	2.081	2.042	2.014	2.020	2.047	2.040
C^2–O^2	2.054	2.048	2.047	2.097	2.103	2.099	2.049	2.053	2.059	2.043	2.048
C^3–O^3	2.054	2.049	2.047	2.092	2.096	2.091	2.049	2.060	2.049	2.043	2.048
Mn–H^1				0.171	0.168	0.168	0.375	0.369	0.372	0.373	0.370
Mn–H^2				0.166	0.166	0.172					
H–H(Mn)				0.631	0.632	0.622					

The reaction of *fac*-**2**^{R} with H_2 can be formally considered as a ring opening of the bicyclic [1,1,0] structure and should be facilitated for the molecules having higher geometrical strain. The deviation of valent angles from ideal tetrahedral geometry (109.5°) for the bridging sp^3-carbon atom in *fac*-**2**^{R} revealed lower distortion for *fac*-**2**^{H} (R−C−P 125.2°, P−C−P 109.4°, H−C−Mn 135.7°) compared to the bridge-substituted derivatives (*fac*-**2**^{Me}: R−C−P 126.9°, P−C−P 105.1°, R−C−Mn 142.8; *fac*-**2**^{Ph}: R−C−P 127.6°, P−C−P 104.7°, R−C−Mn 134.7°). In order to get more precise estimation of the influence of this parameter, we have performed the scan of potential energy of *fac*-**2**^{R} upon increasing the dihedral angle Mn−P−C−P (Figure S54).

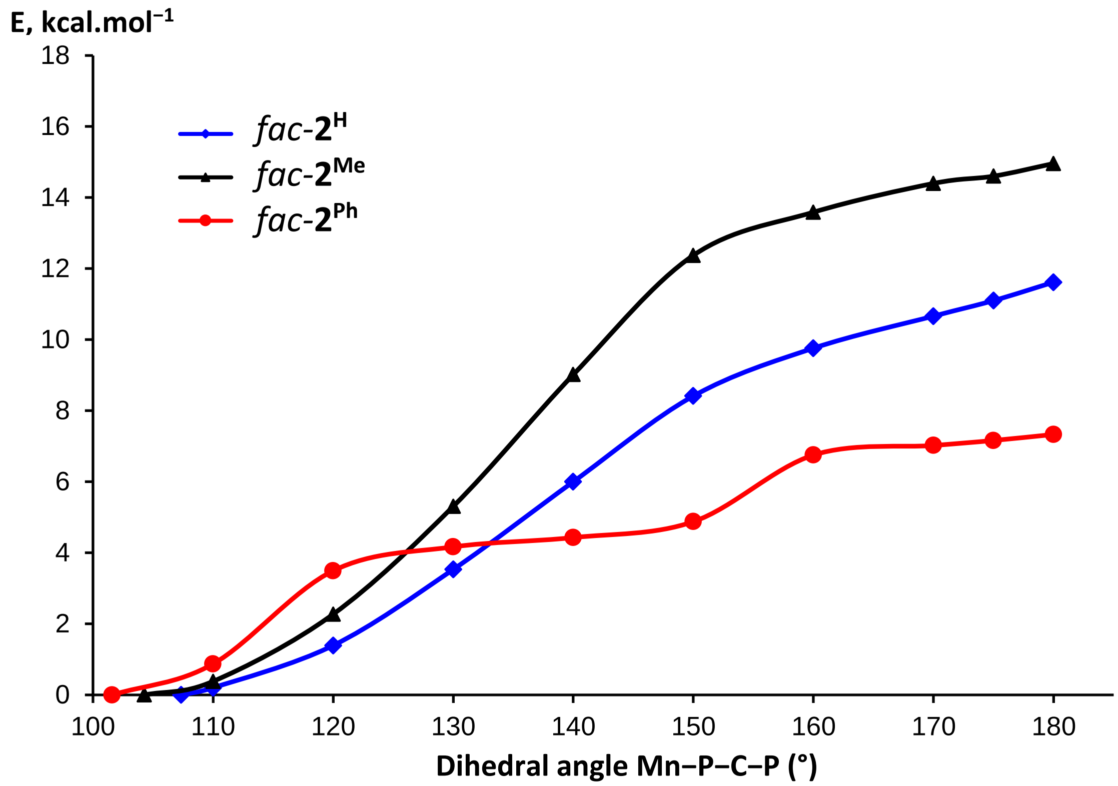
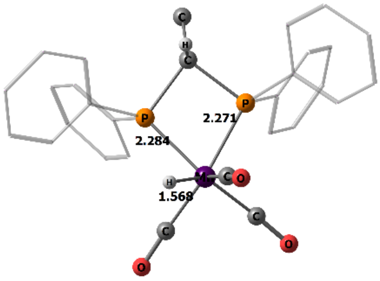


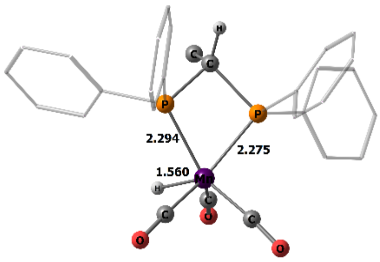
Figure S54. The potential energy profile for complexes *fac*-**2**^{R} upon increasing the dihedral angle Mn−P−C−P up to 180°

These results are consistent with an easier Mn−C bond dissociation in the *fac*-**2**^{Ph} > *fac*-**2**^{Me} > *fac*-**2**^{H} order due to both reduced Mn−C bond strength (according to WBI data) and higher energy of strain release. The energy values obtained at the final deformation point (15.0, 11.6, and 7.3 kcal.mol^{-1} for *fac*-**2**^{H}, *fac*-**2**^{Me}, and *fac*-**2**^{Ph}, respectively) correlate with the corresponding values of **TS1**^{R} (ΔE = 7.0-7.5 kcal.mol^{-1}). This qualitative estimation indicates that the Mn−C bond dissociation roughly represents 2/3 of the overall ΔG^{298} for the *fac*-**2**^{R} +H_2 → *fac*-**4**^{R} process, while the H_2 binding increment remains close in the series of complexes.

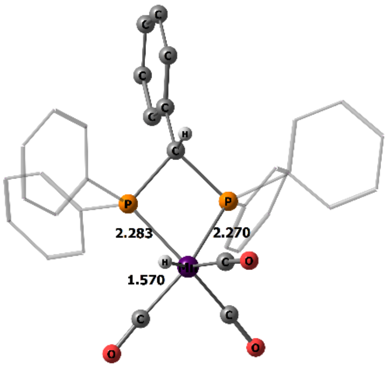
The geometry of the transition states **TS3**^{R} and **TS4**^{R} responsible for the isomerization of hydrides *fac,syn*-**3**^{R} into *fac,anti*-**3**^{R} and the associated thermodynamic values are shown in Figure S55. In order to illustrate better the synchronous rotation of $[Mn(CO)_3H]$ moiety in the transformations *fac,syn*-**3**^{R} → *mer*-**3**^{R} and *mer*-**3**^{R} → *fac,anti*-**3**^{R} animated gif files are provided in the ESI for R = Ph.



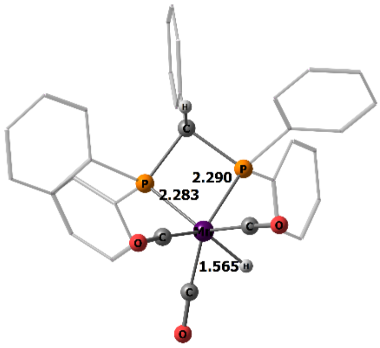
TS3^{Me} 14.3 (15.5)



TS4^{Me} 18.8 (18.6)



TS3^{Ph} 15.0 (15.9)



TS4^{Ph} 16.4 (17.8)

Figure S55. Optimized geometries and thermodynamic data for transition states **TS3^{R}** and **TS4^{R}** (R = Me, upper line; R = Ph, bottom line) responsible for *fac,syn*-**3^{R}** → *mer*-**3^{R}** → *fac,anti*-**3^{R}** isomerization process. Related ΔG^{298} and ΔE (in parenthesis) are given in kcal.mol^{-1} and referred to *fac,syn*-**3^{R}**.

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XYZ coordinates of BP86 optimized species

fac,syn-**1^{Me}**, E(tol)=-5754.33007829

6	-0.269923000	1.077542000	2.305207000
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1	-0.064446000	-1.078158000	-1.718632000
6	2.725550000	-0.937435000	-0.879042000
6	2.605979000	-1.824746000	-1.958701000
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1	3.585581000	-3.300426000	-3.189957000
6	4.902403000	-2.539282000	-1.652220000
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35	0.178533000	-2.886205000	0.601792000
6	-0.071167000	0.751456000	-2.873767000
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fac,anti-**1^{Me}**, E(tol)=-5754.32880493

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1	5.884368000	-2.781386000	-2.361147000
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1	0.889305000	-0.953113000	-3.246535000
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mer-**1**^{Me}, E(tol)=-5754.32163395

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1	5.273034000	-3.050752000	-3.042770000
6	4.189635000	-2.604554000	-1.225069000
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6	3.214833000	-1.803609000	-0.619905000
1	2.966525000	-1.941711000	0.436093000
6	1.950585000	1.913127000	-0.574997000
6	3.335365000	2.129893000	-0.678777000
1	4.015187000	1.284617000	-0.793256000
6	3.853515000	3.427619000	-0.631762000
1	4.932270000	3.578459000	-0.708119000
6	2.999229000	4.523382000	-0.486046000
1	3.406126000	5.535975000	-0.451995000
6	1.620663000	4.316289000	-0.371806000
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1	0.024201000	2.877268000	-0.287750000
6	-2.677610000	-1.342880000	-0.886104000
6	-3.906827000	-1.431798000	-0.205811000
1	-4.155759000	-0.707341000	0.572377000
6	-4.821619000	-2.438664000	-0.518887000
1	-5.769077000	-2.492430000	0.021239000
6	-4.526874000	-3.372194000	-1.517996000
1	-5.243242000	-4.158530000	-1.764020000
6	-3.308026000	-3.295588000	-2.195746000
1	-3.065610000	-4.021040000	-2.975101000
6	-2.386580000	-2.292162000	-1.878591000
1	-1.438257000	-2.267798000	-2.417988000
6	-2.569819000	1.437541000	-0.305234000
6	-2.676110000	2.212232000	0.859510000
1	-2.105131000	1.938092000	1.746467000
6	-3.526880000	3.322464000	0.901786000
1	-3.603009000	3.908559000	1.819751000
6	-4.278867000	3.671220000	-0.222052000
1	-4.942918000	4.537506000	-0.190194000
6	-4.190674000	2.897727000	-1.385693000
1	-4.786504000	3.157201000	-2.263322000
6	-3.349780000	1.784539000	-1.425942000
1	-3.313999000	1.173643000	-2.329507000
15	1.259609000	0.211069000	-0.551915000
15	-1.477026000	-0.048331000	-0.344992000
25	-0.006018000	-0.544563000	1.294006000
8	-2.092958000	-1.291297000	3.253464000
8	0.375325000	2.021254000	2.787921000
8	0.188935000	-3.422991000	0.510785000
35	1.967481000	-1.151523000	2.826390000
6	-0.411099000	1.181102000	-2.852811000
1	-1.264996000	0.893041000	-3.484902000
1	-0.592620000	2.197044000	-2.480078000
1	0.476182000	1.218991000	-3.502039000

fac,syn-**1**^{Ph}, E(tol)=-5946.13022300

6	-0.040799000	-0.828260000	-2.962388000
6	-1.367387000	-2.651468000	-1.902268000
6	1.261885000	-2.685624000	-1.881436000
6	-0.009729000	0.515952000	1.001494000
1	-0.053327000	-0.318101000	1.725308000
6	-2.806451000	-0.619289000	0.817632000
6	-3.888880000	-1.167417000	0.106947000
1	-3.865327000	-1.202068000	-0.984875000
6	-4.997397000	-1.673709000	0.786924000
1	-5.827590000	-2.102901000	0.222395000
6	-5.038655000	-1.639364000	2.184992000
1	-5.903218000	-2.041257000	2.717189000
6	-3.967419000	-1.094674000	2.897020000
1	-3.991690000	-1.066177000	3.988409000
6	-2.854082000	-0.587761000	2.218366000
1	-2.029686000	-0.164642000	2.793261000
6	-2.115010000	1.523418000	-0.929178000
6	-3.098329000	2.253984000	-0.234659000
1	-3.447974000	1.912888000	0.740635000
6	-3.641170000	3.415354000	-0.788037000
1	-4.403737000	3.968687000	-0.235904000
6	-3.214502000	3.864975000	-2.041786000
1	-3.644919000	4.769996000	-2.475691000
6	-2.241388000	3.145484000	-2.740038000
1	-1.907278000	3.482125000	-3.723520000
6	-1.697443000	1.981466000	-2.188769000
1	-0.945751000	1.429668000	-2.749848000
6	2.718599000	-0.790294000	0.921644000
6	2.610860000	-0.989499000	2.305280000
1	1.704255000	-0.705060000	2.839390000
6	3.670319000	-1.556437000	3.021519000
1	3.573619000	-1.703537000	4.099190000
6	4.840219000	-1.941353000	2.362831000
1	5.662415000	-2.391041000	2.923203000
6	4.952158000	-1.753471000	0.981040000
1	5.860470000	-2.055837000	0.455975000
6	3.900415000	-1.180121000	0.265278000
1	4.002013000	-1.035038000	-0.812771000
6	2.241826000	1.346314000	-0.871597000
6	2.223885000	1.571059000	-2.256283000
1	1.684535000	0.889533000	-2.912302000
6	2.917171000	2.652108000	-2.811280000
1	2.898515000	2.806995000	-3.891941000
6	3.637027000	3.519752000	-1.987026000
1	4.179986000	4.362713000	-2.419740000
6	3.671501000	3.297613000	-0.605570000
1	4.240698000	3.965842000	0.043943000
6	2.985335000	2.216799000	-0.050098000
1	3.039017000	2.043534000	1.025547000
6	0.025083000	1.826108000	1.735910000
6	0.073826000	1.824021000	3.143523000
1	0.084036000	0.870396000	3.678033000
6	0.108245000	3.017443000	3.867919000
1	0.145589000	2.988104000	4.959034000
6	0.094033000	4.243831000	3.196184000
1	0.119387000	5.179367000	3.758763000

6	0.047101000	4.262994000	1.799178000
1	0.036631000	5.215253000	1.264906000
6	0.015313000	3.068373000	1.074913000
1	-0.017283000	3.104867000	-0.013899000
15	-1.395464000	-0.003308000	-0.183629000
15	1.377741000	-0.103684000	-0.133798000
25	-0.043035000	-1.556536000	-1.347559000
8	-0.060238000	-0.500014000	-4.087619000
8	-2.191010000	-3.369566000	-2.292310000
8	2.084853000	-3.411961000	-2.256956000
35	-0.131927000	-2.964673000	0.797190000

fac,anti-$\mathbf{1}^{\mathbf{Ph}}$, E(tol)=-5946.12978905

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6	-1.293717000	-1.412208000	-2.850446000
6	1.293699000	-1.412209000	-2.850453000
6	0.000003000	0.350700000	1.244226000
1	0.000002000	-0.325210000	2.111056000
6	-2.282345000	-1.558820000	1.085453000
6	-3.063979000	-2.484414000	0.372009000
1	-3.085173000	-2.454639000	-0.719414000
6	-3.817028000	-3.447759000	1.045989000
1	-4.415778000	-4.160293000	0.475183000
6	-3.795813000	-3.505507000	2.442893000
1	-4.378131000	-4.264018000	2.969777000
6	-3.022523000	-2.589963000	3.161250000
1	-3.000684000	-2.626491000	4.252520000
6	-2.272950000	-1.620269000	2.487751000
1	-1.687563000	-0.909595000	3.074282000
6	-2.711329000	0.995194000	-0.052752000
6	-3.276145000	1.590378000	1.089647000
1	-2.887637000	1.360802000	2.083035000
6	-4.345480000	2.478378000	0.963717000
1	-4.772679000	2.939293000	1.856704000
6	-4.870158000	2.771302000	-0.300166000
1	-5.708493000	3.464598000	-0.396253000
6	-4.318928000	2.176130000	-1.437271000
1	-4.721702000	2.401309000	-2.426846000
6	-3.240588000	1.293824000	-1.317112000
1	-2.797340000	0.853528000	-2.209740000
6	2.282337000	-1.558832000	1.085447000
6	2.272928000	-1.620295000	2.487744000
1	1.687532000	-0.909630000	3.074276000
6	3.022499000	-2.589993000	3.161240000
1	3.000649000	-2.626533000	4.252509000
6	3.795799000	-3.505528000	2.442881000
1	4.378115000	-4.264041000	2.969764000
6	3.817026000	-3.447766000	1.045978000
1	4.415784000	-4.160292000	0.475171000
6	3.063980000	-2.484417000	0.372001000
1	3.085183000	-2.454633000	-0.719422000
6	2.711335000	0.995180000	-0.052756000
6	3.240605000	1.293800000	-1.317113000
1	2.797361000	0.853500000	-2.209742000
6	4.318949000	2.176100000	-1.437269000
1	4.721732000	2.401272000	-2.426843000
6	4.870173000	2.771277000	-0.300164000
1	5.708513000	3.464568000	-0.396249000
6	4.345485000	2.478362000	0.963717000
1	4.772680000	2.939280000	1.856704000
6	3.276146000	1.590367000	1.089644000
1	2.887630000	1.360798000	2.083031000
6	0.000009000	1.768850000	1.747382000
6	0.000016000	2.004334000	3.134661000
1	0.000016000	1.157496000	3.827348000
6	0.000023000	3.306369000	3.642783000
1	0.000029000	3.467061000	4.723061000
6	0.000024000	4.397398000	2.768659000
1	0.000030000	5.416086000	3.161792000
6	0.000018000	4.174677000	1.387756000
1	0.000018000	5.019848000	0.696402000
6	0.000010000	2.874327000	0.879140000
1	0.000005000	2.711310000	-0.202342000
15	-1.389164000	-0.274933000	0.103189000
15	1.389162000	-0.274939000	0.103185000
25	-0.000006000	-1.014976000	-1.652467000
8	-0.000003000	-3.818186000	-0.759367000
8	-2.086673000	-1.708755000	-3.645631000
8	2.086658000	-1.708715000	-3.645651000
35	-0.000007000	1.357645000	-2.637816000

mer-$\mathbf{1}^{\mathbf{Ph}}$, E(tol)=-5946.12287815

6	0.575843000	-2.684976000	0.160211000
6	-0.698098000	-2.542739000	-2.025775000
6	0.244899000	-0.230568000	-2.523025000
6	-0.439528000	0.913704000	0.982421000
1	-0.475628000	0.612834000	2.039339000
6	-2.311687000	-1.379569000	1.333878000
6	-2.751729000	-2.671801000	0.997328000
1	-2.536225000	-3.082903000	0.009293000
6	-3.460918000	-3.444132000	1.919512000
1	-3.791511000	-4.446716000	1.640971000
6	-3.735600000	-2.940395000	3.194597000
1	-4.282342000	-3.547851000	3.918569000
6	-3.301861000	-1.657861000	3.539954000
1	-3.510760000	-1.256948000	4.534096000
6	-2.597292000	-0.880429000	2.615263000
1	-2.277151000	0.121623000	2.907489000
6	-2.855078000	0.395323000	-0.819577000
6	-3.782094000	1.172126000	-0.099877000
1	-3.650140000	1.337908000	0.970476000
6	-4.881262000	1.738028000	-0.746240000
1	-5.588876000	2.344345000	-0.177030000
6	-5.077889000	1.526848000	-2.115978000
1	-5.941221000	1.967622000	-2.618732000
6	-4.170179000	0.746888000	-2.835248000
1	-4.319518000	0.569851000	-3.902187000
6	-3.062491000	0.185660000	-2.190923000
1	-2.365338000	-0.427152000	-2.762413000
6	2.178777000	-0.246617000	1.813022000
6	1.954207000	0.271397000	3.098740000
1	1.160070000	0.998837000	3.277920000
6	2.752516000	-0.133508000	4.172979000
1	2.564938000	0.274046000	5.168744000
6	3.784556000	-1.054733000	3.973420000
1	4.405253000	-1.371791000	4.813977000
6	4.016962000	-1.570263000	2.694515000
1	4.818498000	-2.293391000	2.530883000
6	3.219848000	-1.171940000	1.618930000
1	3.399548000	-1.585824000	0.622328000
6	2.249015000	1.673113000	-0.284904000
6	2.877375000	1.569748000	-1.535454000

1	2.740237000	0.671115000	-2.140066000
6	3.712993000	2.595937000	-1.989034000
1	4.201711000	2.500909000	-2.960782000
6	3.924405000	3.729644000	-1.201425000
1	4.575063000	4.531116000	-1.557866000
6	3.308363000	3.833088000	0.051597000
1	3.476242000	4.714230000	0.674402000
6	2.481189000	2.808596000	0.513127000
1	2.019337000	2.897477000	1.497709000
6	-0.805342000	2.367841000	0.872414000
6	-1.126424000	3.091813000	2.035484000
1	-1.103365000	2.589440000	3.006603000
6	-1.473718000	4.444149000	1.970310000
1	-1.717335000	4.985747000	2.886929000
6	-1.506073000	5.099359000	0.736101000
1	-1.776091000	6.155862000	0.681093000
6	-1.190042000	4.391736000	-0.428315000
1	-1.211728000	4.893738000	-1.397593000
6	-0.843148000	3.041218000	-0.361927000
1	-0.598339000	2.508299000	-1.282150000
15	-1.430898000	-0.408540000	0.031316000
15	1.226040000	0.269903000	0.321843000
25	0.275229000	-1.366014000	-1.083973000
8	0.770400000	-3.564603000	0.886003000
8	-1.314432000	-3.316261000	-2.641667000
8	0.244888000	0.409475000	-3.490619000
35	2.488772000	-2.188043000	-2.097898000

fac-**2^{H}**, E(tol)=-3139.91077958

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6	-1.252513000	-2.547849000	1.574676000
6	1.252255000	-2.548148000	1.574394000
6	0.000013000	-0.636467000	-0.900786000
6	-1.807396000	1.699644000	-0.067044000
6	-2.022505000	2.365979000	1.148602000
1	-1.930688000	1.817998000	2.089285000
6	-2.346733000	3.726737000	1.156002000
1	-2.514862000	4.239521000	2.105315000
6	-2.447773000	4.427419000	-0.048854000
1	-2.696322000	5.490833000	-0.043062000
6	-2.225715000	3.768295000	-1.264233000
1	-2.299331000	4.316646000	-2.205914000
6	-1.910654000	2.408261000	-1.276540000
1	-1.744044000	1.895137000	-2.226583000
6	-2.899591000	-0.879132000	-0.810701000
6	-4.155992000	-0.250676000	-0.786118000
1	-4.268695000	0.732777000	-0.326886000
6	-5.269529000	-0.876933000	-1.353560000
1	-6.240451000	-0.377858000	-1.325454000
6	-5.141372000	-2.131984000	-1.954861000
1	-6.011350000	-2.618112000	-2.401103000
6	-3.894466000	-2.765839000	-1.977203000
1	-3.787075000	-3.749240000	-2.439717000
6	-2.781254000	-2.149251000	-1.402632000
1	-1.816838000	-2.661102000	-1.405161000
6	1.807399000	1.699635000	-0.067029000
6	1.910803000	2.408189000	-1.276552000
1	1.744305000	1.895014000	-2.226588000
6	2.225863000	3.768222000	-1.264280000
1	2.299596000	4.316523000	-2.205981000
6	2.447777000	4.427412000	-0.048909000
1	2.696328000	5.490825000	-0.043145000
6	2.346590000	3.726794000	1.155971000
1	2.514607000	4.239627000	2.105278000
6	2.022366000	2.366035000	1.148604000
1	1.930449000	1.818103000	2.089305000
6	2.899643000	-0.879126000	-0.810603000
6	2.781329000	-2.149182000	-1.402673000
1	1.816897000	-2.661000000	-1.405366000
6	3.894586000	-2.765753000	-1.977177000
1	3.787212000	-3.749104000	-2.439800000
6	5.141510000	-2.131941000	-1.954637000
1	6.011521000	-2.618054000	-2.400831000
6	5.269642000	-0.876954000	-1.353197000
1	6.240577000	-0.377913000	-1.324933000
6	4.156064000	-0.250717000	-0.785816000
1	4.268747000	0.732686000	-0.326471000
1	0.000017000	-1.131683000	-1.876768000
15	-1.438436000	-0.094854000	-0.037475000
15	1.438450000	-0.094866000	-0.037438000
25	-0.000029000	-1.304838000	1.232830000
8	0.000090000	-0.181636000	3.963233000
8	-2.023403000	-3.377021000	1.854521000
8	2.022967000	-3.377638000	1.853778000

TS1^{H}, E(tol)=-3141.06506433

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6	1.314109000	-1.181549000	2.640732000
6	0.008469000	-0.421488000	-1.381987000
6	-2.159906000	1.512008000	-0.506009000
6	-2.776222000	2.132742000	0.591688000
1	-2.768009000	1.646486000	1.570262000
6	-3.392876000	3.379412000	0.444491000
1	-3.865274000	3.855709000	1.306306000
6	-3.391561000	4.018519000	-0.798858000
1	-3.866392000	4.995412000	-0.912140000
6	-2.770816000	3.409265000	-1.895256000
1	-2.760828000	3.909374000	-2.866302000
6	-2.157268000	2.162515000	-1.750001000
1	-1.665002000	1.693306000	-2.605885000
6	-2.723394000	-1.291758000	-0.757976000
6	-4.048917000	-1.056998000	-0.352583000
1	-4.302055000	-0.147678000	0.195968000
6	-5.055736000	-1.975894000	-0.658134000
1	-6.080826000	-1.780503000	-0.335949000
6	-4.756336000	-3.136370000	-1.379855000
1	-5.546450000	-3.849865000	-1.623081000
6	-3.441555000	-3.376439000	-1.790317000
1	-3.200248000	-4.277141000	-2.359269000
6	-2.430538000	-2.464326000	-1.474078000
1	-1.402444000	-2.655126000	-1.790639000
6	2.172345000	1.503457000	-0.480683000
6	2.127056000	2.193237000	-1.702151000
1	1.604288000	1.750945000	-2.554229000
6	2.734692000	3.445234000	-1.828157000
1	2.691369000	3.976014000	-2.781836000
6	3.390357000	4.020882000	-0.734209000
1	3.859323000	5.002303000	-0.831688000
6	3.434179000	3.342343000	0.487613000
1	3.934002000	3.792473000	1.348023000
6	2.824964000	2.090142000	0.615212000

1	2.851618000	1.571719000	1.576946000
6	2.730230000	-1.307187000	-0.759831000
6	2.394931000	-2.572863000	-1.271747000
1	1.343591000	-2.825335000	-1.426322000
6	3.391049000	-3.498576000	-1.591947000
1	3.113607000	-4.474330000	-1.996995000
6	4.737679000	-3.177082000	-1.393682000
1	5.517303000	-3.900624000	-1.641118000
6	5.081114000	-1.922546000	-0.880232000
1	6.130594000	-1.661826000	-0.726787000
6	4.086461000	-0.992066000	-0.567184000
1	4.372580000	-0.011336000	-0.183255000
1	0.015469000	-0.603036000	-2.461777000
15	-1.352585000	-0.134565000	-0.326618000
15	1.366886000	-0.144552000	-0.319470000
25	-0.000655000	-0.627832000	1.527703000
8	0.029033000	2.015908000	2.768520000
8	-2.181163000	-1.443099000	3.374911000
8	2.153694000	-1.492780000	3.384158000
1	0.202310000	-3.264627000	1.228553000
1	-0.442407000	-3.407365000	0.860449000

fac-**4^{H}**, E(tol)=-3141.08322618

6	-0.031170000	1.582620000	1.734872000
6	-1.323384000	-0.374600000	2.821942000
6	1.325741000	-0.334155000	2.814411000
6	0.004131000	-0.264537000	-1.467036000
6	-2.379458000	1.372536000	-0.656202000
6	-3.155624000	1.947673000	0.362784000
1	-3.133013000	1.533020000	1.373009000
6	-3.945779000	3.071883000	0.102929000
1	-4.538001000	3.514767000	0.906676000
6	-3.965069000	3.635695000	-1.176166000
1	-4.576757000	4.517781000	-1.377108000
6	-3.185199000	3.075931000	-2.193607000
1	-3.186175000	3.519100000	-3.191984000
6	-2.394428000	1.953547000	-1.934298000
1	-1.769546000	1.533587000	-2.726174000
6	-2.561059000	-1.486780000	-0.602240000
6	-3.806082000	-1.486815000	0.050747000
1	-4.097411000	-0.644596000	0.681208000
6	-4.686963000	-2.559677000	-0.104129000
1	-5.649772000	-2.546953000	0.411377000
6	-4.339934000	-3.645003000	-0.916886000
1	-5.031240000	-4.481617000	-1.037978000
6	-3.106342000	-3.650834000	-1.573723000
1	-2.830703000	-4.491347000	-2.214794000
6	-2.220419000	-2.580355000	-1.413080000
1	-1.252524000	-2.582182000	-1.920294000
6	2.388778000	1.363202000	-0.660656000
6	2.490637000	1.870424000	-1.966570000
1	1.936833000	1.392696000	-2.778294000
6	3.282194000	2.990009000	-2.233137000
1	3.350733000	3.374607000	-3.253215000
6	3.977351000	3.621565000	-1.195884000
1	4.588985000	4.502253000	-1.403078000
6	3.875491000	3.129207000	0.108153000
1	4.403964000	3.625395000	0.925047000
6	3.084698000	2.006370000	0.374885000
1	2.999956000	1.643524000	1.401544000
6	2.559164000	-1.495790000	-0.575590000
6	2.199735000	-2.625702000	-1.325864000
1	1.216218000	-2.654063000	-1.801230000
6	3.086595000	-3.698049000	-1.466685000
1	2.797130000	-4.566957000	-2.062213000
6	4.339620000	-3.657884000	-0.848409000
1	5.032261000	-4.495369000	-0.955116000
6	4.703923000	-2.537511000	-0.092734000
1	5.681476000	-2.498634000	0.392932000
6	3.822257000	-1.462461000	0.041079000
1	4.126056000	-0.591226000	0.624941000
1	0.005638000	-0.299565000	-2.558415000
15	-1.330554000	-0.121259000	-0.372311000
15	1.334876000	-0.123882000	-0.363152000
25	-0.003580000	-0.207223000	1.596866000
8	-0.050040000	2.734788000	1.869989000
8	-2.154547000	-0.477565000	3.628415000
8	2.165826000	-0.420168000	3.613499000
1	-0.362716000	-1.830068000	1.184466000
1	0.386912000	-1.875947000	1.540328000

TS2^{H}, E(tol)=-3141.05979575

6	-0.035636000	0.227539000	2.657790000
6	-1.345025000	-1.950191000	2.233304000
6	1.296253000	-1.947693000	2.271447000
6	0.013352000	-0.423141000	-1.428441000
6	-1.956498000	1.612917000	-0.304372000
6	-2.425206000	2.197330000	0.883172000
1	-2.405418000	1.628784000	1.815018000
6	-2.913391000	3.508230000	0.879573000
1	-3.273338000	3.954057000	1.809156000
6	-2.931093000	4.245820000	-0.307163000
1	-3.306066000	5.271414000	-0.308252000
6	-2.460208000	3.671098000	-1.493282000
1	-2.468346000	4.245836000	-2.421947000
6	-1.977775000	2.360783000	-1.493994000
1	-1.609127000	1.919919000	-2.423126000
6	-2.800911000	-1.074823000	-0.901184000
6	-4.083370000	-0.810244000	-0.390453000
1	-4.232850000	0.001196000	0.324930000
6	-5.177793000	-1.576226000	-0.797963000
1	-6.168562000	-1.360356000	-0.392427000
6	-5.007056000	-2.613003000	-1.721352000
1	-5.863876000	-3.210409000	-2.039661000
6	-3.734708000	-2.880517000	-2.234739000
1	-3.593978000	-3.685487000	-2.959422000
6	-2.636158000	-2.118036000	-1.826824000
1	-1.643834000	-2.331847000	-2.230030000
6	1.971679000	1.615596000	-0.300491000
6	2.208538000	2.265962000	-1.524942000
1	2.020947000	1.744801000	-2.466887000
6	2.681784000	3.578728000	-1.544863000
1	2.859007000	4.077126000	-2.500460000
6	2.929579000	4.255076000	-0.344005000
1	3.298280000	5.282797000	-0.361976000
6	2.701853000	3.613856000	0.875831000
1	2.891717000	4.136945000	1.815409000
6	2.223640000	2.298961000	0.898918000
1	2.047898000	1.803215000	1.854717000
6	2.818341000	-1.074735000	-0.842390000
6	2.692620000	-2.071758000	-1.822644000
1	1.721978000	-2.251586000	-2.290027000

6	3.803230000	-2.832327000	-2.201826000
1	3.694530000	-3.602064000	-2.969060000
6	5.046656000	-2.608224000	-1.604124000
1	5.912364000	-3.204690000	-1.899391000
6	5.178274000	-1.616727000	-0.625604000
1	6.146111000	-1.437525000	-0.152573000
6	4.072301000	-0.853288000	-0.246487000
1	4.188190000	-0.080012000	0.516378000
1	0.019651000	-0.170800000	-2.498516000
15	-1.347045000	-0.118670000	-0.307466000
15	1.355048000	-0.114884000	-0.283510000
25	-0.013571000	-1.067013000	1.411320000
8	-0.051562000	0.990927000	3.540590000
8	-2.203960000	-2.525055000	2.767305000
8	2.136885000	-2.525394000	2.830763000
1	0.008185000	-1.743216000	-0.502183000
1	0.005242000	-2.339048000	0.295363000

fac-**3**$^{\mathbf{H}}$, E(tol)=-3141.12707023

6	-0.000016000	-1.031048000	2.352235000
6	1.300889000	1.267885000	2.614172000
6	-1.300919000	1.267854000	2.614195000
6	0.000007000	0.231483000	-1.496824000
1	0.000007000	-0.510579000	-2.305990000
6	2.156584000	-1.501634000	-0.403394000
6	2.864147000	-2.000594000	0.704333000
1	2.897929000	-1.422167000	1.630562000
6	3.514830000	-3.233969000	0.633618000
1	4.058322000	-3.608921000	1.503210000
6	3.458079000	-3.991387000	-0.541077000
1	3.957695000	-4.960955000	-0.592298000
6	2.754152000	-3.506103000	-1.646583000
1	2.704235000	-4.092838000	-2.566415000
6	2.110978000	-2.265756000	-1.580830000
1	1.578896000	-1.896437000	-2.459789000
6	2.679350000	1.311717000	-0.792786000
6	3.744032000	0.890096000	-1.608473000
1	3.832841000	-0.158297000	-1.897767000
6	4.704361000	1.806020000	-2.046960000
1	5.526937000	1.463525000	-2.678653000
6	4.617456000	3.150781000	-1.673915000
1	5.371947000	3.863601000	-2.013395000
6	3.566635000	3.576108000	-0.855717000
1	3.497767000	4.622096000	-0.549450000
6	2.605680000	2.662789000	-0.413931000
1	1.793224000	2.993912000	0.236390000
6	-2.156588000	-1.501621000	-0.403372000
6	-2.110965000	-2.265795000	-1.580774000
1	-1.578856000	-1.896520000	-2.459736000
6	-2.754149000	-3.506139000	-1.646484000
1	-2.704220000	-4.092918000	-2.566287000
6	-3.458104000	-3.991364000	-0.540970000
1	-3.957727000	-4.960930000	-0.592157000
6	-3.514869000	-3.233894000	0.633692000
1	-4.058380000	-3.608803000	1.503290000
6	-2.864174000	-2.000524000	0.704366000
1	-2.897952000	-1.422058000	1.630570000
6	-2.679341000	1.311712000	-0.792825000
6	-2.605659000	2.662798000	-0.414019000
1	-1.793190000	2.993939000	0.236277000
6	-3.566613000	3.576107000	-0.855823000
1	-3.497732000	4.622106000	-0.549596000
6	-4.617448000	3.150759000	-1.673993000
1	-5.371939000	3.863571000	-2.013488000
6	-4.704365000	1.805986000	-2.046990000
1	-5.526953000	1.463472000	-2.678658000
6	-3.744034000	0.890070000	-1.608486000
1	-3.832856000	-0.158332000	-1.897742000
1	0.000009000	1.235592000	-1.944416000
15	1.361529000	0.146252000	-0.227205000
15	-1.361521000	0.146260000	-0.227218000
25	-0.000016000	0.600044000	1.570966000
8	0.000167000	-2.059604000	2.904433000
8	2.131805000	1.722072000	3.294475000
8	-2.131889000	1.721984000	3.294472000
1	-0.000028000	2.009527000	0.826390000

fac-**2**$^{\mathbf{Me}}$, E(tol)=-3179.23131944

6	-0.001678000	-0.550775000	2.853261000
6	-1.247036000	-2.514750000	1.660166000
6	1.250276000	-2.510131000	1.662850000
6	-0.000342000	-0.615296000	-0.993665000
6	-1.779387000	1.713880000	-0.030582000
6	-2.015725000	2.340610000	1.202594000
1	-1.946832000	1.760911000	2.125914000
6	-2.333452000	3.701697000	1.251741000
1	-2.517278000	4.181357000	2.215400000
6	-2.407310000	4.446097000	0.070989000
1	-2.650401000	5.510068000	0.109946000
6	-2.165782000	3.828425000	-1.161717000
1	-2.219519000	4.408793000	-2.085408000
6	-1.856554000	2.467528000	-1.214977000
1	-1.679485000	1.989081000	-2.180697000
6	-2.937699000	-0.842014000	-0.738297000
6	-4.121736000	-0.099797000	-0.891023000
1	-4.144500000	0.957200000	-0.623592000
6	-5.281550000	-0.706188000	-1.383490000
1	-6.193084000	-0.114560000	-1.492052000
6	-5.275853000	-2.058435000	-1.734124000
1	-6.181474000	-2.529943000	-2.121340000
6	-4.104939000	-2.807574000	-1.577451000
1	-4.092095000	-3.867905000	-1.838255000
6	-2.948014000	-2.208563000	-1.076254000
1	-2.047654000	-2.809261000	-0.938594000
6	1.779619000	1.713627000	-0.030121000
6	1.857091000	2.467900000	-1.214102000
1	1.679714000	1.990067000	-2.180068000
6	2.167041000	3.828606000	-1.160109000
1	2.221022000	4.409460000	-2.083479000
6	2.408969000	4.445460000	0.072928000
1	2.652643000	5.509276000	0.112470000
6	2.334749000	3.700445000	1.253272000
1	2.518850000	4.179470000	2.217196000
6	2.016278000	2.339563000	1.203395000
1	1.946943000	1.759426000	2.126413000
6	2.936689000	-0.842580000	-0.739063000
6	2.946650000	-2.209415000	-1.075905000
1	2.046438000	-2.809984000	-0.936667000
6	4.103019000	-2.808831000	-1.577869000
1	4.089911000	-3.869384000	-1.837756000
6	5.273735000	-2.059793000	-1.736524000
1	6.178927000	-2.531622000	-2.124355000

6	5.279814000	-0.707266000	-1.386994000
1	6.191215000	-0.115716000	-1.497078000
6	4.120550000	-0.100486000	-0.893696000
1	4.143606000	0.956716000	-0.627102000
15	-1.412910000	-0.083866000	-0.051788000
15	1.412396000	-0.083951000	-0.052040000
25	-0.000033000	-1.291939000	1.233868000
8	-0.002414000	-0.059431000	3.913615000
8	-2.010304000	-3.323743000	2.012732000
8	2.016509000	-3.315486000	2.017329000
6	-0.000357000	-1.141250000	-2.413048000
1	0.885907000	-1.756056000	-2.624665000
1	-0.887673000	-1.754354000	-2.625212000
1	0.000648000	-0.312176000	-3.142799000

TS1^{Me}, E(tol)=-3180.38894130

6	0.001829000	1.025717000	2.298760000
6	-1.323287000	-1.101270000	2.708326000
6	1.325700000	-1.100082000	2.705150000
6	-2.171303000	1.523103000	-0.436037000
6	-2.780073000	2.131552000	0.673529000
1	-2.769136000	1.630192000	1.644284000
6	-3.398056000	3.379651000	0.548237000
1	-3.865311000	3.842983000	1.419884000
6	-3.406335000	4.036487000	-0.686039000
1	-3.882257000	5.014649000	-0.782499000
6	-2.796966000	3.440455000	-1.795417000
1	-2.797147000	3.951582000	-2.760775000
6	-2.184008000	2.190528000	-1.672391000
1	-1.710485000	1.732428000	-2.542990000
6	-2.726689000	-1.287307000	-0.665711000
6	-4.082317000	-0.935847000	-0.550078000
1	-4.361883000	0.079623000	-0.264436000
6	-5.084189000	-1.878172000	-0.802361000
1	-6.132960000	-1.589413000	-0.703731000
6	-4.748708000	-3.180393000	-1.183944000
1	-5.533050000	-3.913734000	-1.382690000
6	-3.402275000	-3.538659000	-1.310879000
1	-3.130155000	-4.552191000	-1.613916000
6	-2.401098000	-2.600793000	-1.048608000
1	-1.350516000	-2.884353000	-1.147533000
6	2.170881000	1.521757000	-0.434342000
6	2.177864000	2.193397000	-1.668496000
1	1.701874000	1.737506000	-2.538888000
6	2.788532000	3.444669000	-1.789727000
1	2.784221000	3.958955000	-2.753399000
6	3.401144000	4.038005000	-0.680738000
1	3.874991000	5.017322000	-0.775690000
6	3.398885000	3.376852000	0.551302000
1	3.868850000	3.837980000	1.422662000
6	2.783553000	2.127305000	0.674742000
1	2.777754000	1.622474000	1.643743000
6	2.727819000	-1.289306000	-0.663205000
6	2.403534000	-2.613006000	-1.010986000
1	1.353995000	-2.907027000	-1.080146000
6	3.406069000	-3.549274000	-1.273412000
1	3.135103000	-4.570997000	-1.548766000
6	4.752288000	-3.179631000	-1.181781000
1	5.537532000	-3.911921000	-1.380942000
6	5.086372000	-1.867416000	-0.834867000
1	6.134881000	-1.569724000	-0.763727000

6	4.083145000	-0.926717000	-0.582034000
1	4.361205000	0.096151000	-0.322737000
15	-1.349286000	-0.119615000	-0.266120000
15	1.350393000	-0.121771000	-0.264898000
25	-0.000374000	-0.579032000	1.590334000
8	0.002943000	2.079071000	2.802834000
8	-2.168555000	-1.393003000	3.453428000
8	2.174475000	-1.386428000	3.448864000
1	0.282031000	-3.210878000	1.346791000
1	-0.399212000	-3.217845000	1.018784000
1	0.014757000	0.255258000	-3.440312000
6	0.002492000	-0.673832000	-2.839902000
1	0.885558000	-1.257936000	-3.146386000
1	-0.890933000	-1.238497000	-3.152333000
6	0.000557000	-0.416628000	-1.353816000

fac-**4^{Me}**, E(tol)=-3180.40709016

6	-0.058650000	1.762256000	1.651286000
6	-1.330805000	-0.055886000	2.893813000
6	1.343318000	0.034439000	2.929832000
6	-2.367447000	1.397124000	-0.562850000
6	-3.618095000	1.559397000	0.058234000
1	-4.017761000	0.770429000	0.700069000
6	-4.359138000	2.726302000	-0.141812000
1	-5.327532000	2.844459000	0.349646000
6	-3.862831000	3.741721000	-0.968043000
1	-4.444811000	4.652271000	-1.126147000
6	-2.618269000	3.588792000	-1.585750000
1	-2.223882000	4.379103000	-2.228421000
6	-1.870779000	2.424708000	-1.378327000
1	-0.888346000	2.309312000	-1.842933000
6	-2.586218000	-1.436915000	-0.443810000
6	-3.394341000	-1.459235000	-1.598490000
1	-3.335183000	-0.643068000	-2.321716000
6	-4.290720000	-2.507630000	-1.820301000
1	-4.905265000	-2.510579000	-2.723353000
6	-4.409312000	-3.542871000	-0.886659000
1	-5.117671000	-4.356377000	-1.056589000
6	-3.625458000	-3.523423000	0.270228000
1	-3.723433000	-4.317651000	1.013555000
6	-2.719233000	-2.480140000	0.486573000
1	-2.127601000	-2.473731000	1.404254000
6	2.524232000	1.200168000	-0.672426000
6	2.914167000	1.412621000	-2.008490000
1	2.536794000	0.760507000	-2.798637000
6	3.785117000	2.453215000	-2.338388000
1	4.074667000	2.606767000	-3.380446000
6	4.286268000	3.295366000	-1.338880000
1	4.965776000	4.110023000	-1.598078000
6	3.911500000	3.089626000	-0.009009000
1	4.297000000	3.741626000	0.777829000
6	3.034649000	2.049981000	0.320740000
1	2.747256000	1.904629000	1.363311000
6	2.446275000	-1.647765000	-0.404668000
6	1.899499000	-2.860060000	-0.856691000
1	0.851666000	-2.887397000	-1.168493000
6	2.683759000	-4.015961000	-0.915367000
1	2.248402000	-4.949001000	-1.280591000
6	4.022915000	-3.976511000	-0.513236000
1	4.636294000	-4.878995000	-0.558624000
6	4.573935000	-2.774912000	-0.055050000

1	5.619270000	-2.736634000	0.259635000
6	3.793220000	-1.616513000	-0.004745000
1	4.239608000	-0.682377000	0.342932000
15	-1.323484000	-0.097124000	-0.251918000
15	1.339898000	-0.166130000	-0.277689000
25	0.023321000	-0.030038000	1.696660000
8	-0.124149000	2.919953000	1.688317000
8	-2.206593000	-0.029911000	3.657596000
8	2.169389000	0.100694000	3.745333000
1	0.388932000	-1.674054000	1.977855000
1	-0.170273000	-1.692289000	1.357938000
1	-0.139638000	0.418769000	-3.462526000
6	-0.047964000	-0.509731000	-2.868922000
1	0.859682000	-1.027997000	-3.220459000
1	-0.898030000	-1.153642000	-3.154555000
6	-0.006984000	-0.284868000	-1.376763000

TS2^{Me}, E(tol)=-3180.38460295

6	0.000179000	0.176991000	2.781851000
6	-1.322703000	-1.964632000	2.283384000
6	1.323334000	-1.964372000	2.283124000
6	-0.000015000	-0.329081000	-1.378485000
6	-2.024771000	1.633807000	-0.217358000
6	-1.989654000	2.427208000	0.940022000
1	-1.593906000	2.013814000	1.867992000
6	-2.469729000	3.740953000	0.915465000
1	-2.440311000	4.343665000	1.825608000
6	-2.988586000	4.275831000	-0.266146000
1	-3.362668000	5.301567000	-0.285940000
6	-3.034099000	3.490710000	-1.424275000
1	-3.444398000	3.901766000	-2.349264000
6	-2.561760000	2.177205000	-1.401078000
1	-2.620833000	1.568461000	-2.305556000
6	-2.794821000	-1.074034000	-0.769470000
6	-4.084773000	-0.775179000	-0.297396000
1	-4.243004000	0.087117000	0.353692000
6	-5.173158000	-1.573003000	-0.658935000
1	-6.169205000	-1.329792000	-0.282824000
6	-4.989218000	-2.676608000	-1.498034000
1	-5.841165000	-3.297830000	-1.782058000
6	-3.708799000	-2.982293000	-1.969321000
1	-3.556488000	-3.842677000	-2.624663000
6	-2.617040000	-2.189295000	-1.604328000
1	-1.618561000	-2.437784000	-1.970786000
6	2.024604000	1.633977000	-0.217359000
6	2.561304000	2.177635000	-1.401089000
1	2.620376000	1.569018000	-2.305651000
6	3.033400000	3.491231000	-1.424173000
1	3.443480000	3.902493000	-2.349168000
6	2.987920000	4.276181000	-0.265927000
1	3.361802000	5.301991000	-0.285639000
6	2.469342000	3.741044000	0.915691000
1	2.439941000	4.343630000	1.825918000
6	1.989514000	2.427207000	0.940139000
1	1.593965000	2.013603000	1.868104000
6	2.794858000	-1.073848000	-0.769666000
6	2.616907000	-2.189563000	-1.603884000
1	1.618320000	-2.438389000	-1.969823000
6	3.708637000	-2.982568000	-1.968930000
1	3.556186000	-3.843323000	-2.623751000
6	4.989207000	-2.676430000	-1.498334000

1	5.841136000	-3.297657000	-1.782398000
6	5.173321000	-1.572361000	-0.659890000
1	6.169490000	-1.328787000	-0.284336000
6	4.084954000	-0.774534000	-0.298288000
1	4.243310000	0.088119000	0.352291000
15	-1.351987000	-0.077075000	-0.212656000
15	1.352012000	-0.076968000	-0.212759000
25	0.000149000	-1.054765000	1.474614000
8	0.000198000	0.878414000	3.716918000
8	-2.173296000	-2.557766000	2.810027000
8	2.174201000	-2.557281000	2.809580000
1	0.000070000	-1.687884000	-0.433687000
1	0.000126000	-2.302850000	0.341844000
1	-0.885779000	-0.359865000	-3.356465000
1	-0.000187000	1.140637000	-3.011849000
1	0.885685000	-0.359708000	-3.356498000
6	-0.000074000	0.048405000	-2.842545000

fac,syn-**3^{Me}**, E(tol)=-3180.44570029

6	-0.146555000	0.670199000	2.655177000
6	1.391430000	-1.456989000	2.520832000
6	-1.188712000	-1.725883000	2.435213000
6	0.061260000	-0.249821000	-1.484821000
1	0.079863000	-1.333618000	-1.688464000
6	2.843967000	-1.058995000	-0.626794000
6	2.708645000	-2.253761000	-1.351859000
1	1.729811000	-2.576311000	-1.712524000
6	3.822509000	-3.056491000	-1.614076000
1	3.699487000	-3.978539000	-2.186185000
6	5.084099000	-2.686433000	-1.139356000
1	5.952948000	-3.316328000	-1.340820000
6	5.225465000	-1.509422000	-0.398259000
1	6.204452000	-1.217343000	-0.012489000
6	4.114930000	-0.700964000	-0.142795000
1	4.241855000	0.215019000	0.437584000
6	2.010201000	1.682646000	-0.389294000
6	2.814036000	2.027388000	-1.494058000
1	3.116869000	1.263145000	-2.212104000
6	3.245354000	3.343261000	-1.673424000
1	3.868388000	3.595036000	-2.534452000
6	2.884146000	4.333881000	-0.752770000
1	3.225764000	5.361739000	-0.892542000
6	2.092298000	4.000913000	0.348475000
1	1.811213000	4.765119000	1.075887000
6	1.658369000	2.683176000	0.528495000
1	1.043907000	2.430521000	1.392292000
6	-2.607116000	-1.377649000	-0.851363000
6	-3.800350000	-0.937451000	-1.449043000
1	-4.016657000	0.129491000	-1.521467000
6	-4.726173000	-1.860545000	-1.945792000
1	-5.650746000	-1.502196000	-2.403729000
6	-4.473897000	-3.231805000	-1.852329000
1	-5.200562000	-3.950840000	-2.236369000
6	-3.291670000	-3.679064000	-1.253198000
1	-3.092054000	-4.748973000	-1.162734000
6	-2.367427000	-2.760093000	-0.751298000
1	-1.457921000	-3.114941000	-0.260468000
6	-2.220779000	1.403804000	-0.191941000
6	-2.880433000	1.733044000	1.006720000
1	-2.811669000	1.059239000	1.863583000
6	-3.617358000	2.914049000	1.115186000

1	-4.124175000	3.149663000	2.053202000
6	-3.694311000	3.794959000	0.031772000
1	-4.258287000	4.725870000	0.120192000
6	-3.043544000	3.478963000	-1.163712000
1	-3.099844000	4.160199000	-2.015604000
6	-2.321602000	2.286527000	-1.281428000
1	-1.844487000	2.051441000	-2.231030000
15	1.381827000	-0.038437000	-0.163014000
15	-1.330101000	-0.207437000	-0.205574000
25	0.042447000	-0.757128000	1.563689000
8	-0.266955000	1.525138000	3.444783000
8	2.253046000	-1.944901000	3.134419000
8	-1.971596000	-2.380954000	2.998311000
1	0.223954000	-2.031245000	0.625441000
6	0.099425000	0.500669000	-2.809204000
1	-0.810549000	0.299687000	-3.396716000
1	0.205652000	1.585428000	-2.681666000
1	0.952522000	0.152088000	-3.412674000

TS3^{Me}, E(tol)=-3180.42102292

6	-1.159741000	0.233347000	2.756291000
6	1.227520000	-0.009473000	2.820306000
6	-0.688256000	-2.209923000	1.855313000
6	0.026571000	-0.253598000	-1.483846000
1	-0.028131000	-1.314765000	-1.779112000
6	2.660231000	-1.419444000	-0.596791000
6	2.568739000	-2.294701000	-1.689426000
1	1.713507000	-2.252645000	-2.366550000
6	3.573863000	-3.238820000	-1.929855000
1	3.487551000	-3.912074000	-2.785506000
6	4.679426000	-3.321216000	-1.080494000
1	5.460929000	-4.060653000	-1.266684000
6	4.778486000	-2.453199000	0.013110000
1	5.637607000	-2.511958000	0.684712000
6	3.777723000	-1.511074000	0.254331000
1	3.866827000	-0.842438000	1.113866000
6	2.266744000	1.397615000	-0.380877000
6	3.170798000	1.575291000	-1.445204000
1	3.366751000	0.757323000	-2.141350000
6	3.840311000	2.789706000	-1.608733000
1	4.539236000	2.914713000	-2.438688000
6	3.624950000	3.838773000	-0.707442000
1	4.155249000	4.785197000	-0.832959000
6	2.738617000	3.667026000	0.358660000
1	2.575596000	4.476190000	1.073642000
6	2.063477000	2.452759000	0.519956000
1	1.376737000	2.311562000	1.357357000
6	-2.705333000	-1.170637000	-0.636894000
6	-3.751323000	-1.325227000	0.291039000
1	-3.718239000	-0.793951000	1.245138000
6	-4.831245000	-2.162899000	0.008703000
1	-5.633588000	-2.274643000	0.740954000
6	-4.880316000	-2.864452000	-1.201253000
1	-5.722320000	-3.524798000	-1.418565000
6	-3.843608000	-2.721960000	-2.126411000
1	-3.872398000	-3.268243000	-3.071768000
6	-2.761578000	-1.879167000	-1.847074000
1	-1.963821000	-1.780873000	-2.585993000
6	-2.052336000	1.602424000	-0.408275000
6	-1.678041000	2.662999000	0.429561000
1	-0.964978000	2.477629000	1.235182000

6	-2.218448000	3.939736000	0.247297000
1	-1.922086000	4.752993000	0.913129000
6	-3.142639000	4.169793000	-0.775030000
1	-3.569919000	5.165113000	-0.914652000
6	-3.528795000	3.116999000	-1.612070000
1	-4.258390000	3.287388000	-2.406835000
6	-2.991390000	1.840855000	-1.429158000
1	-3.319095000	1.024237000	-2.075348000
15	1.351793000	-0.194117000	-0.157090000
15	-1.300636000	-0.072148000	-0.169523000
25	-0.015082000	-0.586992000	1.630212000
8	-1.875839000	0.711729000	3.547008000
8	2.002755000	0.316785000	3.629414000
8	-1.095295000	-3.293462000	2.058155000
1	0.850546000	-1.887608000	1.762516000
6	0.075204000	0.651171000	-2.708404000
1	-0.823706000	0.518262000	-3.330131000
1	0.137372000	1.712406000	-2.432611000
1	0.947814000	0.413778000	-3.336460000

mer-**3^{Me}**, E(tol)=-3180.44090104

6	-1.471046000	-0.763297000	2.732228000
6	0.310864000	1.042184000	2.618212000
6	0.240541000	-2.247610000	1.571526000
6	0.142990000	-0.162859000	-1.410329000
1	0.198645000	-1.219242000	-1.722661000
6	2.766023000	-1.224706000	-0.442066000
6	3.009315000	-1.682622000	-1.748111000
1	2.405136000	-1.320338000	-2.582476000
6	4.031682000	-2.604047000	-1.995943000
1	4.206690000	-2.956905000	-3.014624000
6	4.827153000	-3.069711000	-0.944675000
1	5.624234000	-3.790283000	-1.139216000
6	4.593852000	-2.616102000	0.357579000
1	5.206047000	-2.982109000	1.184371000
6	3.565429000	-1.704701000	0.609515000
1	3.370961000	-1.371246000	1.631645000
6	2.249131000	1.610291000	-0.256604000
6	3.572562000	1.729554000	-0.714339000
1	4.155797000	0.837111000	-0.944611000
6	4.157610000	2.990068000	-0.872418000
1	5.189618000	3.063767000	-1.222320000
6	3.429292000	4.146840000	-0.583682000
1	3.888345000	5.130066000	-0.706320000
6	2.111527000	4.038213000	-0.127781000
1	1.535476000	4.935365000	0.108131000
6	1.529172000	2.780524000	0.042560000
1	0.506803000	2.710294000	0.417979000
6	-2.505749000	-1.393792000	-0.714034000
6	-3.884591000	-1.195856000	-0.521902000
1	-4.252069000	-0.244345000	-0.134229000
6	-4.798089000	-2.210820000	-0.821339000
1	-5.864758000	-2.038212000	-0.662458000
6	-4.350941000	-3.437976000	-1.318180000
1	-5.065167000	-4.229585000	-1.553698000
6	-2.980882000	-3.649878000	-1.500928000
1	-2.618488000	-4.609105000	-1.876616000
6	-2.065611000	-2.640834000	-1.191597000
1	-0.999697000	-2.845291000	-1.313437000
6	-2.221093000	1.456860000	-0.468178000
6	-2.341424000	2.382306000	0.579792000

1	-1.884487000	2.156188000	1.545693000
6	-3.046696000	3.577134000	0.398977000
1	-3.136721000	4.282991000	1.227309000
6	-3.636172000	3.860869000	-0.835293000
1	-4.185410000	4.793746000	-0.979428000
6	-3.529090000	2.941621000	-1.885807000
1	-3.995214000	3.155041000	-2.850230000
6	-2.832945000	1.745064000	-1.703354000
1	-2.778411000	1.026496000	-2.523036000
15	1.427528000	-0.029356000	-0.038796000
15	-1.290388000	-0.109073000	-0.178458000
25	-0.038932000	-0.471458000	1.693753000
8	-2.414231000	-0.948627000	3.395258000
8	0.600736000	1.916443000	3.335455000
8	0.466540000	-3.390701000	1.627785000
1	1.094517000	-0.787122000	2.725506000
6	0.199507000	0.742530000	-2.635078000
1	-0.595455000	0.480619000	-3.349874000
1	0.088612000	1.803481000	-2.374352000
1	1.162914000	0.629132000	-3.156545000

TS4^{Me}, E(tol)=-3180.41602832

6	1.205509000	-0.265004000	2.745333000
6	0.808243000	-2.538116000	1.436317000
6	-1.147480000	-0.647143000	2.819142000
6	-0.030104000	-0.293010000	-1.547264000
1	-0.091454000	0.554179000	-2.246400000
6	-2.029099000	1.453764000	-0.222435000
6	-2.122536000	2.203315000	-1.408311000
1	-1.760129000	1.793187000	-2.352952000
6	-2.685524000	3.483294000	-1.399250000
1	-2.742156000	4.054825000	-2.328219000
6	-3.174465000	4.027067000	-0.208127000
1	-3.614004000	5.026639000	-0.201566000
6	-3.091738000	3.287563000	0.975818000
1	-3.467867000	3.705239000	1.912063000
6	-2.515948000	2.014651000	0.969709000
1	-2.434564000	1.456048000	1.903538000
6	-2.779876000	-1.286845000	-0.712176000
6	-3.912477000	-0.724973000	-1.328017000
1	-3.972493000	0.351906000	-1.489039000
6	-4.980704000	-1.534570000	-1.725265000
1	-5.855870000	-1.078708000	-2.193511000
6	-4.934258000	-2.915847000	-1.517209000
1	-5.771963000	-3.546037000	-1.823331000
6	-3.813497000	-3.484681000	-0.904997000
1	-3.769675000	-4.561660000	-0.729614000
6	-2.748083000	-2.675977000	-0.501371000
1	-1.885490000	-3.129731000	-0.008651000
6	1.679622000	1.739936000	-0.258000000
6	1.331533000	2.543005000	0.837334000
1	0.826261000	2.087188000	1.691193000
6	1.615585000	3.912633000	0.836890000
1	1.342450000	4.520455000	1.702010000
6	2.244773000	4.497997000	-0.263789000
1	2.467978000	5.567075000	-0.265345000
6	2.592334000	3.706886000	-1.364837000
1	3.087277000	4.156099000	-2.228798000
6	2.316255000	2.338119000	-1.361032000
1	2.613768000	1.737746000	-2.222127000
6	2.879690000	-0.821854000	-0.765409000
6	3.730920000	-1.350598000	0.219262000
1	3.418031000	-1.351187000	1.264856000
6	4.975829000	-1.881831000	-0.127244000
1	5.625762000	-2.284798000	0.652128000
6	5.381444000	-1.906174000	-1.464673000
1	6.350508000	-2.329559000	-1.736753000
6	4.537940000	-1.392731000	-2.454374000
1	4.844648000	-1.414706000	-3.502378000
6	3.297182000	-0.849872000	-2.108372000
1	2.657730000	-0.449486000	-2.896919000
15	-1.331203000	-0.257456000	-0.176193000
15	1.284046000	-0.074235000	-0.219893000
25	0.074617000	-0.929203000	1.507517000
8	1.905944000	0.091553000	3.611086000
8	1.235264000	-3.633506000	1.447460000
8	-1.899712000	-0.541047000	3.705572000
1	-0.778187000	-2.234563000	1.447916000
6	0.002125000	-1.619443000	-2.309139000
1	0.819724000	-1.634154000	-3.042589000
1	0.140646000	-2.479261000	-1.637593000
1	-0.940105000	-1.764660000	-2.858570000

fac,anti-**3**^{Me}, E(tol)=-3180.44988322

6	-0.000125000	1.218087000	2.341449000
6	1.298846000	-1.061170000	2.713714000
6	-1.298664000	-1.061425000	2.713859000
6	0.000008000	-0.177797000	-1.485947000
6	2.672413000	-1.314161000	-0.647742000
6	2.588257000	-2.637349000	-0.181809000
1	1.761883000	-2.923112000	0.471897000
6	3.556624000	-3.579475000	-0.539662000
1	3.477952000	-4.602349000	-0.165247000
6	4.626649000	-3.211764000	-1.360426000
1	5.387083000	-3.946451000	-1.633522000
6	4.725113000	-1.895143000	-1.820807000
1	5.563297000	-1.596252000	-2.454094000
6	3.756968000	-0.951733000	-1.466927000
1	3.856869000	0.074948000	-1.822404000
6	2.207257000	1.519540000	-0.416951000
6	2.229144000	2.216121000	-1.636977000
1	1.725091000	1.810708000	-2.516864000
6	2.903382000	3.436591000	-1.746490000
1	2.905791000	3.969090000	-2.700086000
6	3.569911000	3.972338000	-0.641027000
1	4.091978000	4.927618000	-0.726131000
6	3.560806000	3.282793000	0.575758000
1	4.075122000	3.696651000	1.445479000
6	2.881031000	2.067988000	0.688322000
1	2.865784000	1.542645000	1.645938000
6	-2.672383000	-1.314165000	-0.647876000
6	-3.756757000	-0.951772000	-1.467319000
1	-3.856498000	0.074861000	-1.822983000
6	-4.724905000	-1.895160000	-1.821249000
1	-5.562951000	-1.596297000	-2.454732000
6	-4.626628000	-3.211722000	-1.360659000
1	-5.387070000	-3.946388000	-1.633787000
6	-3.556781000	-3.579398000	-0.539645000
1	-3.478250000	-4.602229000	-0.165083000
6	-2.588415000	-2.637294000	-0.181739000
1	-1.762191000	-2.923018000	0.472175000
6	-2.207281000	1.519531000	-0.416923000

6	-2.881321000	2.067715000	0.688325000
1	-2.866248000	1.542172000	1.645835000
6	-3.561125000	3.282512000	0.575870000
1	-4.075660000	3.696160000	1.445561000
6	-3.569981000	3.972320000	-0.640770000
1	-4.092061000	4.927601000	-0.725783000
6	-2.903177000	3.436846000	-1.746195000
1	-2.905387000	3.969559000	-2.699671000
6	-2.228917000	2.216375000	-1.636798000
1	-1.724653000	1.811163000	-2.516656000
1	0.000022000	0.741550000	-2.088400000
15	1.360290000	-0.099505000	-0.177780000
15	-1.360301000	-0.099509000	-0.177822000
25	-0.000026000	-0.446341000	1.635462000
8	-0.000167000	2.270996000	2.845970000
8	2.127730000	-1.477493000	3.420506000
8	-2.127439000	-1.477859000	3.420711000
1	-0.000093000	-1.880543000	0.937747000
6	0.000033000	-1.398810000	-2.402071000
1	-0.890245000	-1.394626000	-3.049115000
1	0.890391000	-1.394677000	-3.048998000
1	-0.000034000	-2.342712000	-1.838792000

fac-**2**$^{\mathbf{Ph}}$, E(tol)=-3371.03640559

6	1.235818000	-1.484981000	2.678145000
6	-0.082162000	0.691637000	3.218132000
6	-1.250205000	-1.608694000	2.533552000
6	0.002827000	-0.646374000	-0.368808000
6	-3.002083000	-0.525214000	-0.107886000
6	-3.301785000	-1.131352000	-1.340251000
1	-2.540162000	-1.209643000	-2.116558000
6	-4.577583000	-1.652577000	-1.574099000
1	-4.796910000	-2.129759000	-2.531660000
6	-5.566939000	-1.564992000	-0.590086000
1	-6.562721000	-1.972387000	-0.777293000
6	-5.277117000	-0.958288000	0.635778000
1	-6.043303000	-0.890660000	1.410808000
6	-4.001273000	-0.443893000	0.878245000
1	-3.779682000	0.022754000	1.840926000
6	-1.661139000	1.977617000	-0.388387000
6	-2.051570000	2.214435000	-1.718171000
1	-2.164054000	1.381662000	-2.415604000
6	-2.305635000	3.516469000	-2.152615000
1	-2.604834000	3.693243000	-3.188113000
6	-2.186169000	4.590941000	-1.262752000
1	-2.393637000	5.607622000	-1.603258000
6	-1.803426000	4.360691000	0.061074000
1	-1.710224000	5.194780000	0.759663000
6	-1.538875000	3.058470000	0.497264000
1	-1.235552000	2.877291000	1.530673000
6	2.964366000	-0.732135000	-0.093944000
6	2.982315000	-2.135362000	0.007390000
1	2.075606000	-2.676022000	0.278904000
6	4.157281000	-2.846556000	-0.241039000
1	4.151376000	-3.935736000	-0.164904000
6	5.334970000	-2.170565000	-0.576417000
1	6.254328000	-2.729638000	-0.762885000
6	5.329284000	-0.776577000	-0.667092000
1	6.244351000	-0.237663000	-0.921851000
6	4.152418000	-0.059868000	-0.430982000
1	4.165560000	1.027743000	-0.508710000
6	1.799492000	1.904836000	-0.296287000
6	1.795672000	2.268803000	-1.652640000
1	1.530569000	1.534359000	-2.415729000
6	2.129676000	3.571757000	-2.029753000
1	2.114776000	3.850751000	-3.085489000
6	2.485366000	4.515295000	-1.059361000
1	2.749886000	5.531906000	-1.357877000
6	2.494941000	4.157686000	0.292105000
1	2.767893000	4.891846000	1.053037000
6	2.145104000	2.859235000	0.674063000
1	2.136072000	2.583034000	1.731387000
6	-0.015612000	-1.780082000	-1.334867000
6	-0.479739000	-3.052236000	-0.951161000
1	-0.804124000	-3.204296000	0.080842000
6	-0.517291000	-4.109476000	-1.863661000
1	-0.881070000	-5.087593000	-1.541137000
6	-0.082118000	-3.920923000	-3.179622000
1	-0.104376000	-4.748464000	-3.891773000
6	0.391340000	-2.665192000	-3.574024000
1	0.741084000	-2.508318000	-4.597046000
6	0.422764000	-1.606654000	-2.662191000
1	0.791428000	-0.628854000	-2.980231000
8	2.007408000	-2.125467000	3.273867000
8	-0.132579000	1.455871000	4.100621000
8	-1.994106000	-2.368324000	3.014047000
15	-1.397657000	0.275858000	0.260586000
15	1.433061000	0.202835000	0.281040000
25	-0.016663000	-0.480411000	1.871332000

TS1$^{\mathbf{Ph}}$, E(tol)=-3372.20168125

6	0.015703000	2.652796000	1.135407000
6	-1.271985000	1.465720000	2.969211000
6	1.380644000	1.476831000	2.926700000
6	-0.022692000	-0.790640000	-0.625503000
6	-2.222222000	1.254534000	-0.987247000
6	-3.059132000	2.256849000	-0.465110000
1	-3.209192000	2.338554000	0.614234000
6	-3.696167000	3.161964000	-1.317547000
1	-4.339503000	3.938893000	-0.899061000
6	-3.499249000	3.081048000	-2.700317000
1	-3.992225000	3.792672000	-3.365995000
6	-2.659651000	2.094645000	-3.225827000
1	-2.495212000	2.031422000	-4.303670000
6	-2.021131000	1.187212000	-2.374565000
1	-1.358939000	0.425861000	-2.790582000
6	-2.683887000	-1.034834000	0.739149000
6	-4.042294000	-0.866246000	0.423047000
1	-4.355857000	-0.052027000	-0.231672000
6	-5.003873000	-1.744580000	0.933862000
1	-6.055614000	-1.599651000	0.677134000
6	-4.623572000	-2.802908000	1.763182000
1	-5.375772000	-3.487715000	2.160103000
6	-3.272565000	-2.981769000	2.080411000
1	-2.964660000	-3.809044000	2.723518000
6	-2.312887000	-2.103136000	1.575396000
1	-1.260335000	-2.255501000	1.822855000
6	2.268110000	1.170242000	-1.023309000
6	2.217256000	0.990221000	-2.415412000
1	1.634546000	0.170638000	-2.838964000
6	2.903137000	1.862039000	-3.266185000
1	2.853376000	1.711681000	-4.346831000

6	3.646584000	2.922278000	-2.738419000
1	4.178403000	3.604172000	-3.405282000
6	3.694274000	3.115113000	-1.354392000
1	4.258928000	3.950406000	-0.934737000
6	3.004464000	2.248210000	-0.502080000
1	3.029212000	2.423618000	0.576027000
6	2.641513000	-1.142154000	0.690547000
6	2.225835000	-2.386775000	1.197079000
1	1.166899000	-2.653382000	1.167259000
6	3.155937000	-3.294545000	1.707490000
1	2.817069000	-4.262159000	2.084030000
6	4.516592000	-2.968762000	1.729510000
1	5.244033000	-3.677258000	2.131066000
6	4.939843000	-1.734816000	1.228048000
1	6.000470000	-1.474143000	1.235845000
6	4.010658000	-0.827428000	0.709076000
1	4.360434000	0.125775000	0.309266000
6	-0.060535000	-1.883487000	-1.590241000
6	1.126902000	-2.462772000	-2.110156000
1	2.096974000	-2.081780000	-1.786653000
6	1.086464000	-3.514104000	-3.024835000
1	2.024257000	-3.930735000	-3.400437000
6	-0.136979000	-4.032638000	-3.465662000
1	-0.166335000	-4.854652000	-4.183416000
6	-1.322026000	-3.474899000	-2.971150000
1	-2.288618000	-3.860501000	-3.304415000
6	-1.287815000	-2.423485000	-2.056373000
1	-2.229606000	-2.013564000	-1.688040000
15	-1.346343000	0.102075000	0.150071000
15	1.348856000	0.052909000	0.117988000
25	0.037365000	1.025725000	1.796316000
8	-0.000698000	3.743350000	0.722996000
8	-2.103015000	1.803921000	3.710183000
8	2.229907000	1.821809000	3.643152000
1	0.650640000	-1.281750000	3.361956000
1	-0.016292000	-0.958682000	3.514335000

fac-**4**^{Ph}, E(tol)=-3372.21922516

6	0.061477000	-2.679426000	-0.582312000
6	-1.233263000	-2.023410000	-2.703307000
6	1.412436000	-1.998657000	-2.653565000
6	-0.024765000	0.779262000	0.626094000
6	-2.328265000	-1.152735000	0.920398000
6	-3.272812000	-2.048024000	0.386378000
1	-3.456198000	-2.073553000	-0.690367000
6	-3.977676000	-2.916134000	1.223080000
1	-4.704041000	-3.610205000	0.794786000
6	-3.744399000	-2.903993000	2.602920000
1	-4.291182000	-3.587175000	3.256254000
6	-2.800539000	-2.024140000	3.139588000
1	-2.607642000	-2.015236000	4.214462000
6	-2.091809000	-1.155152000	2.303104000
1	-1.343988000	-0.480844000	2.723927000
6	-2.590064000	1.090674000	-0.905881000
6	-3.954092000	1.051829000	-0.572626000
1	-4.325310000	0.310112000	0.135337000
6	-4.850633000	1.969253000	-1.132155000
1	-5.906993000	1.923122000	-0.858392000
6	-4.400063000	2.939932000	-2.029248000
1	-5.101065000	3.654882000	-2.464778000
6	-3.042047000	2.993058000	-2.362637000
1	-2.676123000	3.752333000	-3.057065000
6	-2.149002000	2.076017000	-1.806776000
1	-1.090069000	2.140721000	-2.067216000
6	2.385328000	-1.011176000	1.003973000
6	2.245967000	-0.867438000	2.393872000
1	1.538415000	-0.140439000	2.795517000
6	3.001119000	-1.656691000	3.266678000
1	2.881305000	-1.533179000	4.345199000
6	3.899175000	-2.602547000	2.763698000
1	4.483800000	-3.221723000	3.447313000
6	4.033249000	-2.764427000	1.381170000
1	4.718267000	-3.514185000	0.979518000
6	3.277689000	-1.978276000	0.506912000
1	3.373970000	-2.136071000	-0.569626000
6	2.537100000	1.224354000	-0.856746000
6	2.016496000	2.428017000	-1.364209000
1	0.949185000	2.635798000	-1.262742000
6	2.853737000	3.372739000	-1.961531000
1	2.432166000	4.307434000	-2.337799000
6	4.227397000	3.129209000	-2.064399000
1	4.883235000	3.867803000	-2.529934000
6	4.756386000	1.940068000	-1.555406000
1	5.829053000	1.744685000	-1.620173000
6	3.919806000	0.994490000	-0.953663000
1	4.356692000	0.081626000	-0.547154000
6	-0.074152000	1.866261000	1.598806000
6	1.105462000	2.473466000	2.103144000
1	2.080708000	2.121882000	1.759971000
6	1.053620000	3.518650000	3.025741000
1	1.987800000	3.955227000	3.388246000
6	-0.173611000	4.007308000	3.488836000
1	-0.211618000	4.823639000	4.212617000
6	-1.351134000	3.426731000	3.003248000
1	-2.322566000	3.789938000	3.348305000
6	-1.305341000	2.379524000	2.082847000
1	-2.244122000	1.952682000	1.724266000
15	-1.330629000	-0.074206000	-0.192698000
15	1.348136000	-0.009199000	-0.146980000
25	0.064963000	-1.268010000	-1.693369000
8	0.065173000	-3.620922000	0.093620000
8	-2.050759000	-2.537696000	-3.349124000
8	2.258243000	-2.494841000	-3.277497000
1	-0.323774000	0.138187000	-2.585817000
1	0.485473000	0.019852000	-2.737407000

TS2^{Ph}, E(tol)=-3372.19169078

6	0.027671000	2.032111000	-2.353344000
6	1.296052000	0.007985000	-3.338762000
6	-1.340039000	0.054846000	-3.326111000
6	-0.005781000	-0.890951000	0.590325000
6	1.959354000	1.491955000	0.688938000
6	2.556790000	2.529664000	-0.049230000
1	2.638482000	2.447211000	-1.135253000
6	3.045522000	3.668039000	0.596894000
1	3.505489000	4.466433000	0.010991000
6	2.932331000	3.787799000	1.985469000
1	3.307814000	4.680514000	2.489991000
6	2.330195000	2.765225000	2.724962000
1	2.233886000	2.856106000	3.808974000
6	1.847585000	1.620755000	2.083544000
1	1.381567000	0.829495000	2.671815000

6	2.821701000	-1.074480000	-0.373595000
6	4.121612000	-0.596054000	-0.140599000
1	4.277214000	0.433377000	0.184846000
6	5.227437000	-1.435358000	-0.313748000
1	6.231037000	-1.046994000	-0.127634000
6	5.050617000	-2.760005000	-0.718735000
1	5.914479000	-3.414229000	-0.852581000
6	3.758577000	-3.244498000	-0.951820000
1	3.608881000	-4.279653000	-1.265704000
6	2.653647000	-2.408583000	-0.786674000
1	1.653455000	-2.804650000	-0.970573000
6	-1.937903000	1.487330000	0.771330000
6	-1.968062000	1.473279000	2.177295000
1	-1.639224000	0.588336000	2.724404000
6	-2.416177000	2.593326000	2.882127000
1	-2.430844000	2.572991000	3.973968000
6	-2.843822000	3.734334000	2.194943000
1	-3.191239000	4.608776000	2.749257000
6	-2.821475000	3.754129000	0.797617000
1	-3.149301000	4.642851000	0.254482000
6	-2.368330000	2.637953000	0.088222000
1	-2.350717000	2.660747000	-1.003030000
6	-2.854533000	-1.014314000	-0.379921000
6	-2.725529000	-2.353121000	-0.792414000
1	-1.735822000	-2.788576000	-0.942319000
6	-3.857209000	-3.142483000	-1.000571000
1	-3.738829000	-4.181938000	-1.313657000
6	-5.136246000	-2.606375000	-0.811291000
1	-6.020662000	-3.224051000	-0.980005000
6	-5.273764000	-1.276986000	-0.406702000
1	-6.266720000	-0.848392000	-0.255120000
6	-4.141419000	-0.484444000	-0.189916000
1	-4.266150000	0.550415000	0.132087000
6	0.006077000	-1.620918000	1.873120000
6	-1.187874000	-2.111216000	2.454759000
1	-2.143498000	-1.918005000	1.965875000
6	-1.172176000	-2.844794000	3.641884000
1	-2.115655000	-3.204769000	4.059290000
6	0.034107000	-3.121112000	4.294608000
1	0.044712000	-3.694068000	5.223799000
6	1.226256000	-2.648487000	3.736277000
1	2.179975000	-2.851113000	4.229495000
6	1.214415000	-1.914016000	2.549148000
1	2.161997000	-1.564016000	2.136782000
15	1.345130000	0.021342000	-0.219852000
15	-1.354358000	0.044253000	-0.199753000
25	-0.011406000	0.248708000	-2.127338000
8	0.059732000	3.174237000	-2.587796000
8	2.134992000	-0.149486000	-4.129435000
8	-2.190413000	-0.078705000	-4.108639000
1	-0.022106000	-1.405431000	-0.927876000
1	-0.036805000	-1.424560000	-1.945971000

fac,syn-**3**$^{\mathbf{Ph}}$, E(tol)=-3372.24806241

6	-0.104938000	-1.366324000	-2.907439000
6	-1.336939000	-3.091739000	-1.401711000
6	1.246691000	-3.063088000	-1.428214000
6	0.005214000	0.345800000	1.025128000
1	-0.004390000	-0.402023000	1.835496000
6	-2.736311000	-0.877783000	1.002071000
6	-3.837446000	-1.510354000	0.396814000
1	-3.872751000	-1.624764000	-0.688919000
6	-4.891520000	-1.995008000	1.172994000
1	-5.737076000	-2.486985000	0.687945000
6	-4.861034000	-1.857738000	2.565246000
1	-5.683866000	-2.240682000	3.172434000
6	-3.772943000	-1.228739000	3.174569000
1	-3.743498000	-1.111477000	4.260020000
6	-2.716032000	-0.739942000	2.398099000
1	-1.884410000	-0.237680000	2.894490000
6	-2.179080000	1.143971000	-0.930292000
6	-3.184904000	1.890960000	-0.289136000
1	-3.510820000	1.620611000	0.716436000
6	-3.778532000	2.978412000	-0.933813000
1	-4.559525000	3.546539000	-0.423857000
6	-3.378095000	3.335583000	-2.225737000
1	-3.848043000	4.182475000	-2.730349000
6	-2.381211000	2.598572000	-2.871109000
1	-2.068703000	2.864292000	-3.883098000
6	-1.788770000	1.507016000	-2.228922000
1	-1.019945000	0.931429000	-2.743916000
6	2.635039000	-1.089126000	1.044511000
6	2.236736000	-1.968545000	2.067614000
1	1.181107000	-2.223012000	2.190472000
6	3.180737000	-2.552996000	2.913591000
1	2.850136000	-3.229071000	3.704936000
6	4.543065000	-2.288179000	2.737232000
1	5.282007000	-2.752351000	3.393656000
6	4.951878000	-1.438641000	1.707014000
1	6.013555000	-1.236314000	1.550094000
6	4.006451000	-0.840645000	0.867008000
1	4.346615000	-0.181308000	0.067942000
6	2.249998000	0.981451000	-0.925788000
6	2.382216000	0.957220000	-2.323016000
1	1.944203000	0.133767000	-2.888614000
6	3.082110000	1.967554000	-2.990283000
1	3.179490000	1.930470000	-4.077175000
6	3.655979000	3.015622000	-2.266131000
1	4.200586000	3.807131000	-2.785429000
6	3.538301000	3.045117000	-0.871888000
1	3.990881000	3.858060000	-0.300199000
6	2.845576000	2.033655000	-0.202728000
1	2.777613000	2.060533000	0.885361000
6	0.066120000	1.711514000	1.645144000
6	0.295968000	1.816996000	3.031642000
1	0.424231000	0.906398000	3.623090000
6	0.371155000	3.061755000	3.660282000
1	0.551218000	3.115349000	4.736202000
6	0.212440000	4.233293000	2.913327000
1	0.263855000	5.208565000	3.401864000
6	-0.010872000	4.145693000	1.535928000
1	-0.132047000	5.054387000	0.942479000
6	-0.078037000	2.900189000	0.905831000
1	-0.243589000	2.855153000	-0.170261000
15	-1.378591000	-0.298796000	-0.099257000
15	1.356367000	-0.394388000	-0.095354000
25	-0.056727000	-1.855584000	-1.168933000
8	-0.161500000	-1.175531000	-4.061183000
8	-2.129364000	-3.934813000	-1.539504000
8	2.081887000	-3.862154000	-1.571529000
1	-0.087537000	-2.351295000	0.342083000

TS3^{Ph}, E(tol)=-3372.22269309

6	1.288328000	-1.968809000	-2.469945000
6	0.773217000	-3.254234000	-0.225656000
6	-1.088446000	-2.247109000	-2.442004000
6	-0.049889000	0.365534000	1.071655000
1	0.005721000	-0.325583000	1.930414000
6	-2.632180000	-1.168325000	1.067795000
6	-3.549521000	-2.075374000	0.506595000
1	-3.481452000	-2.336623000	-0.552003000
6	-4.546966000	-2.652529000	1.293939000
1	-5.251359000	-3.355216000	0.843931000
6	-4.638180000	-2.339548000	2.655181000
1	-5.413902000	-2.797696000	3.272096000
6	-3.730477000	-1.441533000	3.221113000
1	-3.794729000	-1.190958000	4.282246000
6	-2.733784000	-0.855624000	2.431887000
1	-2.041750000	-0.147841000	2.890630000
6	-2.289294000	0.844269000	-0.924543000
6	-3.263306000	1.613283000	-0.261098000
1	-3.475328000	1.439917000	0.795393000
6	-3.976344000	2.595524000	-0.951280000
1	-4.729898000	3.185473000	-0.425132000
6	-3.732051000	2.818765000	-2.311040000
1	-4.296202000	3.583183000	-2.849722000
6	-2.772612000	2.053594000	-2.979377000
1	-2.585392000	2.213127000	-4.043352000
6	-2.056481000	1.070524000	-2.289184000
1	-1.314679000	0.461466000	-2.810220000
6	2.722729000	-0.794532000	1.031678000
6	2.836779000	-0.404097000	2.375466000
1	2.088198000	0.247896000	2.828773000
6	3.920093000	-0.836380000	3.148916000
1	3.994465000	-0.527112000	4.193824000
6	4.901703000	-1.656732000	2.587706000
1	5.745335000	-1.994951000	3.192908000
6	4.796180000	-2.048123000	1.248424000
1	5.555602000	-2.694641000	0.803861000
6	3.712714000	-1.624962000	0.476754000
1	3.631637000	-1.951747000	-0.562534000
6	2.066070000	1.140914000	-0.960943000
6	1.738959000	1.363114000	-2.306971000
1	1.053407000	0.677901000	-2.809105000
6	2.290776000	2.441631000	-3.005087000
1	2.031789000	2.595962000	-4.054702000
6	3.179763000	3.308959000	-2.364748000
1	3.617057000	4.147864000	-2.910394000
6	3.517682000	3.092088000	-1.024331000
1	4.216921000	3.762063000	-0.519440000
6	2.968167000	2.014786000	-0.326245000
1	3.252740000	1.850159000	0.714265000
6	-0.143431000	1.778003000	1.574687000
6	-0.148492000	2.018829000	2.962789000
1	-0.082531000	1.174177000	3.654553000
6	-0.232117000	3.316562000	3.472529000
1	-0.233351000	3.475838000	4.552985000
6	-0.313272000	4.406478000	2.600200000
1	-0.378067000	5.422727000	2.994287000
6	-0.310318000	4.184338000	1.220042000
1	-0.373482000	5.027698000	0.529383000
6	-0.227055000	2.885730000	0.711012000
1	-0.227472000	2.734143000	-0.368216000
15	-1.334584000	-0.468322000	-0.041157000
15	1.322475000	-0.291332000	-0.057049000
25	0.099019000	-1.881648000	-1.117686000
8	2.038578000	-2.110090000	-3.355293000
8	1.187645000	-4.207939000	0.322709000
8	-1.817757000	-2.548654000	-3.301795000
1	-0.748495000	-2.977805000	-0.379946000

mer-**3^{Ph}**, E(tol)=-3372.23990259

6	0.190384000	-2.545199000	-1.852834000
6	-1.429657000	-1.080776000	-3.057447000
6	0.161513000	0.834545000	-2.762326000
6	0.070724000	0.373585000	1.027926000
1	0.102422000	-0.256254000	1.927583000
6	-2.102211000	-1.646950000	0.857224000
6	-2.704781000	-2.687414000	0.129761000
1	-2.672250000	-2.674381000	-0.961433000
6	-3.337644000	-3.744212000	0.788563000
1	-3.800382000	-4.543325000	0.205774000
6	-3.366477000	-3.784870000	2.185843000
1	-3.851798000	-4.616377000	2.700889000
6	-2.763654000	-2.759866000	2.920369000
1	-2.777418000	-2.785782000	4.012250000
6	-2.139371000	-1.696199000	2.261262000
1	-1.680114000	-0.904655000	2.857375000
6	-2.687048000	0.988050000	-0.116874000
6	-3.444962000	1.283253000	1.030679000
1	-3.244790000	0.767376000	1.971139000
6	-4.472425000	2.226398000	0.975881000
1	-5.051444000	2.447353000	1.875184000
6	-4.762993000	2.882490000	-0.225823000
1	-5.570446000	3.616697000	-0.267037000
6	-4.021232000	2.589837000	-1.372516000
1	-4.244854000	3.091505000	-2.316298000
6	-2.986902000	1.650084000	-1.317098000
1	-2.412273000	1.423947000	-2.216440000
6	2.282168000	-1.607472000	0.676286000
6	2.302962000	-1.770030000	2.070135000
1	1.738243000	-1.098766000	2.719406000
6	3.055052000	-2.794300000	2.654771000
1	3.055642000	-2.910406000	3.740739000
6	3.801172000	-3.663533000	1.855049000
1	4.385611000	-4.464288000	2.312723000
6	3.792311000	-3.504959000	0.465562000
1	4.369400000	-4.181210000	-0.168459000
6	3.036428000	-2.487630000	-0.120026000
1	3.030879000	-2.377600000	-1.206612000
6	2.741179000	0.985759000	-0.343522000
6	3.264912000	1.272000000	-1.613166000
1	2.830788000	0.802051000	-2.496966000
6	4.347306000	2.147531000	-1.750441000
1	4.745975000	2.360914000	-2.744402000
6	4.910928000	2.747350000	-0.622038000
1	5.751959000	3.435620000	-0.729450000
6	4.395800000	2.463686000	0.648331000
1	4.833744000	2.928373000	1.534232000
6	3.322123000	1.583392000	0.789337000
1	2.937191000	1.365439000	1.786894000
6	0.058150000	1.818604000	1.445059000
6	0.035804000	2.143997000	2.813567000
1	0.036481000	1.344049000	3.559265000
6	0.015361000	3.475646000	3.238208000

1	-0.000518000	3.702768000	4.306513000
6	0.015518000	4.510711000	2.299346000
1	-0.000201000	5.552093000	2.627209000
6	0.036568000	4.201594000	0.935265000
1	0.037834000	5.001223000	0.191637000
6	0.058027000	2.871556000	0.512358000
1	0.079326000	2.650414000	-0.556147000
15	-1.331882000	-0.267870000	-0.104238000
15	1.380474000	-0.250154000	-0.196726000
25	-0.070916000	-0.755501000	-1.936741000
8	0.374337000	-3.691865000	-1.937059000
8	-2.303335000	-1.294521000	-3.803160000
8	0.337848000	1.777907000	-3.427134000
1	1.094009000	-1.011000000	-2.953778000

TS4^{Ph}, E(tol)=-3372.21973573

6	-1.317659000	-2.962623000	-1.161040000
6	-0.749389000	-1.255805000	-3.055322000
6	1.029833000	-3.061851000	-1.319534000
6	0.090753000	0.223980000	1.050717000
1	0.094300000	-0.616326000	1.764974000
6	-2.694351000	-0.917788000	0.925054000
6	-3.897081000	-1.249470000	0.273045000
1	-4.005110000	-1.069632000	-0.799340000
6	-4.958615000	-1.811028000	0.983791000
1	-5.882962000	-2.065050000	0.460854000
6	-4.837699000	-2.050178000	2.357113000
1	-5.668015000	-2.490948000	2.912540000
6	-3.648230000	-1.724648000	3.012947000
1	-3.546082000	-1.903973000	4.085413000
6	-2.581743000	-1.163197000	2.301637000
1	-1.666206000	-0.909833000	2.838500000
6	-2.088826000	1.301740000	-0.746355000
6	-3.000225000	2.033242000	0.038391000
1	-3.279727000	1.678063000	1.031633000
6	-3.559720000	3.216783000	-0.448079000
1	-4.266388000	3.773632000	0.171048000
6	-3.220051000	3.685879000	-1.721896000
1	-3.664081000	4.608209000	-2.102685000
6	-2.316750000	2.965452000	-2.507737000
1	-2.051414000	3.318488000	-3.506465000
6	-1.757288000	1.779306000	-2.022385000
1	-1.058310000	1.213634000	-2.639215000
6	2.707914000	-1.203491000	0.729294000
6	2.381845000	-2.095309000	1.766691000
1	1.336933000	-2.276249000	2.030383000
6	3.380785000	-2.790162000	2.450748000
1	3.107385000	-3.471937000	3.258804000
6	4.722921000	-2.627037000	2.091149000
1	5.503656000	-3.176861000	2.620631000
6	5.055551000	-1.769819000	1.039954000
1	6.098419000	-1.648687000	0.739122000
6	4.057076000	-1.060598000	0.363907000
1	4.336420000	-0.394983000	-0.453782000
6	2.200909000	1.084482000	-0.941511000
6	2.103156000	1.344265000	-2.316350000
1	1.521559000	0.668258000	-2.946853000
6	2.747043000	2.450418000	-2.880432000
1	2.666391000	2.634690000	-3.953753000
6	3.492789000	3.312208000	-2.072195000
1	3.994973000	4.177324000	-2.510664000
6	3.598588000	3.061851000	-0.699260000
1	4.181167000	3.731116000	-0.062636000
6	2.961029000	1.954703000	-0.135528000
1	3.063250000	1.764486000	0.933859000
6	0.193876000	1.506777000	1.823995000
6	0.382162000	1.450220000	3.219178000
1	0.450918000	0.476897000	3.712431000
6	0.488114000	2.615079000	3.982277000
1	0.634032000	2.544024000	5.062345000
6	0.406111000	3.866475000	3.363483000
1	0.485587000	4.779897000	3.956682000
6	0.222716000	3.939216000	1.979369000
1	0.160120000	4.911324000	1.485791000
6	0.120716000	2.773681000	1.215572000
1	-0.017309000	2.852086000	0.137562000
15	-1.318489000	-0.258245000	-0.112177000
15	1.350942000	-0.387642000	-0.227023000
25	-0.109093000	-1.659713000	-1.448647000
8	-2.057557000	-3.856733000	-1.037375000
8	-1.113812000	-1.090505000	-4.160224000
8	1.739659000	-3.985310000	-1.292775000
1	0.867167000	-1.402657000	-2.644141000

fac,anti-**3^{Ph}**, E(tol)=-3372.25086260

6	0.000157000	-3.014708000	-0.704063000
6	-1.290768000	-1.859478000	-2.741411000
6	1.291005000	-1.859305000	-2.741425000
6	-0.000054000	0.441016000	0.967757000
1	-0.000040000	-0.217680000	1.851149000
6	-2.482347000	-1.201640000	1.022853000
6	-3.253466000	-2.247828000	0.486986000
1	-3.161582000	-2.503416000	-0.571056000
6	-4.127413000	-2.973452000	1.299479000
1	-4.717344000	-3.784669000	0.867916000
6	-4.235096000	-2.672044000	2.661032000
1	-4.911611000	-3.245746000	3.297807000
6	-3.467378000	-1.638747000	3.205076000
1	-3.543177000	-1.399445000	4.268072000
6	-2.597892000	-0.905173000	2.391203000
1	-2.012940000	-0.096506000	2.834109000
6	-2.467640000	1.073694000	-0.721439000
6	-3.360530000	1.716536000	0.155834000
1	-3.418748000	1.413999000	1.202542000
6	-4.190426000	2.740716000	-0.303838000
1	-4.875297000	3.232426000	0.390304000
6	-4.149925000	3.130142000	-1.647028000
1	-4.805474000	3.926366000	-2.006193000
6	-3.273860000	2.490499000	-2.527481000
1	-3.242654000	2.780608000	-3.579831000
6	-2.436141000	1.469404000	-2.067979000
1	-1.749660000	0.973110000	-2.756137000
6	2.482427000	-1.201390000	1.022906000
6	2.597966000	-0.904890000	2.391250000
1	2.012973000	-0.096249000	2.834146000
6	3.467509000	-1.638393000	3.205127000
1	3.543304000	-1.399064000	4.268117000
6	4.235287000	-2.671651000	2.661096000
1	4.911845000	-3.245298000	3.297875000
6	4.127610000	-2.973092000	1.299550000
1	4.717589000	-3.784280000	0.867997000
6	3.253610000	-2.247538000	0.487052000

1	3.161733000	-2.503154000	-0.570984000	6	-0.000301000	3.498020000	3.241684000
6	2.467517000	1.073954000	-0.721381000	1	-0.000352000	3.706907000	4.313784000
6	2.435961000	1.469694000	-2.067911000	6	-0.000328000	4.549610000	2.320625000
1	1.749515000	0.973355000	-2.756071000	1	-0.000399000	5.585029000	2.667354000
6	3.273577000	2.490879000	-2.527400000	6	-0.000265000	4.265172000	0.951236000
1	3.242325000	2.781013000	-3.579742000	1	-0.000287000	5.078472000	0.222601000
6	4.149596000	3.130581000	-1.646945000	6	-0.000175000	2.942457000	0.503948000
1	4.805065000	3.926876000	-2.006100000	1	-0.000128000	2.738203000	-0.567454000
6	4.190156000	2.741123000	-0.303765000	15	-1.370783000	-0.289171000	-0.131559000
1	4.874993000	3.232878000	0.390378000	15	1.370792000	-0.289023000	-0.131518000
6	3.360364000	1.716853000	0.155894000	25	0.000091000	-1.425159000	-1.569719000
1	3.418629000	1.414293000	1.202593000	8	0.000384000	-4.056426000	-0.177970000
6	-0.000144000	1.872932000	1.418013000	8	-2.104107000	-2.123212000	-3.534835000
6	-0.000210000	2.174456000	2.793028000	8	2.104871000	-2.123000000	-3.534320000
1	-0.000192000	1.360894000	3.523882000	1	0.000007000	0.003618000	-2.258297000