Supporting Information of the manuscript entitled:

Homo- and Heterobimetallic Transition Metal Cluster derived from [Cp*Fe(η^5-E_5)] (E = P, As) – Unprecedented Structural Motifs of the resulting Polypnictogen Ligands

Sabrina B. Dinauer,[a] Robert Szlosek,[a] Martin Piesch,[a] Gábor Balázs,[a] Stephan Reichl,[a] Lukas Prock,[a] Christoph Riesinger,[a] Marc D. Walter[b] and Manfred Scheer*[a]

[a] S. B. Dinauer, R. Szlosek, Dr. M. Piesch, Dr. G. Balázs, Dr. Stephan Reichl, L. Prock, Dr. C. Riesinger, Prof. Dr. M. Scheer
Institute of Inorganic Chemistry
University of Regensburg, 93040 Regensburg (Germany)
E-mail: manfred.scheer@chemie.uni-regensburg.de

[b] Prof. Dr. M. D. Walter
Institute of Inorganic and Analytical Chemistry
Technical University of Braunschweig
38106 Braunschweig (Germany)
E-mail: mwalter@tu-bs.de

Author Contributions

Sabrina B. Dinauer – performing experimental work, writing of original draft.

Robert Szlosek – performing all calculations, co-writing final manuscript.

Martin Piesch – performing experimental work (first syntheses of **1-Ni** and **2-Ni**).

Stephan Reichl – performing experimental work (first synthesis of **1-Mn**).

Christoph Riesinger – finalization of all single crystal X-ray structures.

Lukas Prock – performing experimental work (synthesis of [Cp'''Fe(μ-Br)]$_2$.

Gábor Balázs – co-writing final manuscript.

Marc D. Walter – performing experimental work (synthesis of [{Cp'''Mn(THF)(μ-I)}$_2$] and co-writing final manuscript.

Manfred Scheer – project administration, funding acquisition, co-writing final manuscript.

All authors contributed to preparing the manuscript.

Table of Contents

1 Experimental Part

1.1 Synthetic procedures and experimental details

All manipulations were performed using dry nitrogen standard Schlenk techniques or an argon filled glove box. Solvents and deuterated solvents were dried, degassed, and distilled by using standard procedures. The compounds [(Cp*Fe(η^5-E$_5$)][1] (E = P (**1**), As (**2**)), [K(dme)$_2$]$_2$[(Cp*Fe(η^4-P$_5$)],[2] KC$_8$[3], [Cp'''Fe(μ-Br)]$_2$,[4] [Cp'''Cr(μ-Cl)]$_2$[5], [Cp'''Mn(thf)(μ-I)]$_2$,[6] [Cp'''Ni(μ-Br)]$_2$[7] and Ag[FAl][8] ([FAl]$^-$ = [FAl{O(1-C$_6$F$_5$)C$_6$F$_{10}$}$_3$]$^-$) were synthesized according to literature known procedures.

NMR spectra were recorded on a Bruker Avance 400 (^{1}H: 400.132 MHz, ^{19}F: 376.498 MHz, ^{31}P: 161.975 MHz) or 300 (^{1}H: 300.131 MHz) spectrometer. Chemical shifts are referenced to SiMe$_4$ (^{1}H NMR), CFCl$_3$ (^{19}F NMR) and 85% H$_3$PO$_4$ (^{31}P NMR) as external standard. Chemical shifts are given in ppm and coupling constants J in Hertz [Hz] without considering their sign.

Magnetic susceptibilities and effective magnetic moments μ_{eff} of paramagnetic compounds in solution were determined by ^{1}H NMR spectroscopy using the Evans method.[9]

LIFDI mass spectra were recorded using a Finnigan MAT 95 mass spectrometer and FD mass spectra were recorded using a Jeol AccuTOF GCX mass spectrometer by the analytical department of the University of Regensburg. All compounds were dissolved in the corresponding solvent under inert atmosphere. According to the mass/charge (m/z) ratio and the corresponding isotope pattern the observed fragments were assigned.

Data for elemental analysis (CHN) was accomplished by a Vario micro cube apparatus by the department of central analyses of the University of Regensburg. All compounds were filled in tin capsules under N$_2$ or Argon atmosphere prior to the measurements.

The X-band EPR measurements were performed with a MiniScope MS400 device with a frequency of 9.44 GHz and a rectangular resonator TE102 of the company Magnettech GmbH. The compounds were dissolved in a glovebox under N$_2$ inert gas atmosphere, placed in tip-sealed pasteur pipettes, and sealed with rubber caps. The measurements were conducted at room temperature and 77 K, respectively.

General Information

To screen the best reaction conditions all reactions were performed at first using 1.0 eq **1** or **2**, 2.5 eq KC$_8$ and 1.0 eq [Cp'''M(μ-X)]$_2$ and then optimized as described for each compound separately.

1.2 Synthesis of [(Cp*Fe)(Cp'''Cr)(μ,$\eta^{5:5}$-P_5)] (1-Cr)

a) A freshly prepared solution of [(Cp*Fe(η^5-P_5)] (200 mg, 0.578 mmol, 1.0 eq) and KC_8 (195 mg, 1.445 mmol, 2.5 eq) in THF (5 mL) was cooled to -80°C. Then a dark blue solution of [Cp'''Cr(μ-Cl)]$_2$ (370 mg, 0.578 mmol, 1.0 eq) in THF (5 mL) was slowly added at -80°C. The mixture turned dark red and was allowed to reach room temperature overnight. The solvent was removed *in vacuo*. Then the residue was dissolved in a small amount of CH_2Cl_2, silica gel was added and the solvent was removed *in vacuo*. The preabsorbed compound was purified by column chromatographic workup (SiO_2, hexane, 8 x 2.5 cm). Using hexane as an eluent **1-Cr** can be obtained as dark red fraction. After removing the solvent in vacuo, the residue was dissolved in CH_2Cl_2 and layered with CH_3CN. After storage at room temperature for a few days, **1-Cr** can be obtained as dark red blocks. The supernatant was decanted off and the crystalline compound dried in vacuo.

Yield:	85 mg (0.134 mmol, 23 %).
^{1}H NMR (CD_2Cl_2, 293 K):	*δ* [ppm] = 1.52 (s, br, 27H, C_5H_2*tBu*$_3$), -0.99 (s, br, 15H, C_5*Me*$_5$). Signals for C_5*H*$_2$*t*Bu_3 could not be found within the ^{1}H NMR spectrum of **1-Cr**.
EPR (X-band, thf solution, 298 K):	*g* = 1.918.
Evans-NMR (CD_2Cl_2, 293 K):	μ_{eff} = 1.21 μ_B corresponding to ~1.0 unpaired electron.
LIFDI-MS (toluene):	*m/z* = 631.13 ([**1-Cr**]$^+$, 100%).
Elemental Analysis	calculated (%) for $C_{27}H_{44}CrFeP_5$: C: 51.36, H: 7.02 found [%]: C: 51.40, H: 6.97.

b) A freshly prepared solution of [(Cp*Fe(η^5-P_5)] (200 mg, 0.578 mmol, 1.0 eq) and KC_8 (195 mg, 1.445 mmol, 2.5 eq) in THF (5 mL) was cooled to -80°C. Then a dark blue solution of [Cp'''Cr(μ-Cl)]$_2$ (185 mg, 0.289 mmol, 0.5 eq) in THF (5 mL) was slowly added at -80°C. The mixture turned dark red and was allowed to reach room temperature overnight and was filtered over diatomaceous earth. The solvent was removed *in vacuo*. Then the residue was dissolved in a small amount of CH_2Cl_2, and an excess of acetonitrile was added. After 12 hours storage at room temperature **1-Cr** can be obtained as dark red rods. The supernatant was decanted off and the crystalline compound washed with acetonitrile and dried in vacuo.

Yield:	80 mg (0.127 mmol, 44 % related to [Cp'''Cr(μ-Cl)]$_2$).

The recorded ^{1}H NMR data and the X-band EPR data (solid and solution) matches the spectroscopic data of **1-Cr** obtained via method a.

1.3 Synthesis of [(Cp*Fe)(Cp'''Cr)$_2$(μ_3,$\eta^{2:3:3}$-As$_4$)(μ_3-As)] (2-Cr)

a) A freshly prepared solution of [(Cp*Fe(η^5-As$_5$)] (100 mg, 0.177 mmol, 1.0 eq) and KC_8 (55 mg, 0.407 mmol, 2.3 eq) in THF (5 mL) was cooled to -80°C. Then a dark blue solution of [Cp'''Cr(µ-Cl)]$_2$ (114 mg, 0.177 mmol, 1.0 eq) in THF (3 mL) was slowly added at -80°C. The mixture turned dark brown and was allowed to reach room temperature overnight. The solvent was removed *in vacuo*. Then the residue was dissolved in a small amount of CH_2Cl_2, silica gel was added and the solvent was removed *in vacuo*. The preabsorbed compound was purified by column chromatographic workup (SiO_2, hexane, 8 x 2.5 cm). Using hexane as an eluent **2-Cr** can be obtained as dark brown fraction. After removing the solvent in vacuo, the residue was dissolved in CH_2Cl_2 and layered with CH_3CN. After storage at room temperature for a few days, **2-Cr** can be obtained as light green-blue blocks. The supernatant was decanted off and the crystalline compound dried in vacuo.

Yield:	50 mg (0.044 mmol, 25 %).
^{1}H NMR (CD_2Cl_2, 293 K):	*δ* [ppm] = 1.57 (s, br, 30H, C_5H_2*tBu$_3$*), -3.17 (s, br, 15H, C_5*Me$_5$*). Signals for the second Cp''' ligand (C_5H_2*tBu$_3$*) and C_5*H$_2$t*Bu$_3$ could not be found within the ^{1}H NMR spectrum of **2-Cr**.
EPR (X-band):	broad, intense signal with unresolved hyperfine coupling in thf solution (293 K or 77 K) or as solid (298 K and 77 K) (see Figure S 27).
Evans-NMR (CD_2Cl_2, 293 K):	μ_{eff} = 1.36 μ_B corresponding to ~1.0 unpaired electron.
FD-MS (CH_2Cl_2):	*m/z* = 1136.12 ([**2-Cr**]$^+$, 100%).

1.4 Synthesis of [(Cp*Fe)(Cp'''Mn)(μ,$\eta^{5:5}$-P_5)] (1-Mn)

a) A freshly prepared solution of [(Cp*Fe(η^5-P_5)] (103.4 mg, 0.299 mmol, 1.0 eq) and KC_8 (101.1 mg, 0.748 mmol, 2.5 eq) in THF (5 mL) was cooled to -80°C. Then a light greenish solution of [Cp'''Mn(thf)(μ-I)]$_2$ (292.4 mg, 0.299 mmol, 1.0 eq) in THF (5 mL) was slowly added at -80°C. The mixture turned dark green and was allowed to reach room temperature overnight. The solvent was removed *in vacuo*. Then the residue was extracted with *n*-pentane and filtered over diatomaceous earth. Reducing the solvent in vacuo and storing the concentrated solution at 8°C yielded **1-Mn** as brownish green plates. The supernatant was decanted off and the crystalline compound dried in vacuo. Due to the high sensitivity of this compound towards moisture and oxygen it is not fully characterized, although the ^{31}P NMR spectrum of the reaction solution indicates a selective formation of **1-Mn** (cf. Figure S 5).

Yield: a few crystals

^{1}H NMR (C_6D_6, 293 K): *δ* [ppm] = 2.89 (s, 2H, C_5*H_2*tBu$_3$), 1.34 (s, 18H, C_5H_2*tBu$_3$*), 1.22 (s, 9H, C_5H_2*tBu$_3$*), 0.88 (s, 15H, C_5*Me$_5$*).

^{31}P{^{1}H} NMR (C_6D_6, 298 K): *δ* [ppm] = -38.4 (s, 5P, **1-Mn**).

^{31}P{^{1}H} NMR (C_6D_6, 298 K): *δ* [ppm] = -38.4 (s, 5P, **1-Mn**).

LIFDI-MS (toluene): *m/z* = 345.91 ([**1**]$^+$, 100%).

b) A freshly prepared solution of [(Cp*Fe(η^4-P_5)]$^{2-}$ (0.151 mmol, 1.0 eq) in THF (5 mL) was cooled to -80°C. Then a light greenish solution of [Cp'''Mn(thf)(μ-I)]$_2$ (70.0 mg, 0.076 mmol, 0.5 eq) in THF (5 mL) was slowly added at -80°C. The mixture turned dark green and was allowed to reach room temperature overnight. The ^{31}P NMR spectrum of the reaction solution measured with C_6D_6 capillary and PPh_3 (n = 0.016 mmol) shows the formation of **1-Mn** along with signals for **1** and [(Cp*Fe)$_2$(μ,$\eta^{4:4}$-P_{10})]$^{2-}$ indicating redox processes (cf. Figure S 7).[2]

1.5 Reaction of [Cp*Fe(η^5-As_5)], KC_8 and [Cp'''Mn(thf)(μ-I)]$_2$

A freshly prepared solution of [(Cp*Fe(η^5-As_5)] (169.0 mg, 0.299 mmol, 1.0 eq) and KC_8 (101.1 mg, 0.748 mmol, 2.5 eq) in THF (5 mL) was cooled to -80°C. Then a light greenish solution of [Cp'''Mn(thf)(μ-I)]$_2$ (292.4 mg, 0.299 mmol, 1.0 eq) in THF (5 mL) was slowly added at -80°C. The mixture turned dark green and was allowed to reach room temperature overnight turning dark brown. The solvent was removed *in vacuo*. Then the residue was extracted with *n*-hexane and filtered over diatomaceous earth. Storing a concentrated solution in hexane at -30°C or storing a mixture of hexane and hexamethyldisiloxane (1:1) at -30°C did not lead to single crystals. ^{1}H NMR spectroscopy suggests the formation of one major compound and one minor compound (see Figure S 8 and Figure S 9). Apart from that a broad singlet for [(Cp''')$_2$Mn] can be assigned[10] along with signals for HCp'''. However, we were not able to characterize the product of this reaction due to its sensitivity towards moisture and oxygen and the missing SC-XRD.

1.6 Synthesis of [(Cp*Fe)(Cp'''Fe)$_2$(μ_3,$\eta^{2:1:1}$-P_2)(μ,$\eta^{3:3}$-P_3)] (1-Fe)

a) [(Cp*Fe(η^5-P_5)] (200 mg, 0.578 mmol, 1.0 eq), KC_8 (195 mg, 1.445 mmol, 2.5 eq) and [Cp'''Fe(μ-Br)]$_2$ (340 mg, 0.460 mmol, 0.8 eq) were weighed in a Schlenk tube and DME (10 mL) was added. The mixture turned dark brown and was stirred for 3 hours at room temperature. The solvent was removed *in vacuo*. Then the residue was dissolved in a small amount of CH_2Cl_2, silica gel was added and the solvent was removed *in vacuo*. The preabsorbed compound was purified by column chromatographic workup (SiO_2, hexane, 7 x 2.5 cm). Using hexane as an eluent **1-Fe** can be obtained as dark brown fraction. After removing the solvent in vacuo, the residue was dissolved in CH_2Cl_2 and layered with CH_3CN. After storage at room temperature for a few days, **1-Fe** can be obtained as dark brown blocks. The supernatant was decanted off and the crystalline compound dried in vacuo.

Yield:	115 mg (0.124 mmol, 21 %).
^{1}H NMR (thf-d$_8$, 293 K):	δ [ppm] = 2.93 (s, br, 2H, C_5*H_2*tBu$_3$), 2.46 (s, br, 2H, C_5*H_2*tBu$_3$), 1.64 (s, 36H, C_5H_2*tBu$_3$*), 1.59 (s, 18H, C_5H_2*tBu$_3$*), 1.01 (s, 15H, C_5*Me$_5$*).
^{31}P{^{1}H} NMR (thf-d$_8$, 293 K):	δ [ppm] = 385.4 (d, J_{PP} = 98 Hz, 2P, P_A), 376.5 (d, J_{PP} = 371 Hz, 1P, P_B), -66.6 (dt, J_{PP} = 382 Hz, J_{PP} = 99 Hz, 1P, P_M), -231.8 (t, J_{PP} = 382 Hz, 1P, P_X).
^{31}P NMR (thf-d$_8$, 293 K):	δ [ppm] = 385.4 (d, J_{PP} = 98 Hz, 2P, P_A), 376.5 (d, J_{PP} = 371 Hz, 1P, P_B), -66.6 (dt, J_{PP} = 382 Hz, J_{PP} = 99 Hz, 1P, P_M), -231.8 (t, J_{PP} = 382 Hz, 1P, P_X).
FD-MS (CH_2Cl_2):	*m/z* = 924.92 ([**1-Fe**]$^+$, 100%).
Elemental Analysis	calculated (%) for $C_{44}H_{73}Fe_3P_5$: C: 57.17, H: 7.96 found [%]: C: 57.11, H: 8.01.

b) When a 1.0:2.5:0.8 stoichiometry of [(Cp*Fe(η^5-P_5)] (0.144 mmol) to KC_8 (0.360 mmol) to [Cp'''Fe(μ-Br)]$_2$ (0.106 mmol) is used, even after column chromatography traces of [Cp'''Fe(μ-Br)]$_2$ are still present, which can just be determined by X-band EPR spectroscopy (cf. Figure S 28). To obtain analytically pure **1-Fe** 0.8 eq [Cp'''Fe(μ-Br)]$_2$ must be used. In that case, after 3 hours stirring the X-band EPR spectrum remains silent and pure **1-Fe** is isolated. Nevertheless, in some cases minor impurities of [Cp'''Fe(μ-Br)]$_2$ can still be detected by X-band EPR spectroscopy.

c) When 0.5 eq of [Cp'''Fe(μ-Br)]$_2$ are used in the same one pot reaction in DME and the reaction is stirred at room temperature for 16 hours, no formation of **1-Fe** is observed. The ^{31}P

NMR spectrum of the reaction solution in dme with C_6D_6 capillary shows solely signals for $[(Cp^*Fe)_2(\mu,\eta^{4:4}\text{-}P_{10})]^{2-}$ (see Figure S 12).[2]

1.7 Synthesis of $[(Cp^*Fe)(Cp'''Fe)_2(\mu_3,\eta^{2:1:1}\text{-}As_2)(\mu,\eta^{3:3}\text{-}As_3)]$ (2-Fe)

a) $[(Cp^*Fe(\eta^5\text{-}As_5)]$ (163 mg, 0.289 mmol, 1.0 eq), KC_8 (98 mg, 0.723 mmol, 2.5 eq) and $[Cp'''Fe(\mu\text{-}Br)]_2$ (170 mg, 0.231 mmol, 0.8 eq) were weighed in a Schlenk tube and DME (10 mL) was added. The mixture turned dark green brown and was stirred for 3 hours at room temperature. The solvent was removed *in vacuo*. Then the residue was dissolved in a small amount of CH_2Cl_2, silica gel was added and the solvent was removed *in vacuo*. The preabsorbed compound was purified by column chromatographic workup (SiO_2, hexane, 7 x 2.5 cm). Using hexane as an eluent **2-Fe** can be obtained as dark brown fraction. After removing the solvent in vacuo, the residue was dissolved in CH_2Cl_2 and layered with CH_3CN. After storage at room temperature for a few days, **2-Fe** can be obtained as dark brown plates. The supernatant was decanted off and the crystalline compound dried in vacuo.

Yield:	65 mg (0.057 mmol, 20 %).
^{1}H NMR (CD_2Cl_2, 293 K):	δ [ppm] = 1.56 (s, br, $C_5H_2tBu_3$), 1.48 (s, br, $C_5H_2tBu_3$), 1.41 (s, br, $C_5H_2tBu_3$), 0.83 (s, br, C_5Me_5). The signals at 1.56, 1.48 and 1.41 ppm are overlapping. Due to the overlap of the signals and the broad shape no rational integration of the signals is possible (see Figure S 13).
FD-MS (CH_2Cl_2):	*m/z* = 1144.02 ([**2-Fe**]$^+$, 100%).
Elemental Analysis	calculated (%) for $C_{44}H_{73}Fe_3As_5$: C: 46.19, H: 6.43 found [%]: C: 46.58, H: 6.29.

When a 1.0:2.5:0.8 stoichiometry of $[(Cp^*Fe(\eta^5\text{-}As_5)]$ to KC_8 to $[Cp'''Fe(\mu\text{-}Br)]_2$ (0.106 mmol) is used, even after column chromatography traces of $[Cp'''Fe(\mu\text{-}Br)]_2$ are still present, which can just be determined by X-band EPR spectroscopy (cf. Figure S 28). To obtain analytically pure **2-Fe** 0.8 eq $[Cp'''Fe(\mu\text{-}Br)]_2$ must be used. In that case, after 3 hours stirring the X-band EPR spectrum remains silent and pure **2-Fe** is isolated. Nevertheless, in some cases minor impurities of $[Cp'''Fe(\mu\text{-}Br)]_2$ can still be detected by X-band EPR spectroscopy.

1.8 Synthesis of [(Cp*Fe)(Cp'''Ni)$_2$(μ_3,$\eta^{2:1:1}$-P_2)(μ_3,$\eta^{2:2:2}$-P_3)] (1-Ni)

[(Cp*Fe(η^5-P_5)] (1000 mg, 2.89 mmol, 1.0 eq), KC_8 (1000 mg, 7.40 mmol, 2.5 eq) and [Cp'''Ni(µ-Br)]$_2$ (2150 mg, 2.89 mmol, 1.0 eq) were weighed in a Schlenk tube and DME (50 mL) was added. The mixture turned dark red and was stirred for 30 min at room temperature. The solvent was removed *in vacuo*. Then the residue was dissolved in pentane and filtered over diatomaceous earth. Then the solvent was removed *in vacuo*. Then the residue was dissolved in a small amount of CH_2Cl_2, silica gel was added and the solvent was removed *in vacuo*. The preabsorbed compound was purified by column chromatographic workup (SiO_2, pentane, 15 x 4.5 cm). Using toluene as an eluent **1-Ni** can be obtained as dark red fraction. After removing the solvent in vacuo, a dark red-brown powder was obtained. Despite several attempts no single crystals of **1-Ni** could be obtained. Structural proof of the proposed complex **1-Ni** was done by coordination to silver (see Synthesis of [{(Cp*Fe)(Cp'''Ni)$_2$(µ3,η2$^{:1:1-P2}$)(µ3,η2$^{:2:2-P3}$)}Ag]$_2$[FAl]$_2$ (3-Ag)).

Yield:	1530 mg (1.64 mmol, 57 %)
^{1}H NMR (tol-d$_8$, 253 K):	*δ* [ppm] = 5.61 (s, br, 2H, C_5H_2tBu$_3$), 5.58 (s, br, 2H, C_5H_2tBu$_3$), 1.83 (s, 15H, C_5Me_5), 1.55 (s, 18H, $C_5H_2tBu_3$), 1.50 (s, 18H, $C_5H_2tBu_3$), 1.47 (s, 18H, $C_5H_2tBu_3$).
^{31}P{^{1}H} NMR (tol-d$_8$, 253 K):	*δ* [ppm] = 390.0 (t, J_{PP} = 156 Hz, 1P, P_3), 280.7 (d, J_{PP} = 156 Hz, J_{PP} = 24 Hz, 2P, P_3), 152.8 (s, 2P, P_2).
^{31}P NMR (tol-d$_8$, 253 K):	*δ* [ppm] = 390.0 (t, J_{PP} = 156 Hz, 1P, P_3), 280.7 (d, J_{PP} = 156 Hz, J_{PP} = 24 Hz,2P, P_3), 152.8 (s, 2P, P_2).
FD-MS (CH_2Cl_2):	*m/z* = 928.18 ([**1-Ni**]$^+$, 100%).
Elemental Analysis	calculated (%) for $C_{44}H_{73}FeNi_2P_5$: C: 56.82, H: 7.91 found [%]: C: 57.29, H: 7.75.

When the reaction is performed using a stoichiometry of [(Cp*Fe(η^5-P_5)] (200 mg, 0.578 mmol, 1.0 eq), KC_8 (198 mg, 1.445 mmol, 2.5 eq) and [Cp'''Ni(µ-Br)]$_2$ (215 mg, 0.289 mmol, 0.5 eq) in dme for 30 min, the ^{31}P{^{1}H} NMR spectrum of the reaction solution shows no set of signals for **1-Ni**. Instead, small multiplets for [(Cp*Fe)$_2$(µ,$\eta^{4:4}$-P_{10})]$^{2-}$ can be assigned[2] and a broad signal at δ = 32.9 ppm is observed (see Figure S 17). Purification by column chromatography (SiO_2, hexane, 12 x 2.5 cm) eluted an orange-brown fraction using a 1:1 mixture of hexane/CH_2Cl_2. From a concentrated solution in CH_2Cl_2 layered with acetonitrile no single crystals could be formed. The formed compound could not be unequivocally characterized.

1.9 Synthesis of [{(Cp*Fe)(Cp'''Ni)$_2$(μ$_3$,η$^{2:1:1}$-P$_2$)(μ$_3$,η$^{2:2:2}$-P$_3$)}Ag]$_2$[FAl]$_2$ (3-Ag)

A solution of Ag[FAl] (160 mg, 0.107 mmol, 1 eq) in *o*-DFB (5 mL) was added to a stirred solution of **1-Ni** (100 mg, 0.107 mmol, 1 eq) in *o*-DFB (5 mL). The brown mixture was stirred for 2 h at room temperature. Then the solvent was removed in vacuo and the residue washed with hexane. The residue was dried in vacuo, dissolved in *o*-DFB and layered with hexane. After storage at room temperature for 2 days, **3-Ag** can be obtained as dark brown blocks. The supernatant was decanted off and the crystalline compound dried in vacuo.

Yield:	57 mg (0.055 mmol, 51 %)
^{1}H NMR (thf-d$_8$, 293 K):	Signals can not be properly assigned due to decomposition in solution and rearrangement processes (see Figure S 19 to Figure S 20).
^{31}P NMR (thf-d$_8$, 293 K):	δ [ppm] = 430.6 (t, J_{PP} = 151 Hz, br), 248.8 (d, J_{PP} = 151 Hz, br), 88.2 (br).
^{19}F{^{1}H} (thf-d$_8$, 293 K):	δ [ppm] = -112.0 (d, J_{FF} = 275 Hz, 6F), -116.2 (d, J_{FF} = 281 Hz, 6F), -121.2 (d, J_{FF} = 281 Hz, 3F), -127.0 (s, 6F), -129.8 (d, J_{FF} = 281 Hz, 6F), -136.9 (d, J_{FF} = 281 Hz, 6F), -141.0 (d, J_{FF} = 281 Hz, 3F), -154.8 (s, 3F), -165.2 (t, J_{FF} = 20 Hz, 6F), -170.7 (s, 1F).
ESI-MS (CH$_2$Cl$_2$, pos. mode):	*m/z* = 928.18 ([**3-Ag**]$^{2+}$, 100%)
ESI-MS (CH$_2$Cl$_2$, neg. mode):	*m/z* = 1037.15 ([FAl]$^{-}$, 100%)
Elemental Analysis	calculated (%) for $C_{160}H_{146}Fe_2Ni_4P_{10}O_6Al_2F_{92}Ag_2$: C: 39.72, H: 3.04 found [%]: C: 39.86, H: 3.16.

Compound **3-Ag** is hard to re-dissolve after crystallization even in thf. Apart from that, **3-Ag** shows decomposition over time in solution at room temperature, which was monitored in the ^{31}P{^{1}H} and ^{31}P NMR spectrum. Therefore, the data quality for the corresponding NMR spectra are of poor quality as many species can be observed (see Figure S 19 and Figure S 20). Dissolving crystals of **3-Ag** in thf-d$_8$ at -80°C and measuring an ^{1}H NMR spectrum at -80°C did not improve the spectrum quality. As the solubility of **3-Ag** at lower temperatures is very poor and in the corresponding spectrum already at -80°C many signals can be observed an attribution of the signals is not possible (see Figure S 21). Presumably, in solution rearrangement processes and decomposition is present.

1.10 Synthesis of [(Cp*Fe)(Cp'''Ni)$_2$(μ$_3$,η$^{3:2:2}$-As$_4$)(μ$_3$-As)] (2-Ni)

[(Cp*Fe(η^5-As$_5$)] (100 mg, 0.177 mmol, 1 eq) and [Cp'''Ni(μ-Br)]$_2$ (132 mg, 0.177 mmol, 1.0 eq) were weighed in a Schlenk tube and DME (10 mL) was added. Then a suspension of KC_8 (68 mg, 0.400 mmol, 2.3 eq) in DME (10 mL) was added at room temperature to afford a dark brown color change. The mixture was stirred for 3 hours at room temperature. Then the solvent was removed *in vacuo*. Then the residue was dissolved in pentane and filtered over diatomaceous earth. After removing the solvent in vacuo, the residue was dissolved in CH_2Cl_2 and layered with CH_3CN. After storage at room temperature for a few days, **2-Ni** can be obtained as dark brown blocks. The supernatant was decanted off and the crystalline compound washed with CH_3CN (5 x 3 mL) and dried in vacuo.

Yield:	71 mg (0.061 mmol, 35 %).
^{1}H NMR (C_6D_6, 293 K):	*δ* [ppm] = 5.47 (s, br, 2H, C_5*H*$_2$*t*Bu$_3$), 5.34 (s, br, 2H, C_5*H*$_2$*t*Bu$_3$), 1.70 (s, 18H, C_5H_2*tBu*$_3$), 1.53 (s, 15H, C_5*Me*$_5$), 1.52 (s, 18H, C_5H_2*tBu*$_3$), 1.44 (s, 18H, C_5H_2*tBu*$_3$).
LIFDI-MS (toluene):	*m/z* = 1147.99 ([**2-Ni**]$^+$, 100%).
Elemental Analysis	calculated (%) for $C_{44}H_{73}FeNi_2As_5$: C: 45.96, H: 6.40 found [%]: C: 45.50, H: 6.19.

2 NMR spectroscopic investigations

2.1 1-Cr

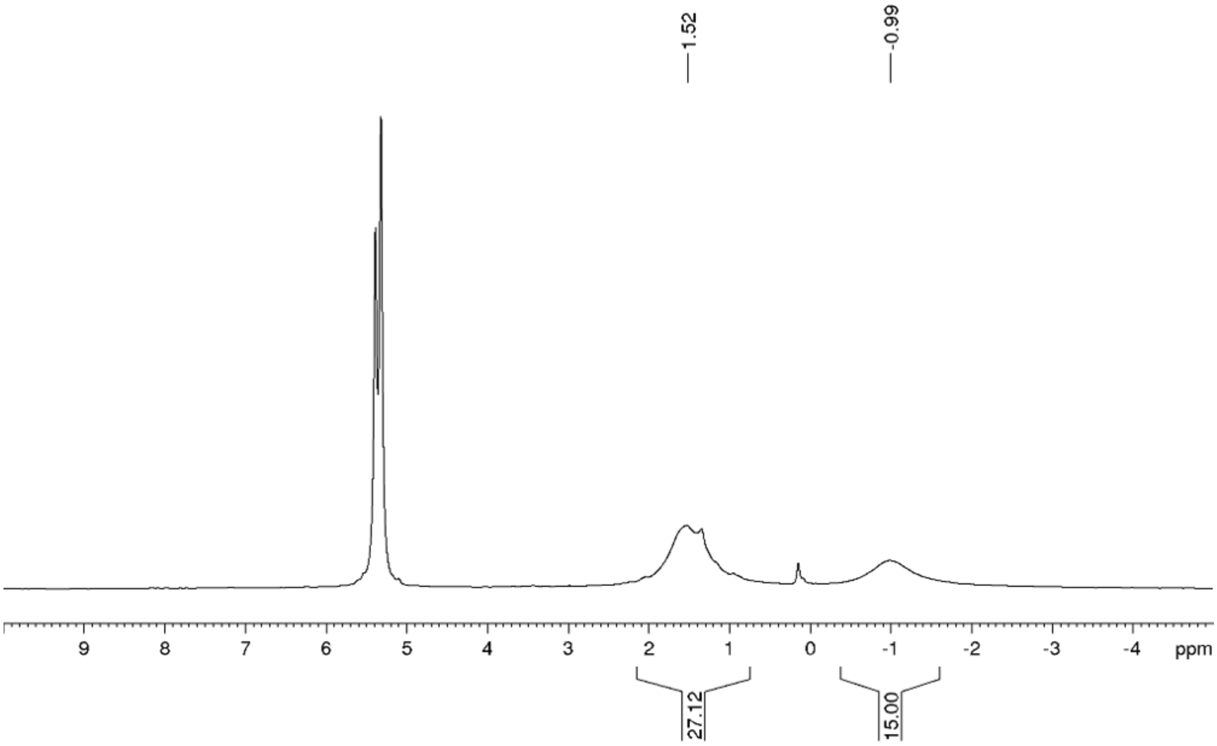


Figure S 1. ^{1}H NMR spectrum for **1-Cr** in CD_2Cl_2 recorded at room temperature. 8.0 mg of **1-Cr** were dissolved in 2.2 mL CD_2Cl_2 and filled in an Evans NMR tube with pure CD_2Cl_2 in the outer tube in order to determine the number of unpaired electrons via Evans NMR method.

2.2 2-Cr

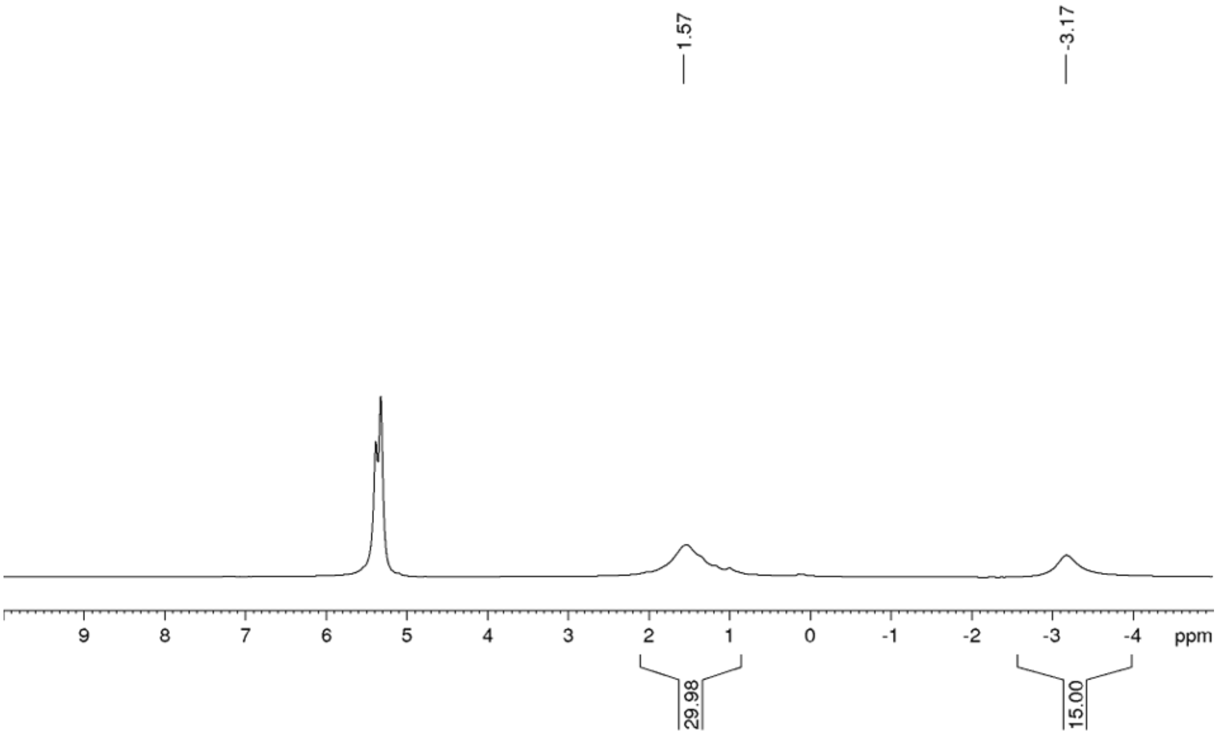


Figure S 2. [1]H NMR spectrum for **2-Cr** in CD_2Cl_2 recorded at room temperature. 10.0 mg of **2-Cr** were dissolved in 1.8 mL CD_2Cl_2 and filled in an Evans NMR tube with pure CD_2Cl_2 in the outer tube in order to determine the number of unpaired electrons via Evans NMR method.

2.3 1-Mn

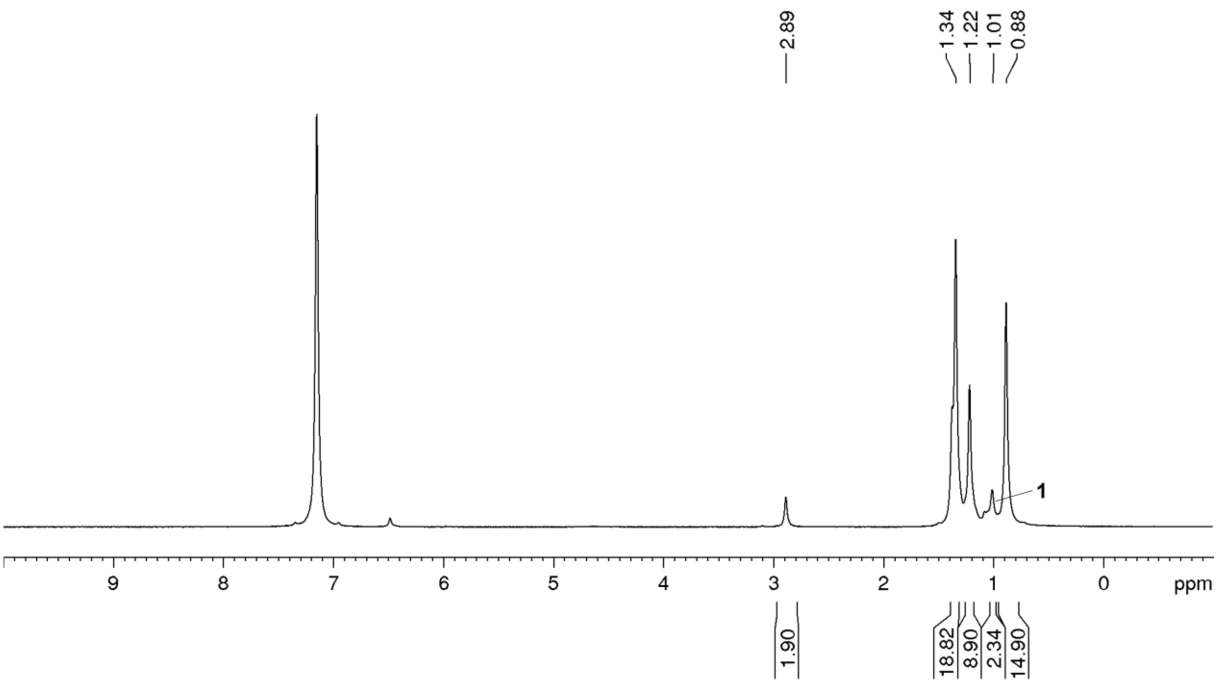


Figure S 3. [1]H NMR spectrum for **1-Mn** in C_6D_6 recorded at room temperature. Minor impurities of **1** can be observed.

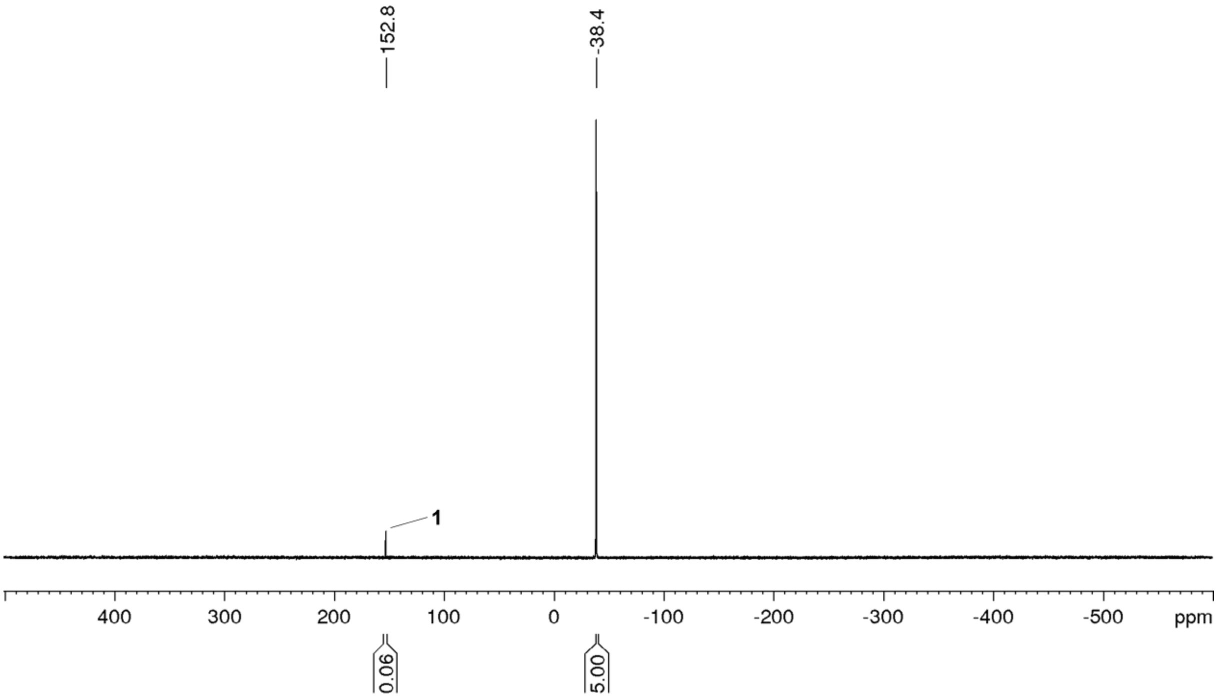


Figure S 4. ^{31}P NMR spectrum for **1-Mn** in C_6D_6 recorded at room temperature. Minor impurities of **1** can be observed.

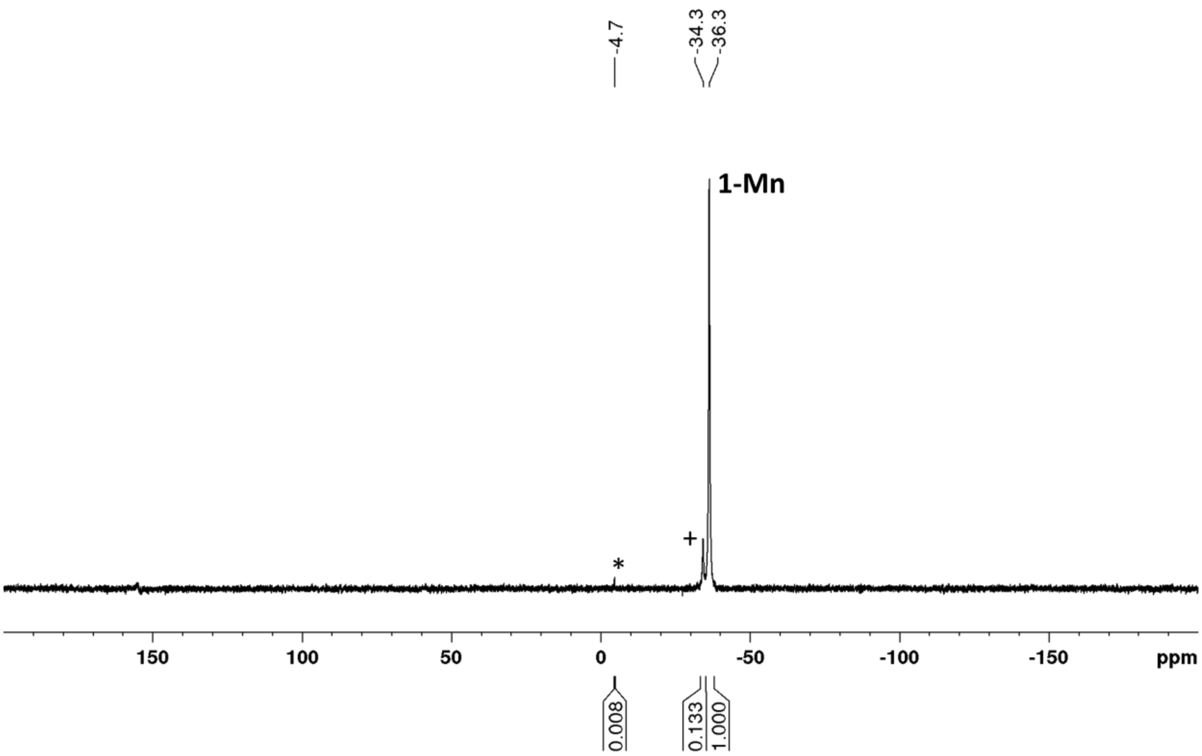


Figure S 5. ^{31}P NMR spectrum for the reaction solution of **1-Mn** in thf with a C_6D_6-capillary and 0.02 mmol PPh_3 recorded at room temperature (signal marked with * = PPh_3, signal marked with + = unidentified by-product).

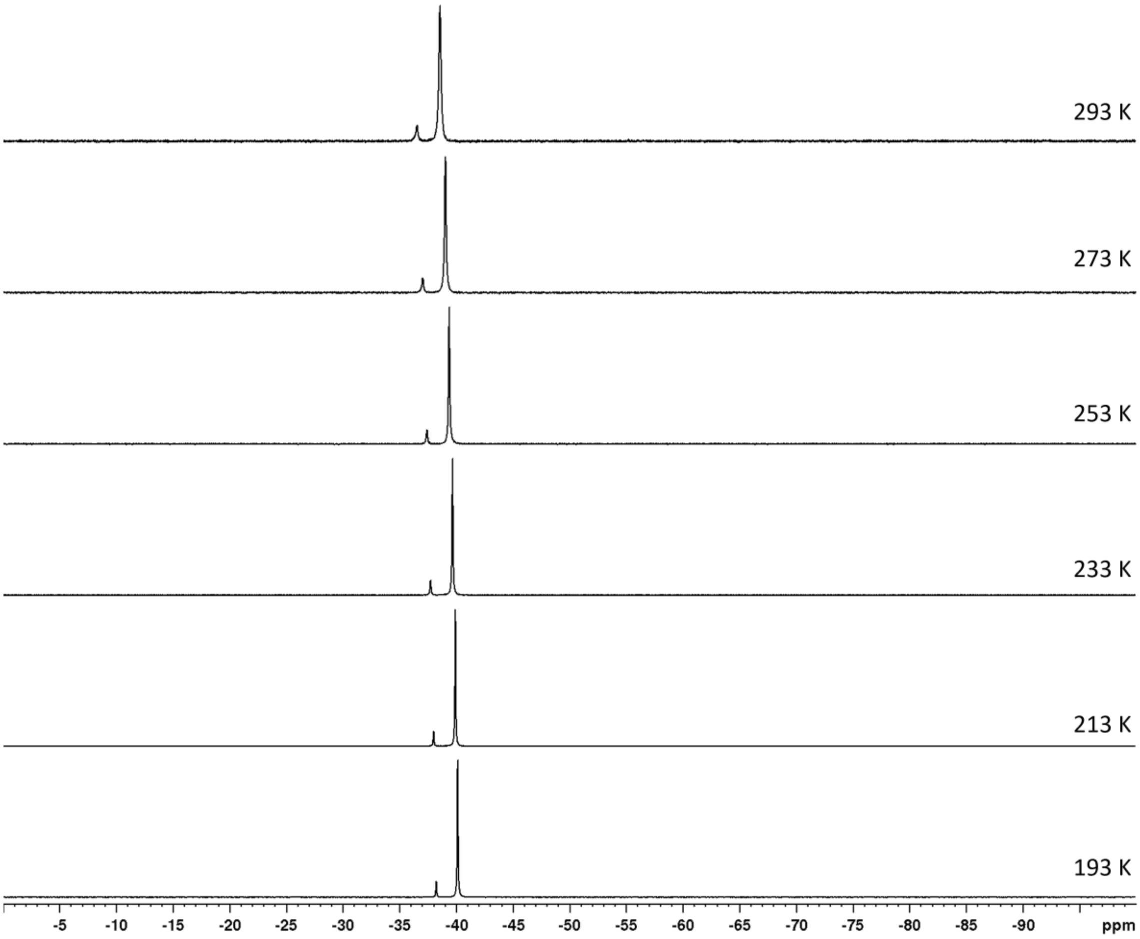


Figure S 6. Variable temperature $^{31}P\{^1H\}$ NMR spectra for the reaction solution of **1-Mn** recorded in thf-d_8.

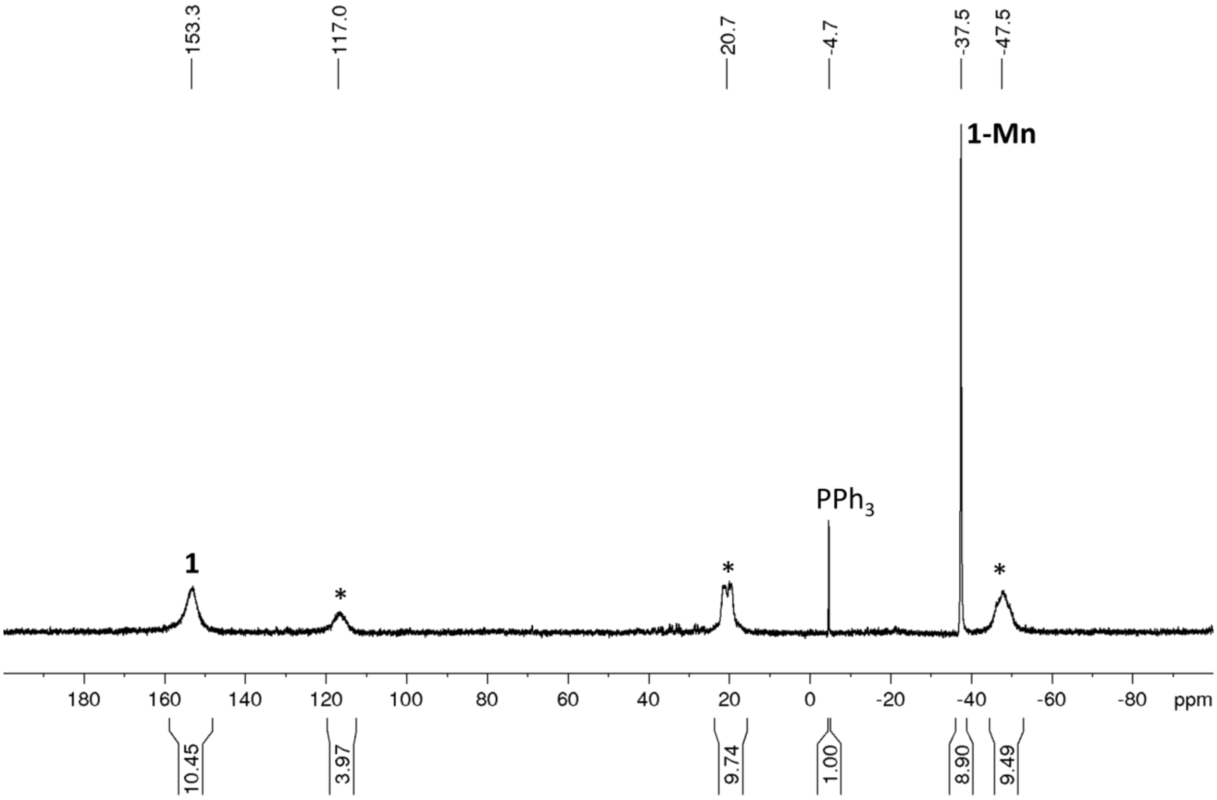


Figure S 7. ^{31}P NMR spectrum for the reaction solution of 1.0 eq $[Cp^*Fe(\eta^4\text{-}P_5)]^{2-}$ (0.151 mmol) and 0.5 eq $[Cp'''Mn(THF)(\mu\text{-}I)]_2$ (0.076 mmol) in thf with a C_6D_6-capillary containing 0.016 mmol PPh_3 recorded at room temperature (signal marked with * = redox by-product = $[(Cp^*Fe)_2(\mu,\eta^4\text{:}\eta^4\text{-}P_{10})]^{2-}$).[2]

2.4 2-Mn

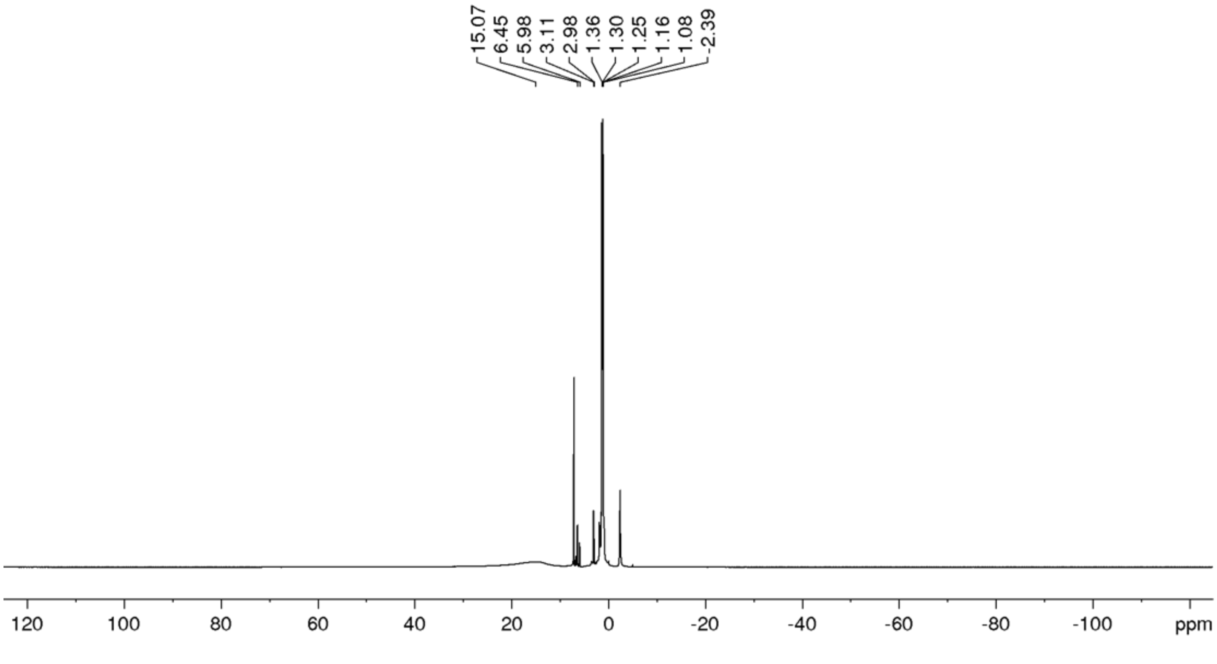


Figure S 8. ^{1}H NMR spectrum for the reaction of $[Cp^*Fe(\eta^5\text{-}As_5)]$, KC_8 and $[Cp'''Mn(THF)(\mu\text{-}I)]_2$ after extraction with hexane in C_6D_6 recorded at room temperature. Signal at δ [ppm] = 15.07 can be assigned to the formation of $[(Cp''')_2Mn]$.[10]

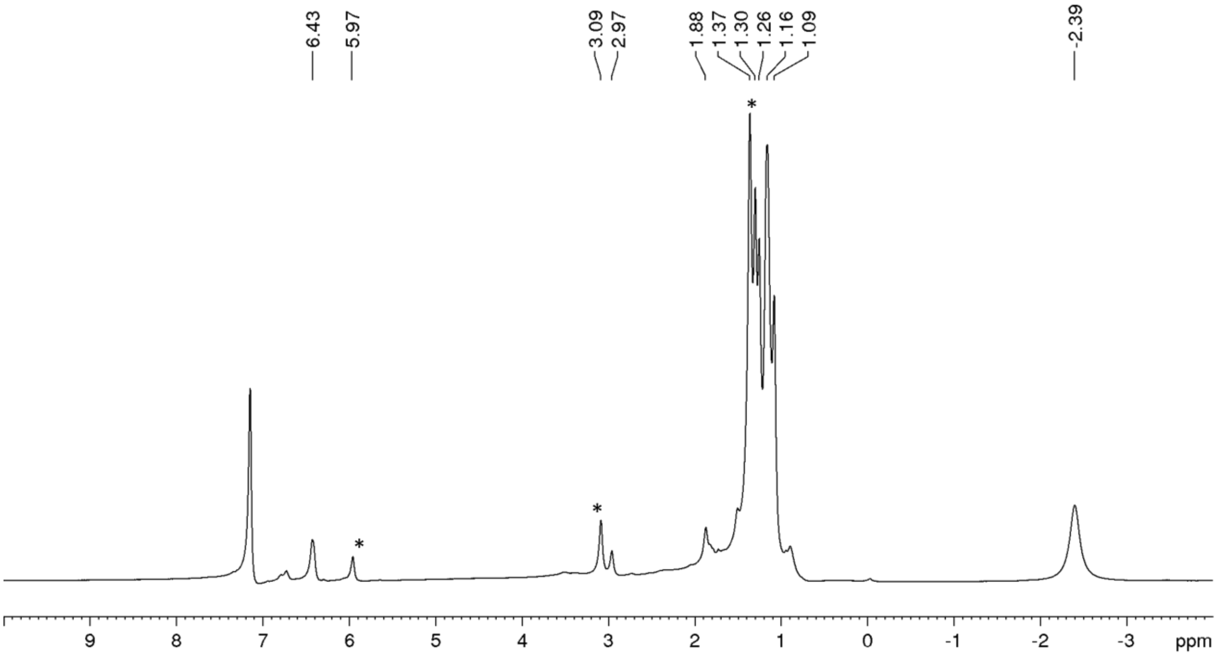


Figure S 9. [1]H NMR spectrum for the reaction of [Cp*Fe(η^5-As_5)], KC_8 and [Cp'''Mn(THF)(µ-I)]$_2$ after extraction with hexane in C_6D_6 recorded at room temperature. Only the area between δ/ppm = 10 ppm to -4 is depicted. Signals for HCp''' are marked with *.

2.5 1-Fe

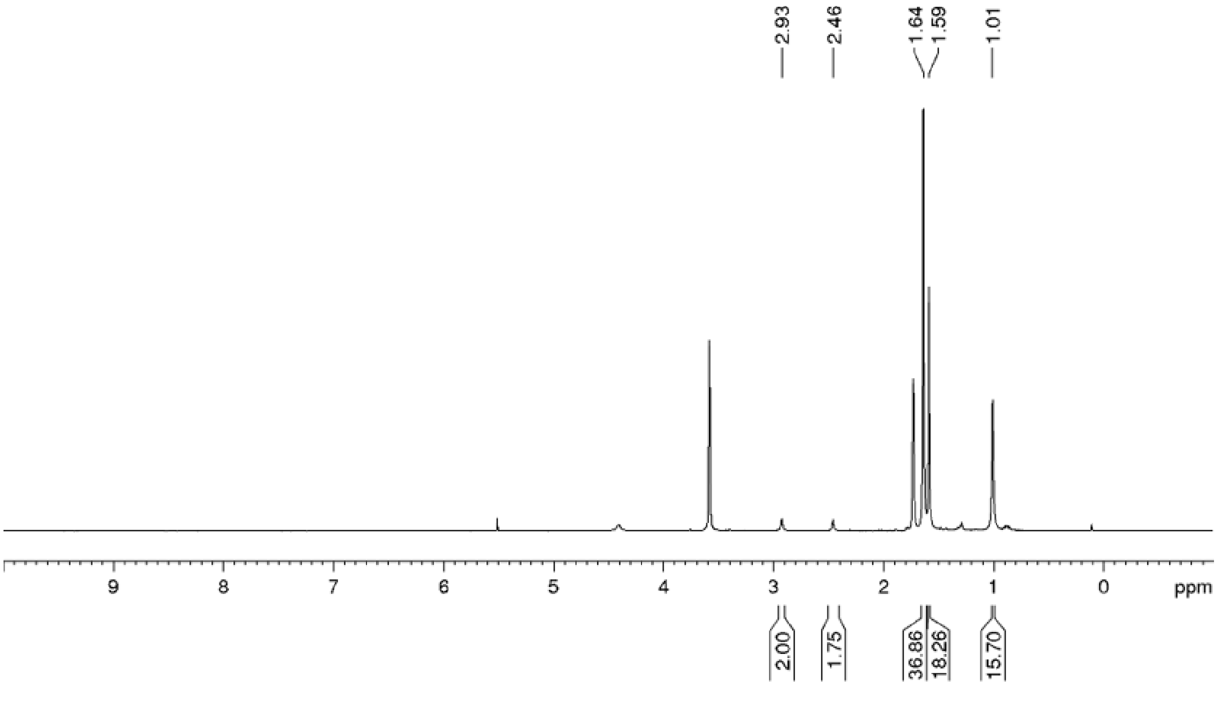


Figure S 10. [1]H NMR spectrum for **1-Fe** in thf-d_8 recorded at room temperature.

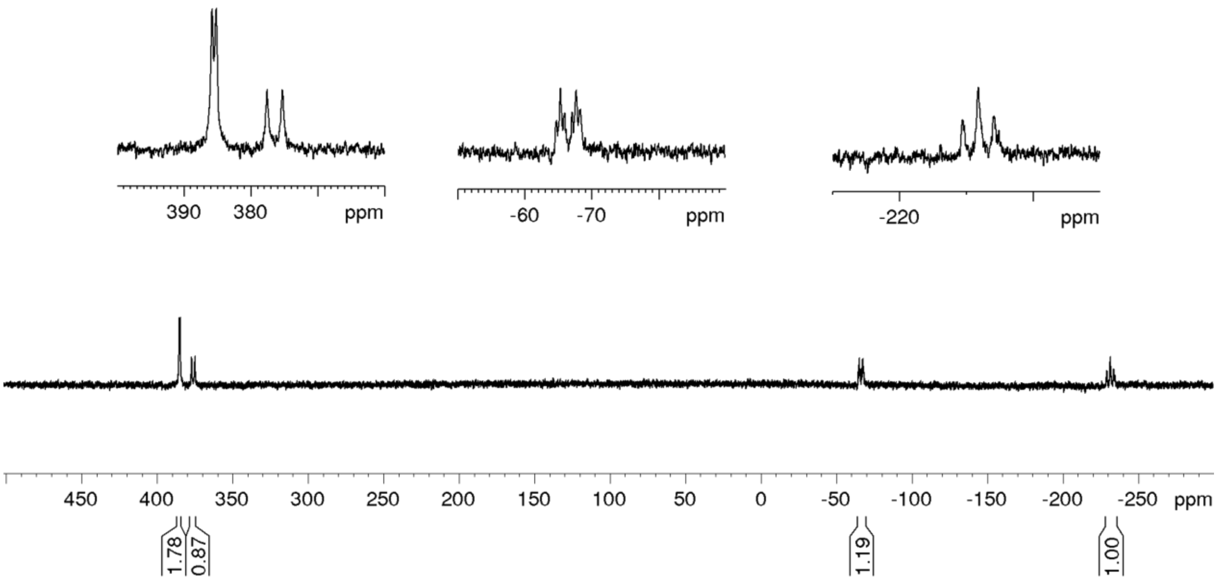


Figure S 11. ^{31}P NMR spectrum for **1-Fe** in thf-d_8 recorded at room temperature.

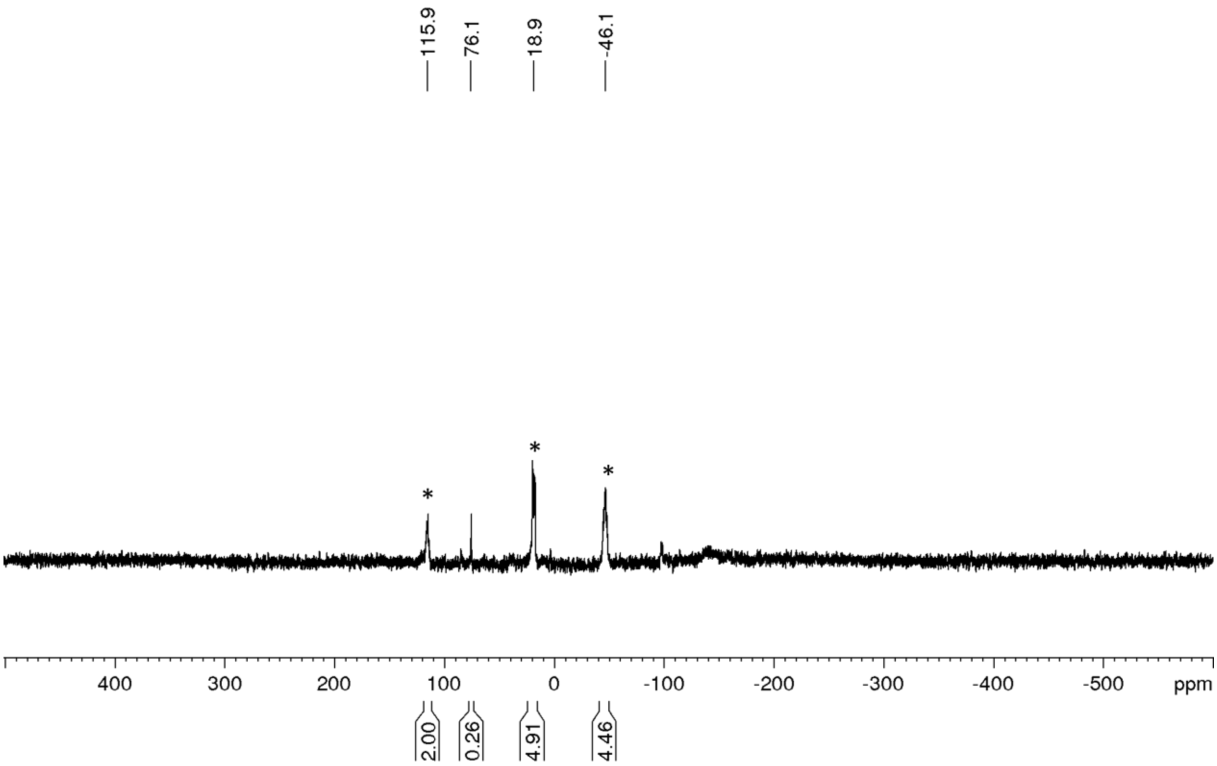


Figure S 12. ^{31}P NMR spectrum for the reaction solution of 1.0 eq [Cp*Fe(η^4-P_5)]$^{2-}$ (0.144 mmol) and 0.5 eq [Cp'''Fe(μ-Br)]$_2$ (0.072 mmol) in dme with a C_6D_6-capillary recorded at room temperature (signal marked with * = redox product = [(Cp*Fe)$_2$(μ,η^4:η^4-P_{10})]$^{2-}$).[2]

2.6 2-Fe

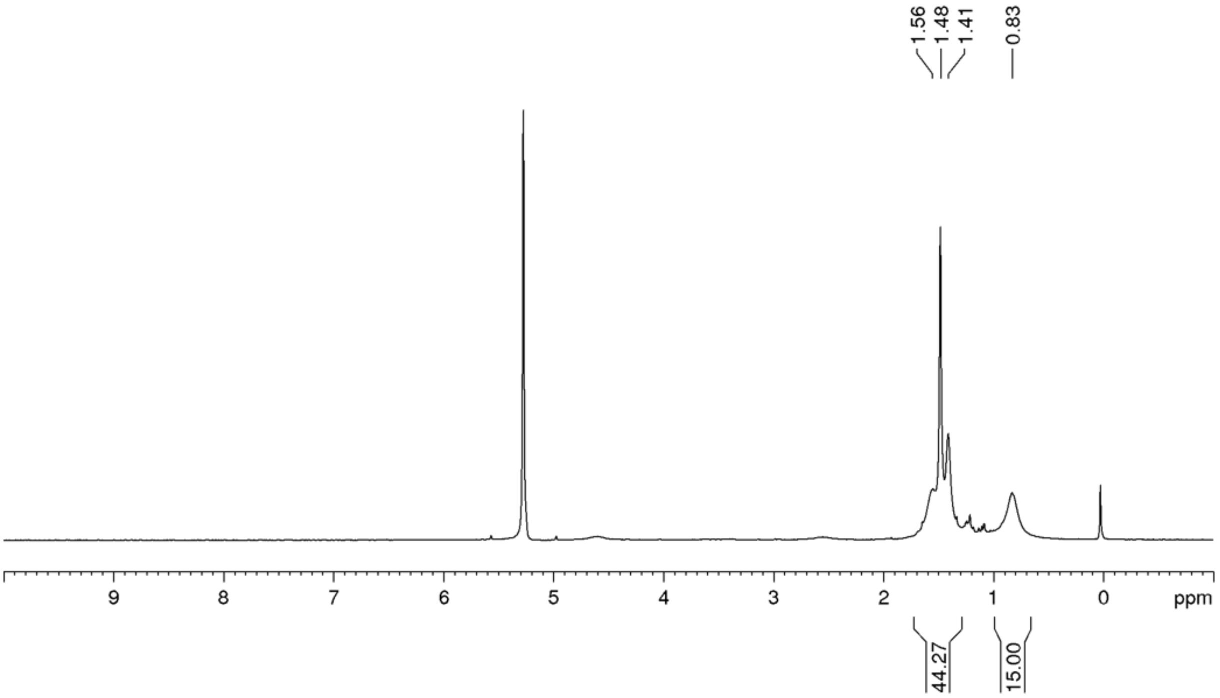


Figure S 13. ^{1}H NMR spectrum for **2-Fe** in CD_2Cl_2 recorded at room temperature.

2.7 1-Ni

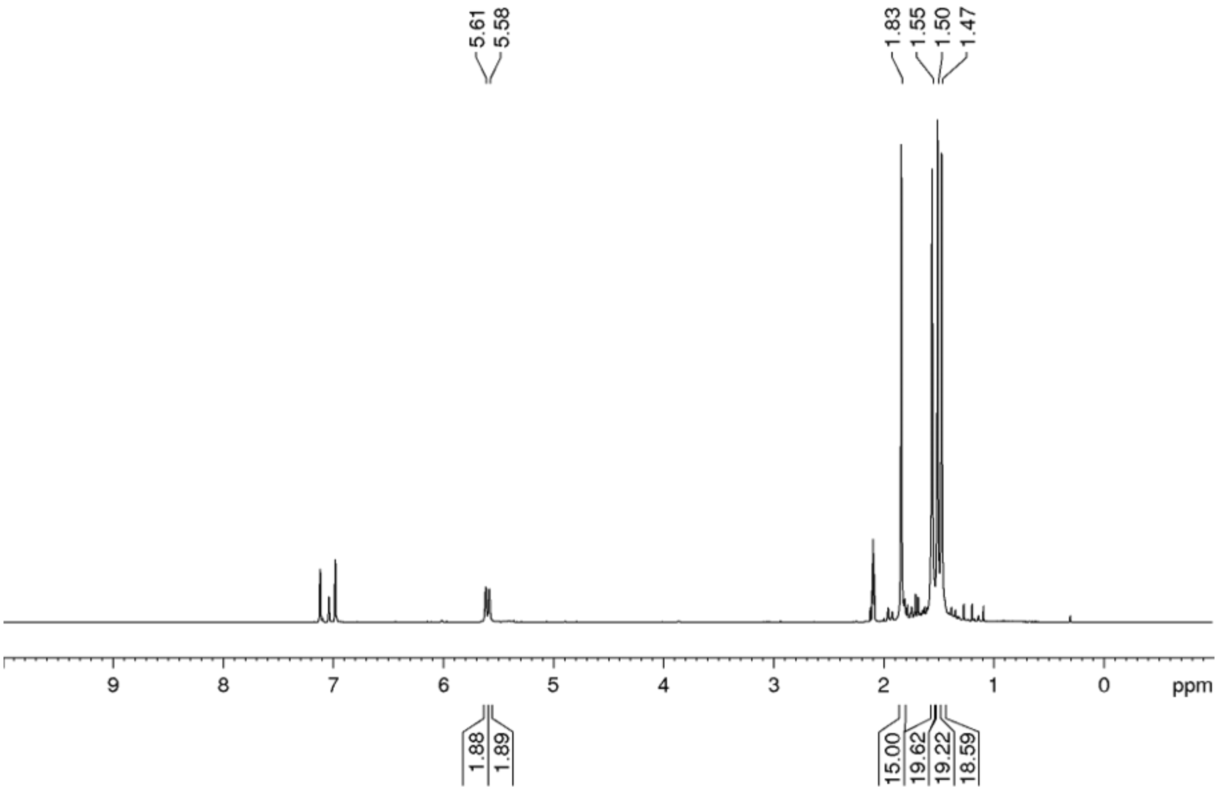


Figure S 14. ^{1}H NMR spectrum for **1-Ni** in tol-d_8 recorded at 253 K.

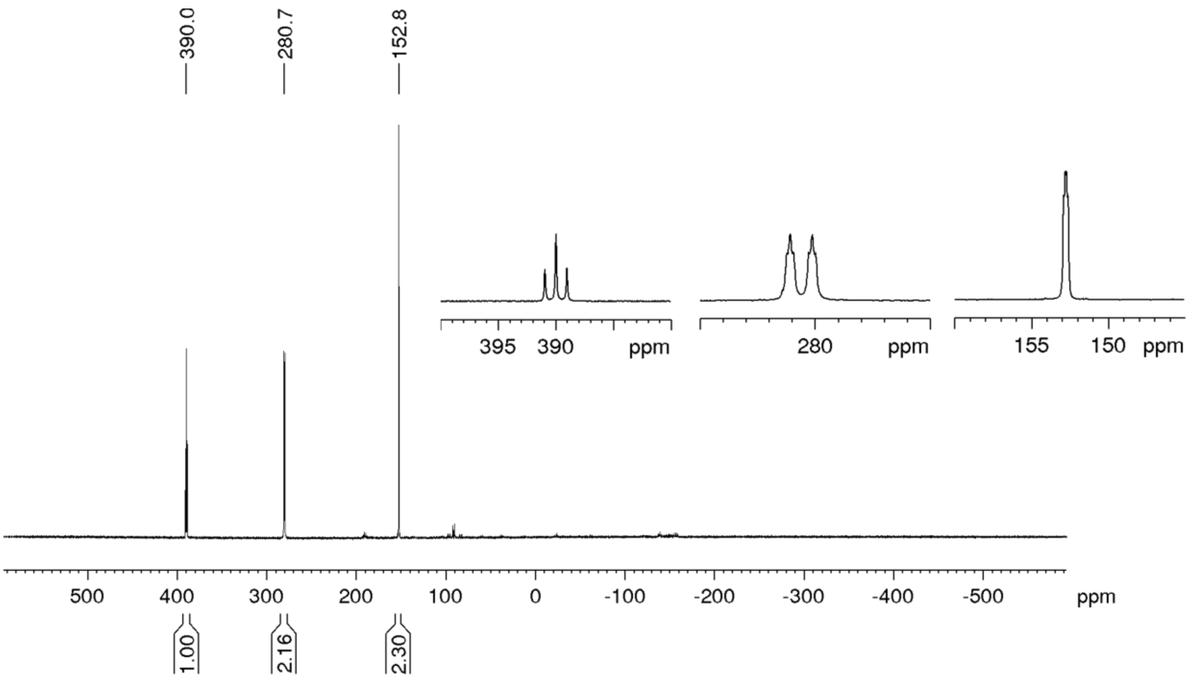


Figure S 15. ^{31}P NMR spectrum for **1-Ni** in tol-d_8 recorded at 253 K.

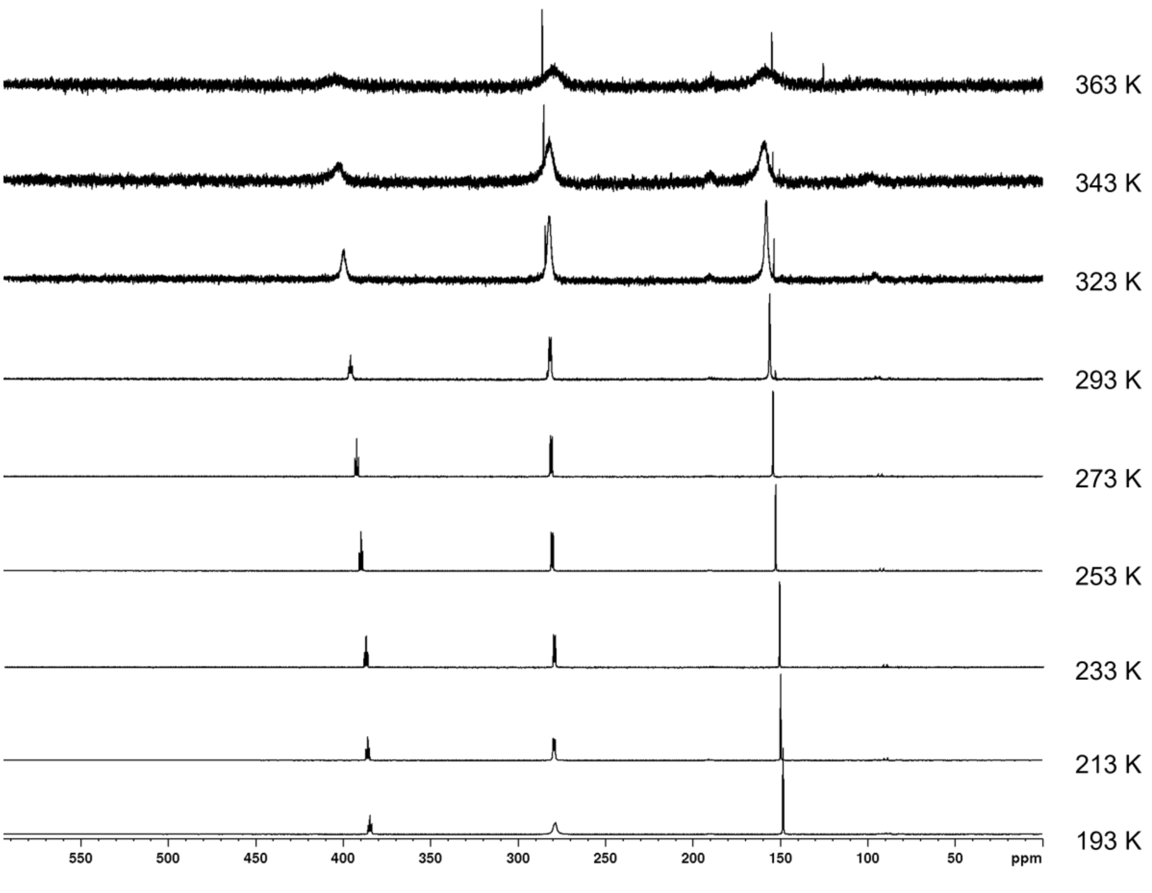


Figure S 16. Variable temperature ^{31}P NMR spectra for **1-Ni** recorded in thf-d_8.

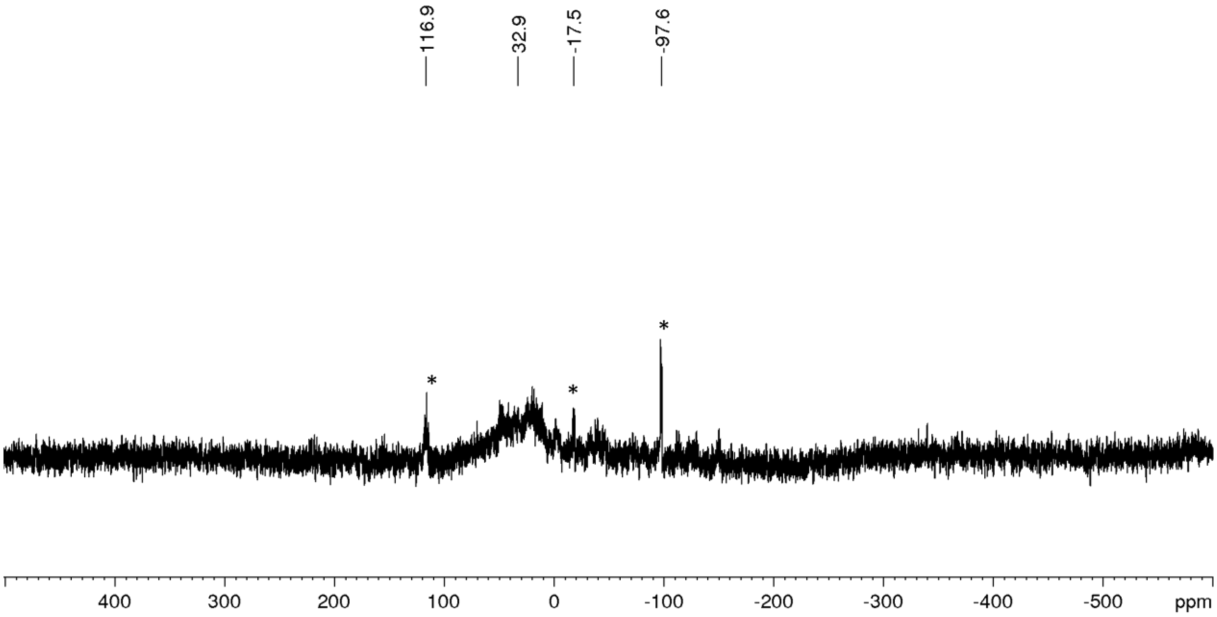


Figure S 17. $^{31}P\{^{1}H\}$ NMR spectrum for the reaction solution of 1.0 eq $[Cp^{*}Fe(\eta^{4}-P_{5})]^{2-}$ (0.578 mmol) and 0.5 eq $[Cp'''Ni(\mu-Br)]_2$ (0.289 mmol) in DME with a C_6D_6-capillary recorded at room temperature (signal marked with * = redox product = $[(Cp^{*}Fe)_2(\mu,\eta^{4}:\eta^{4}-P_{10})]^{2-}$).[2]

2.8 2-Ni

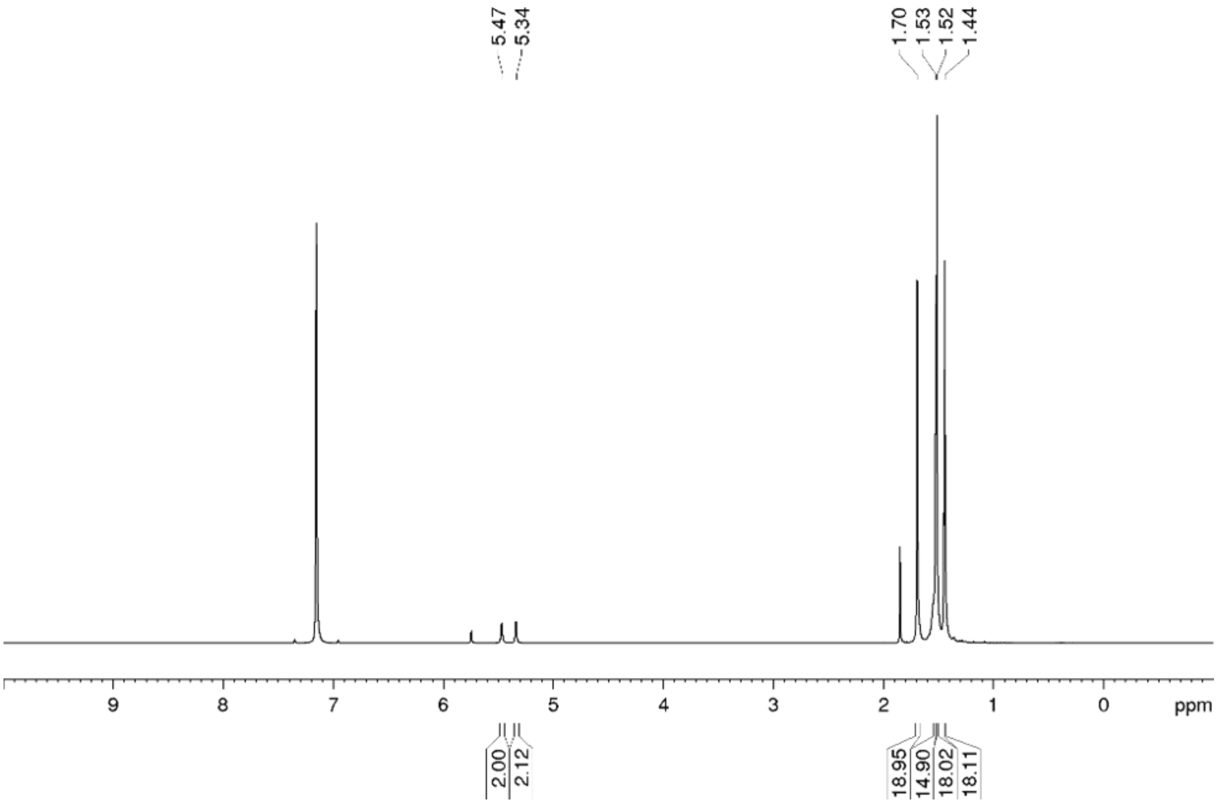


Figure S 18. ^{1}H NMR spectrum for **2-Ni** in C_6D_6 recorded at room temperature.

2.9 3-Ag

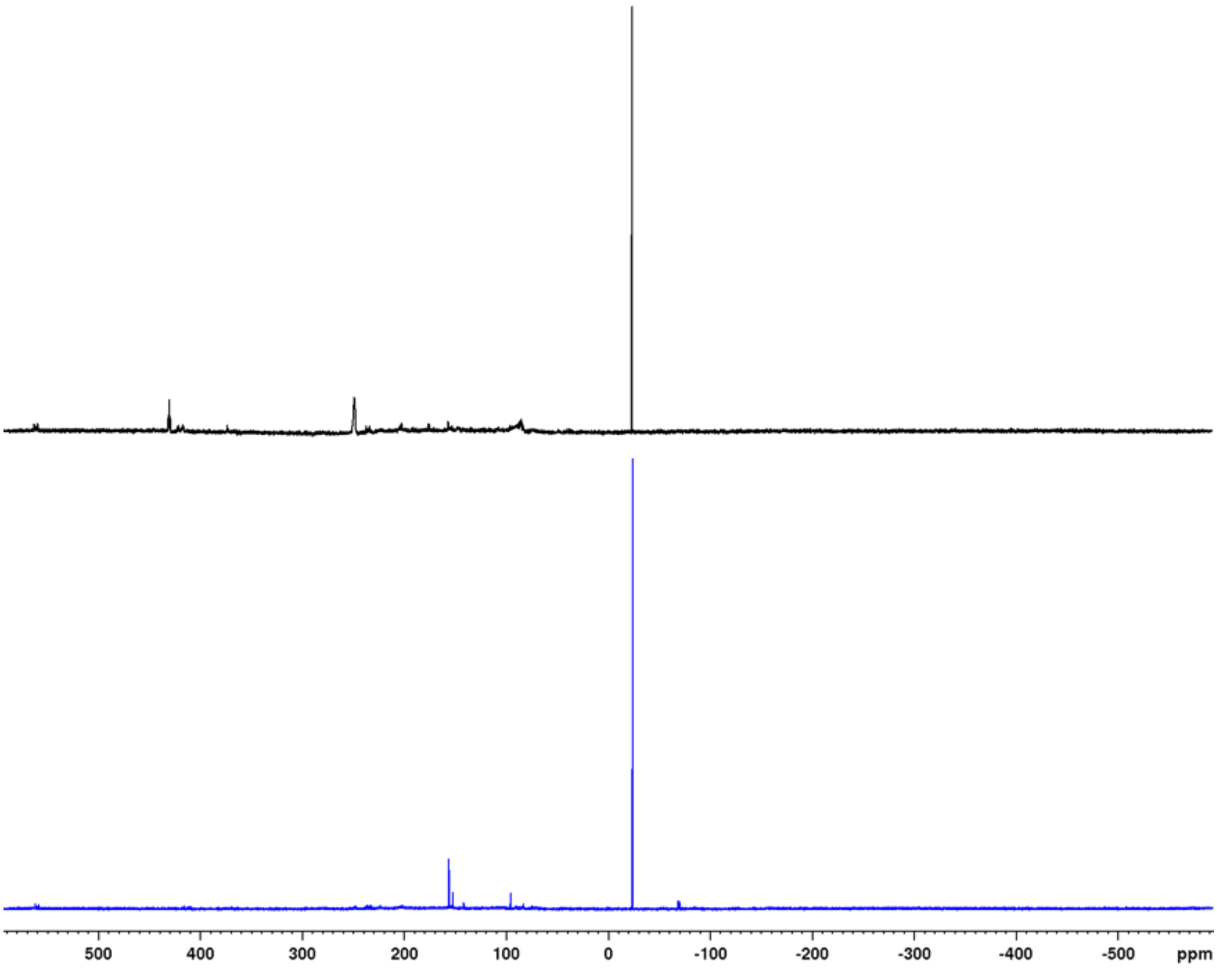


Figure S 19. $^{31}P\{^1H\}$ (top, black) and ^{31}P (bottom, blue) NMR spectra for **3-Ag** in thf-d_8 recorded at 273 K. The signal at δ = -22 ppm is attributed to an impurity. The signals at δ/ppm = 430.6, 249.1 and 86.6 in the $^{31}P\{^1H\}$ NMR spectrum are assigned to the complex **3-Ag**. Upon measurement of the ^{31}P NMR spectrum of the same sample already changes in the spectrum can be observed within a few hours.

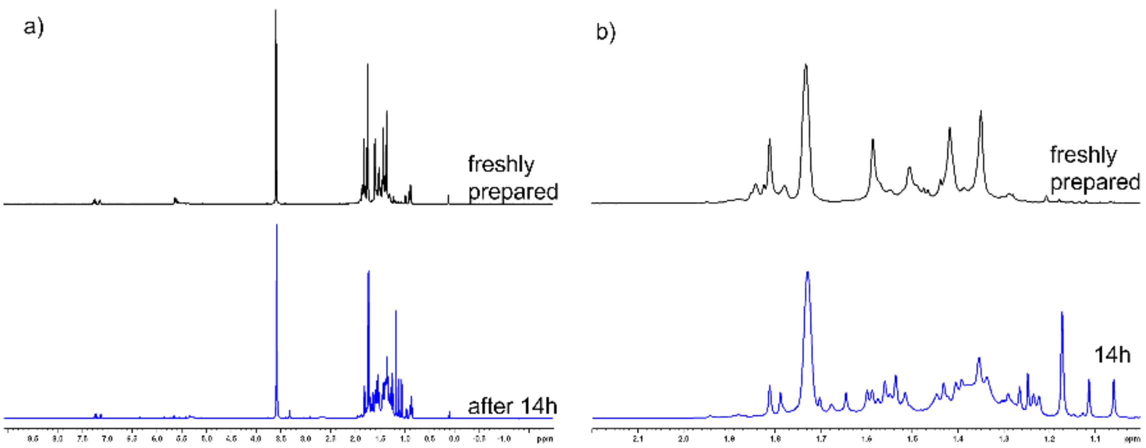


Figure S 20. a) ^1H NMR spectra for **3-Ag** in thf-d_8 recorded at 273 K of a freshly prepared sample (top, black) and after 14h (bottom, blue); b) zoom for a better view in the aliphatic C-H region.

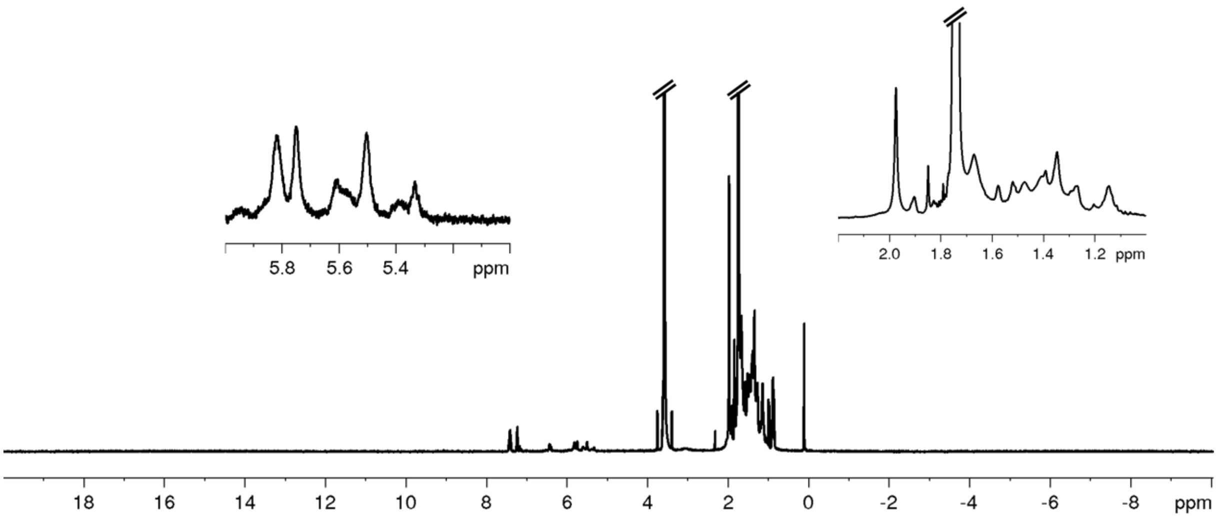


Figure S 21. ^{1}H NMR spectrum for **3-Ag** in THF-d_8 recorded at 193 K. The sample was freshly prepared and dissolved at 193 K prior to the measurement.

2.10 Syntheses starting from $[K(dme)_2]_2[Cp^*Fe(\eta^4\text{-}P_5)]$

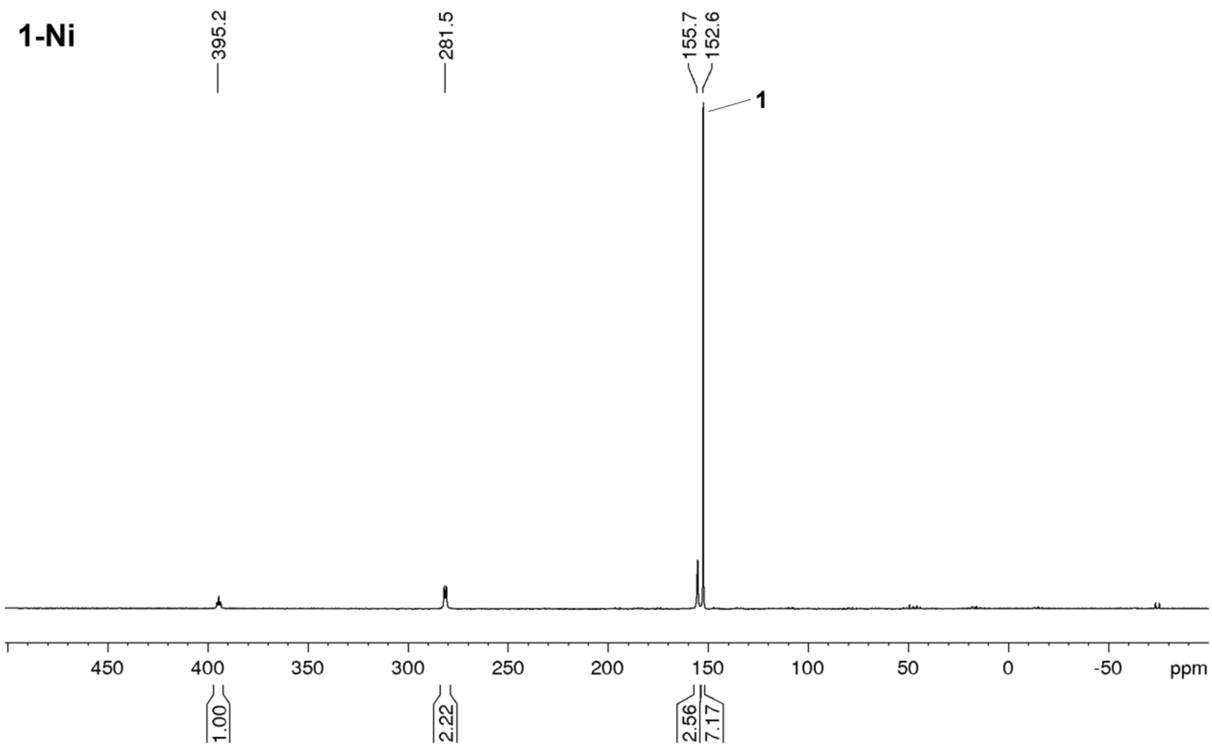


Figure S 22. Experimental $^{31}P\{^{1}H\}$ NMR spectrum (dme|C_6D_6 capillary) for the reaction mixture of $[K(dme)_2]_2[Cp^*Fe(\eta^4\text{-}P_5)]$ with $[Cp'''Ni(\mu\text{-}Br)]_2$ recorded at room temperature.

1-Cr

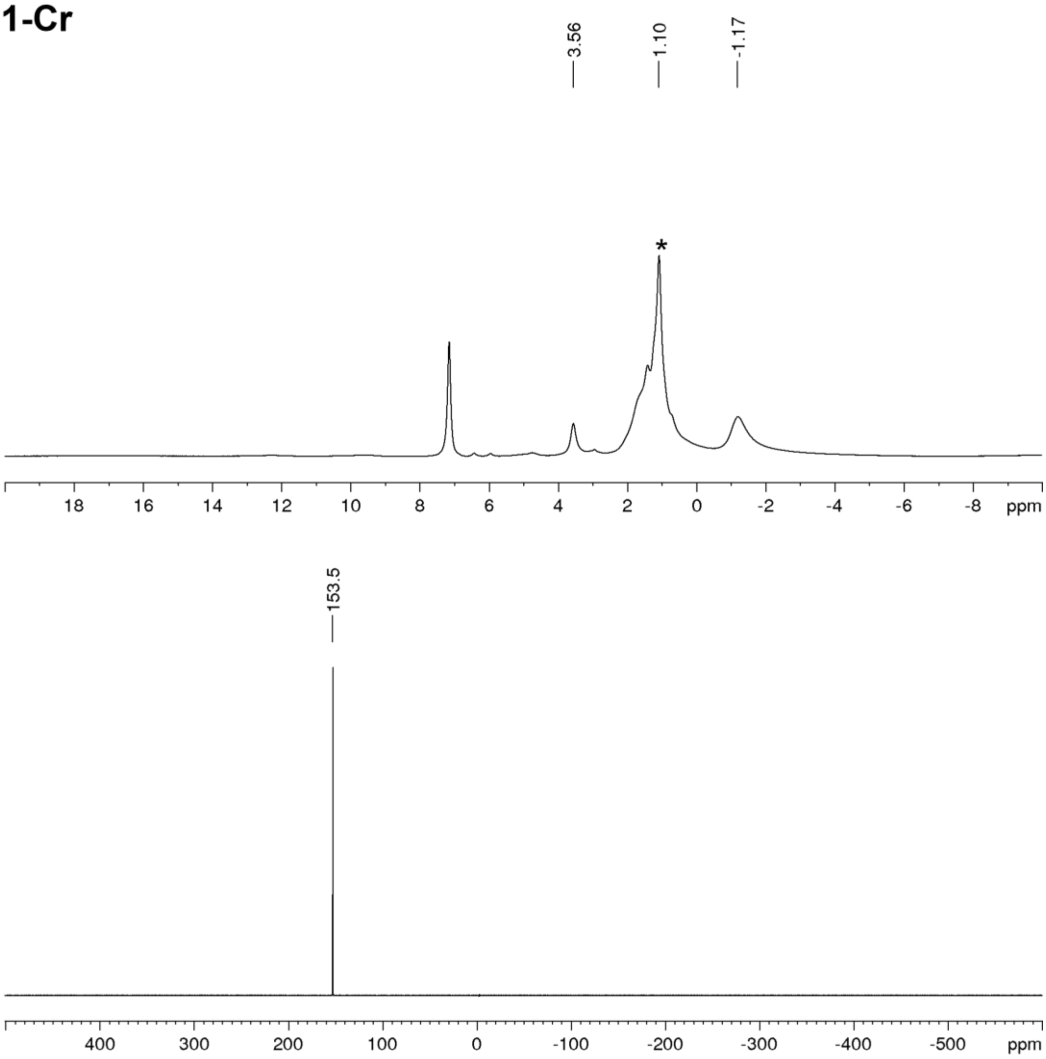


Figure S 23. Experimental ^{1}H (top) and ^{31}P (bottom) NMR spectrum (C_6D_6) for the reaction mixture of $[K(dme)_2]_2[Cp^*Fe(\eta^4-P_5)]$ with $[Cp'''Cr(\mu-Cl)]_2$ recorded at room temperature. Signal marked with * corresponds to **1**.

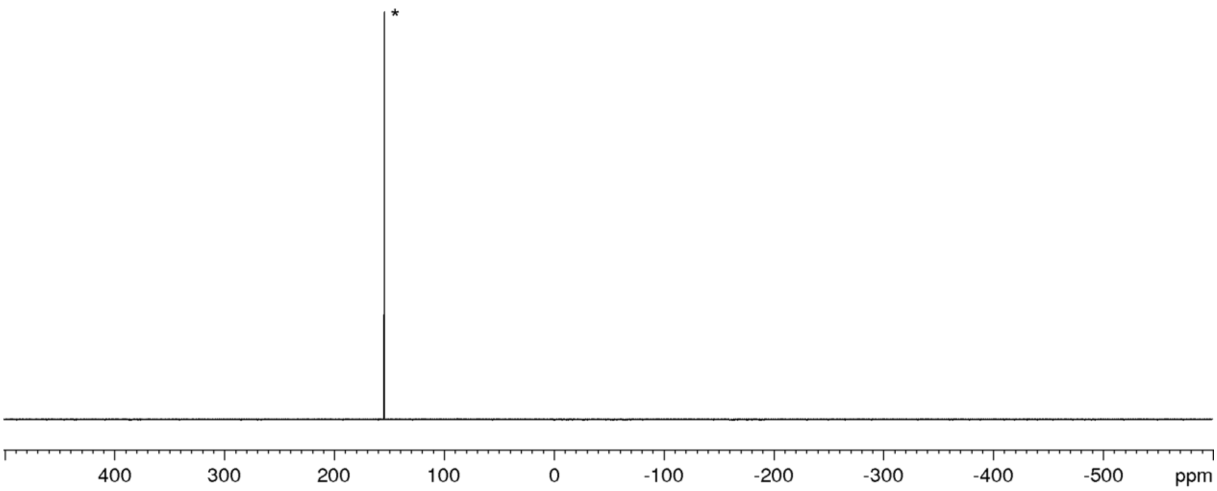


Figure S 24. Experimental ^{31}P NMR spectrum (C_6D_6) for the reaction mixture of $[K(dme)_2]_2[Cp^*Fe(\eta^4-P_5)]$ with $[Cp'''Fe(\mu-Br)]_2$ recorded at room temperature. Signal marked with * corresponds to **1**. No signals for **1-Fe** observed.

3 EPR studies

3.1 1-Cr

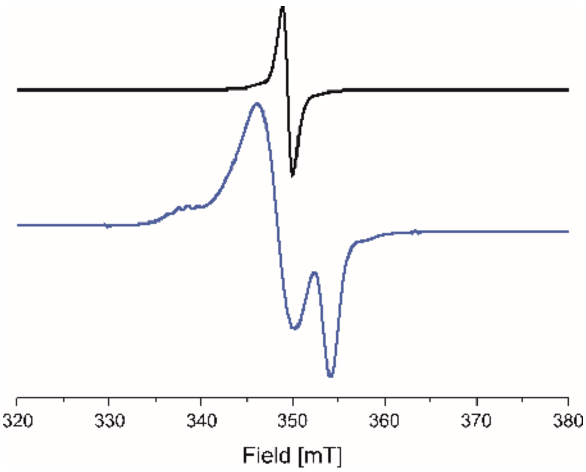


Figure S25. X-band EPR spectrum for **1-Cr** in thf solution at 298 K (black, top) or at 77 K (blue, bottom). *g* value for the sample at 298 K: g_{iso} = 1.918.

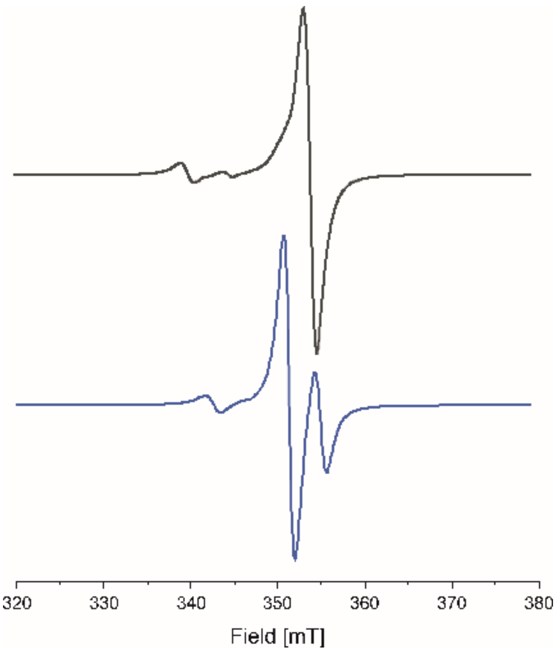


Figure S 26. X-band EPR spectrum for **1-Cr** in solid state at 298 K (black, top) or at 77 K (blue, bottom).

3.2 2-Cr

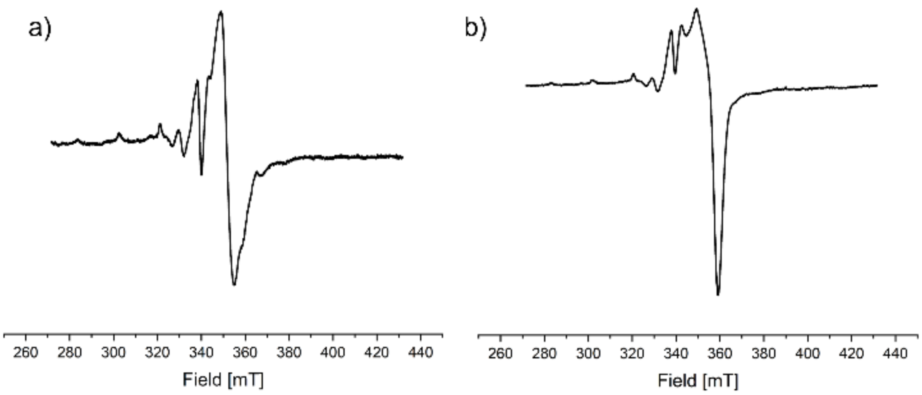


Figure S 27. X-band EPR spectrum for **2-Cr** in thf solution at 298 K (a) and 77 K (b).

3.3 Impurities within 1-Fe and 2-Fe

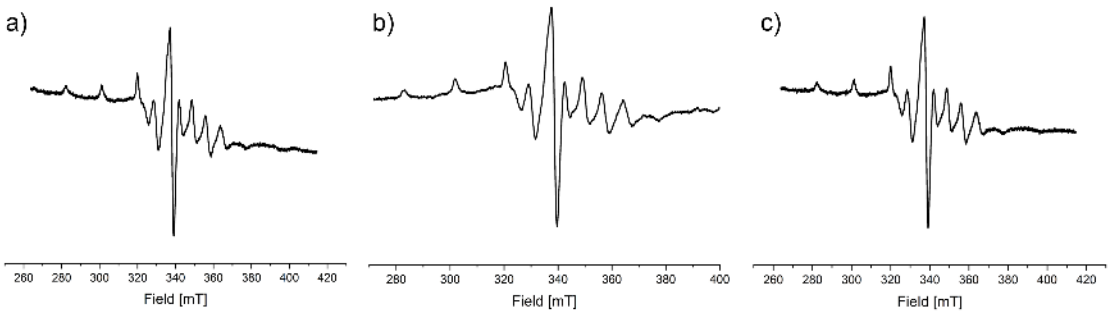


Figure S 28. Comparison of X-band EPR spectra for samples of (a) **1-Fe** (thf solution of crystals at 77 K, using 1.0 eq [Cp'''Fe(μ-Br)]$_2$), (b), **2-Fe** (crystals at 77 K, using 1.0 eq [Cp'''Fe(μ-Br)]$_2$) with (c) solid [Cp'''Fe(μ-Br)]$_2$ at 77 K.

4 Details on single crystal X-ray structure analysis

The X-ray diffraction experiments were performed on either a Xcalibur, AtlasS2, Gemini ultra (**2-Ni**) or GV1000 TitanS2 (**3-Ag**) diffractometer applying Cu-K_α radiation (λ = 1.54178 Å) or using a XtaLAB Synergy R, DW System with a HyPix-Arc 150 detector using Cu-Kα radiation from a rotating anode (**1-Cr**, **2-Cr**, **1-Mn**, **1-Fe**, **2-Fe**, **2-Ni**). All measurements were performed at 123 K, except for **1-Mn** (100 K). Data collection and reduction were performed with CrysAlisPro 1.171.40.14a (**3-Ag**), CrysAlisPro 1.171.41.83a (**1-Mn**) or 171.43.36a (**1-Cr**, **2-Cr**, **1-Mn**, **1-Fe, 2-Fe**, **2-Ni**). For the compounds (**1-Cr**, **2-Cr**, **1-Fe, 2-Fe, 2-Ni**, **3-Ag**) a numeric absorption correction based on gaussian integration over a multifaceted crystal model was used. All structures were solved by direct methods with ShelXT[11] and Olex2[12] and refined by full-matrix least-squares method against F^2 in anisotropic approximation using ShelXL.[11] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined in calculated positions riding on pivot atom model for all compounds. Visualisation of the crystal structures was performed with Olex2 (1.3alpha).[12]

CCDC-2347421 (**1-Cr**), CCDC-2347422 (**2-Cr**), CCDC-2347423 (**1-Mn**), CCDC-2347424 (**1-Fe**), CCDC-2347425 (**2-Fe**) CCDC-2347426 (**2-Ni**) and CCDC-2347427 (**3-Ag**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; Fax: + 44-1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

4.1 Crystallographic information

Table S1. Crystallographic data for all compounds.

	1-Cr	**2-Cr**	**1-Mn**	**1-Fe**
CCDC	2347421	2347422	2347423	2347424
Formula	$C_{27}H_{44}FeCrP_5$	$C_{44}H_{73}FeCr_2As_5$	$C_{27}H_{44}FeMnP_5$	$C_{44}H_{73}Fe_3P_5$
$D_{calc.}$/ g cm^{-3}	1.393	1.607	1.405	1.358
μ/mm^{-1}	9.454	10.306	9.935	9.500
Formula Weight	631.32	1136.47	634.26	924.42
Colour	Dark red	Light green blue	Brownish green	Dark brown
Shape	Block shaped	Block shaped	Plate shaped	Block shaped
Size/mm^3	0.42 x 0.27 x 0.21	0.46 x 0.13 x 0.11	0.26 x 0.23 x 0.12	0.13 x 0.10 x 0.05
T/K	123.01(10)	123.00(10)	100.00(10)	123.00(10)
Crystal System	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space Group	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P2_1/n$
a/Å	12.1473(10)	19.5158(2)	12.14780(10)	19.23420(10)
b/Å	13.60100(10)	10.89260(10)	13.55300(10)	10.87860(10)
c/Å	18.5936(2)	22.9447(2)	18.5913(2)	22.55640(10)
α/°	90	90	90	90
β/°	101.4680(10)	105.5730(10)	101.6500(10)	106.6420(10)
γ/°	90	90	90	90
V/Å^3	3010.62(5)	4698.47(8)	2997.80(5)	4522.03(6)
Z	4	4	4	4
Z'	1	1	1	1
Wavelength/Å	1.54184	1.54184	1.54184	1.54184
Radiation type	Cu K_α	Cu K_α	Cu K_α	Cu K_α
θ_{min}/°	4.011	2.645	4.007	2.669
θ_{max}/°	74.178	71.657	75.220	75.254
Measured Refl.	61137	39500	59246	39583
Independent Refl.	5942	8904	6140	8917
Reflections with I > 2(I)	5673	8450	5702	8333
R_{int}	0.0496	0.0283	0.0573	0.0229
Parameters	321	492	321	492
Restraints	0	0	0	0
Largest Peak	0.621	0.580	0.558	0.365
Deepest Hole	-0.626	-0.654	-0.471	-0.308
GooF	1.026	1.059	1.056	1.080
wR_2 (all data)	0.0908	0.0725	0.0962	0.0617
wR_2	0.0900	0.0717	0.0939	0.0609
R_1 (all data)	0.0328	0.0296	0.0376	0.0254
R_1	0.0318	0.0278	0.0345	0.0231

	2-Fe	3-Ag	2-Ni
CCDC	2347425	2347427	2347426
Formula	$C_{44}H_{73}Fe_3As_5$	$C_{80}H_{73}FeNi_2P_5AgAlF_{46}O_3$	$C_{44}H_{73}FeNi_2As_5$
$D_{calc.}$/ g cm^{-3}	1.649	1.674	1.624
μ/mm^{-1}	11.670	5.352	7.484
Formula Weight	1144.17	2419.35	1149.89
Colour	Dark brown	Dark brown	Dark brown
Shape	Plate shaped	Block shaped	Block shaped
Size/mm^3	0.19 x 0.05 x 0.05	0.21 x 0.14 x 0.12	0.44 x 0.18 x 0.15
T/K	123.00(10)	122.98(10)	123.01(10)
Crystal System	Monoclinic	Triclinic	Triclinic
Space Group	$P2_1/n$	P-1	P-1
a/Å	19.3733(2)	14.9140(6)	12.4331(2)
b/Å	10.87080(10)	19.2206(9)	12.5276(2)
c/Å	22.7856(2)	19.5632(9)	17.9814(3)
α/°	90	63.886(4)	72.5910(10)
β/°	106.2280(10)	79.623(4)	70.5950(10)
γ/°	90	72.650(4)	64.918(2)
V/Å^3	4608.48(8)	4798.5(4)	2351.07(8)
Z	4	2	2
Z'	1	1	1
Wavelength/Å	1.54184	1.54184	1.54184
Radiation type	Cu K_α	Cu K_α	Cu K_α
θ_{min}/°	2.653	2.643	3.965
θ_{max}/°	73.487	74.270	73.011
Measured Refl.	40677	31575	33114
Independent Refl.	8821	18494	8990
Reflections with I > 2(I)	7899	14896	8889
R_{int}	0.0342	0.0225	0.0228
Parameters	492	1275	502
Restraints	0	0	18
Largest Peak	0.573	0.767	0.519
Deepest Hole	-0.457	-0.508	-0.653
GooF	1.052	0.902	1.155
wR_2 (all data)	0.0630	0.0593	0.0663
wR_2	0.0614	0.0583	0.0661
R_1 (all data)	0.0316	0.0314	0.0265
R_1	0.0268	0.0254	0.0260

4.2 1-Cr

Compound **1-Cr** crystallizes in the monoclinic space group $P2_1/n$ in form of dark red block shaped crystals from a concentrated solution in CH_2Cl_2 layered with acetonitrile at room temperature. The asymmetric unit contains one molecule of **1-Cr**.

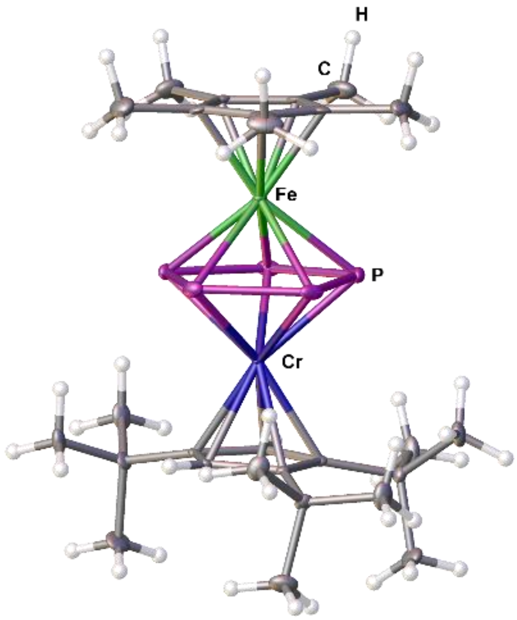


Figure S 29. Molecular structure of **1-Cr** in solid state. Thermal ellipsoids are drawn with 50 % probability level.

4.3 2-Cr

Compound **2-Cr** crystallizes in the monoclinic space group $P2_1/n$ in form of light green-blue block shaped crystals from a concentrated solution in CH_2Cl_2 layered with acetonitrile at room temperature. The asymmetric unit contains one molecule of **2-Cr**.

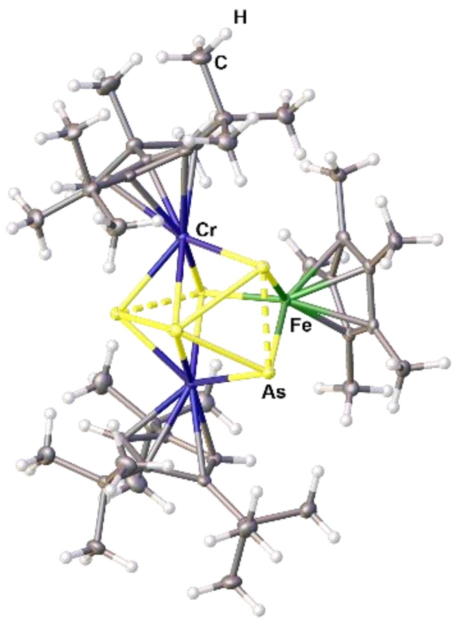


Figure S 30. Molecular structure of **2-Cr** in solid state. Thermal ellipsoids are drawn with 50 % probability level.

4.4 1-Mn

Compound **1-Mn** crystallizes in the monoclinic space group $P2_1/n$ in form of brownish green plate shaped crystals from a concentrated solution in pentane at 8°C. The asymmetric unit contains one molecule of **1-Mn**.

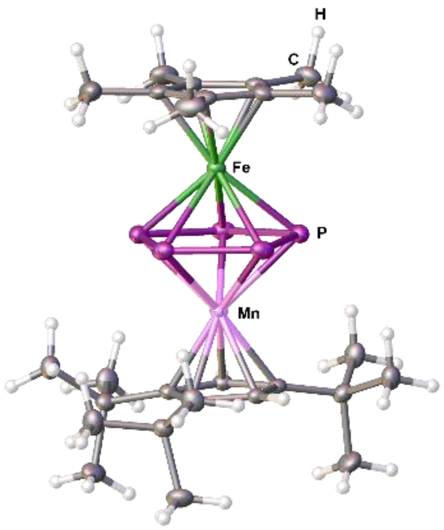


Figure S 31. Molecular structure of **1-Mn** in solid state. Thermal ellipsoids are drawn with 50 % probability level.

4.5 1-Fe

Compound **1-Fe** crystallizes in the monoclinic space group $P2_1/n$ in form of dark brown block shaped crystals from a concentrated solution in CH_2Cl_2 layered with acetonitrile at room temperature. The asymmetric unit contains one molecule of **1-Fe**.

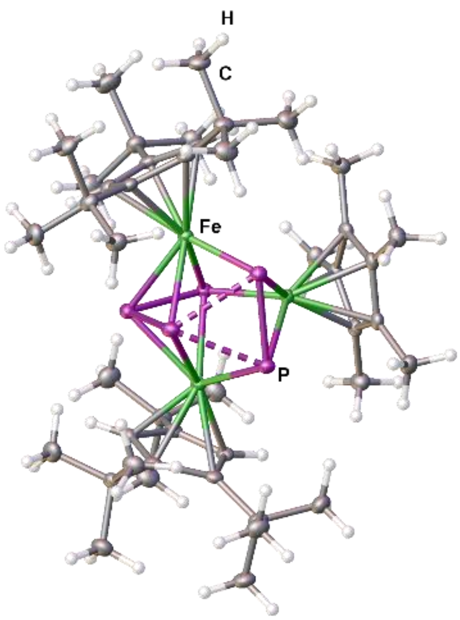


Figure S 32. Molecular structure of **1-Fe** in solid state. Thermal ellipsoids are drawn with 50 % probability level.

4.6 2-Fe

Compound **2-Fe** crystallizes in the monoclinic space group $P2_1/n$ in form of dark brown plate shaped crystals from a concentrated solution in CH_2Cl_2 layered with acetonitrile at room temperature. The asymmetric unit contains one molecule of **2-Fe**.

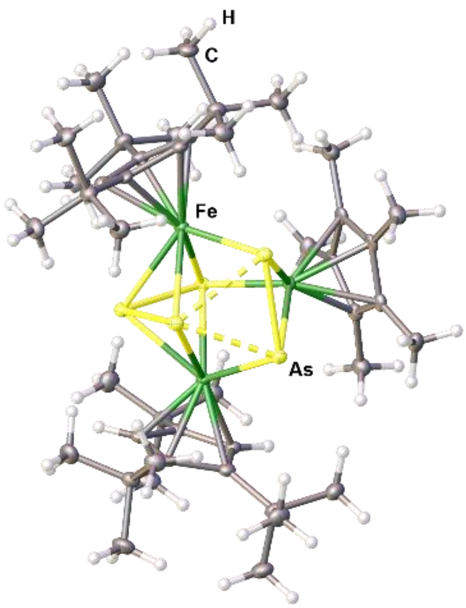


Figure S 33. Molecular structure of **2-Fe** in solid state. Thermal ellipsoids are drawn with 50 % probability level.

4.7 3-Ag

Compound **3-Ag** crystallizes in the triclinic space group *P*-1 in form of dark brown block shaped crystals from a concentrated solution in *o*-DFB layered with hexane at room temperature. The asymmetric unit contains one half molecule of **3-Ag** and one anion.

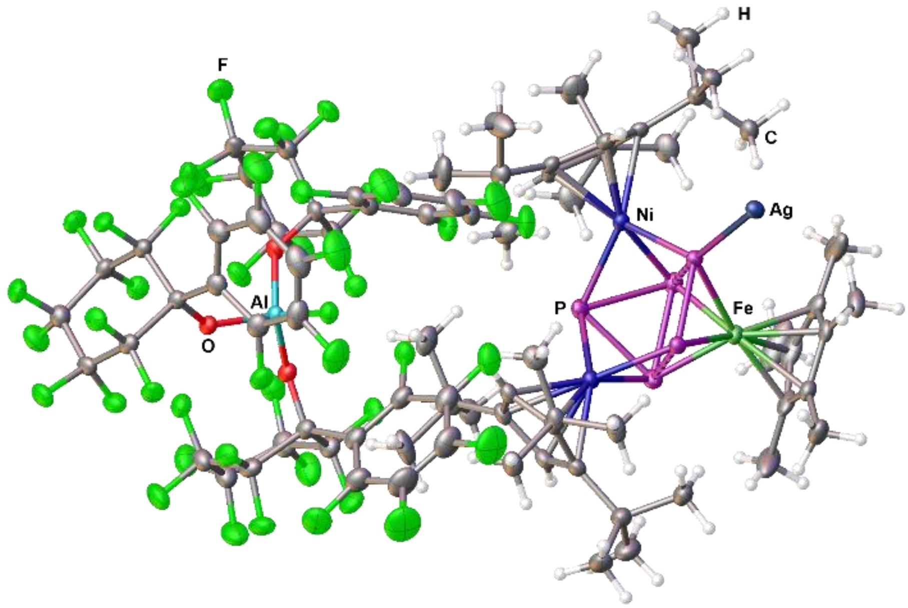


Figure S 34. Molecular structure of **3-Ag** in solid state. Thermal ellipsoids are drawn with 50 % probability level.

4.8 2-Ni

Compound **2-Ni** crystallizes in the triclinic space group *P*-1 in form of dark brown block shaped crystals from a concentrated solution in CH_2Cl_2 layered with acetonitrile at room temperature. The asymmetric unit contains one molecule of **2-Ni**. Within the solid-state structure As1 is slightly disordered over two positions (occupancy of 0.91 and 0.09). A solvent mask was calculated, and 9 electrons were found in a volume of 328 Å^3 in 1 void per unit cell. This is consistent with the presence of 0.2 CH_3CN molecules per asymmetric unit which account for 9 electrons per unit cell.

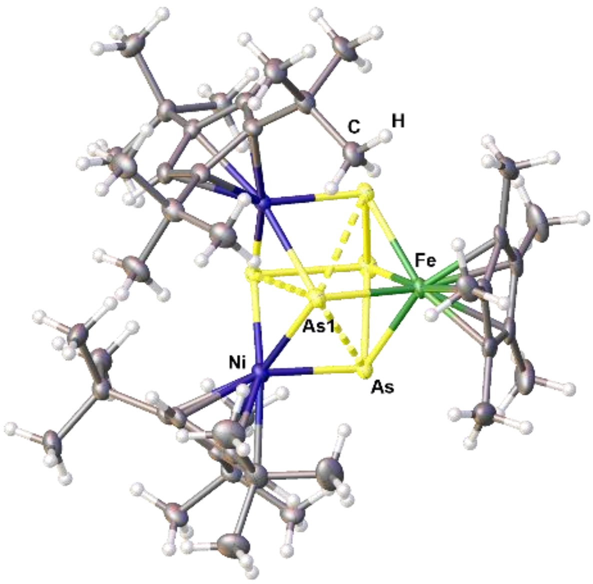


Figure S 35. Molecular structure of **2-Ni** in solid state depicting the part with the higher occupancy. Thermal ellipsoids are drawn with 50 % probability level.

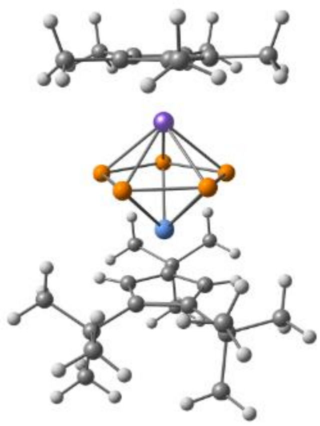
5 Computational Details

The Gaussian 16[13] program was used for all calculations. Density functional theory (DFT) in form of BP86[14] (Becke's exchange and Perdew 86 correlation functional) with TZVP basis set was employed.[15] Subsequent analytical frequency analysis was carried out to confirm the presence of true minima on the potential energy surface. For **3-Ag** no frequency analysis was calculated due to computational costs. Electronic densities were analysed by Natural Bond Orbital analysis (NBO 7.0)[16] at the same level of theory. Long range empirical dispersion correction in form of GD3BJ[17] was applied. Figures concerning the DFT calculations for the supporting information were created with Chemcraft.[18]

Table S 2. Total energies for the optimized geometries (BP86/TZVP level of theory).

	E_{total} [Ha]	H_{total} [Ha]	G_{total} [Ha]
1-Cr doublet	-5071.1398997	-5071.1389555	-5071.2557023
2-Cr triplet	-16254.842309	-16254.8413648	-16255.0067975
2-Cr singlet	-16254.8474274	-16254.8464832	-16255.0077907
1-Mn singlet	-5177.6788506	-5177.6779064	-5177.7938715
1-Fe singlet	-7219.6216898	-7219.6207456	-7219.7794774
2-Fe singlet	-16693.419148	-16693.4182038	-16693.5849332
2-Ni singlet	-17182.7572175	-17182.7562733	-17182.92398
1-Ni singlet	-7708.918155	-7708.9172108	-7709.0799273

1-Cr (doublet)



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P	3.108800000	4.638300000	7.440400000
P	1.527700000	5.125800000	6.021800000
P	1.752500000	1.609500000	6.207400000
P	3.303100000	2.469400000	7.498900000
C	3.856300000	2.322100000	3.641300000
H	3.608000000	1.422700000	3.462300000
C	3.849300000	4.588600000	3.676700000
H	3.597800000	5.491800000	3.523500000
C	4.950400000	4.172400000	4.502200000
C	4.957900000	2.714600000	4.475000000
C	2.207200000	3.475900000	1.965200000

C	3.191000000	3.459300000	3.122800000
C	-0.847700000	3.901800000	8.225700000
C	-0.626100000	2.500100000	8.414800000
C	0.905900000	3.644300000	9.712600000
C	0.096500000	4.610200000	9.028200000
C	5.994300000	1.626400000	4.816300000
C	5.977500000	5.206300000	4.992700000
C	1.399500000	2.174400000	1.883900000
H	2.012800000	1.410800000	1.852700000
H	0.846900000	2.182900000	1.074600000
H	0.822700000	2.098200000	2.672500000
C	0.464900000	2.340800000	9.325200000
C	6.409400000	5.094700000	6.465100000
H	5.722500000	5.495000000	7.038200000
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H	6.522600000	4.150500000	6.701700000
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H	-1.725700000	1.656800000	6.916800000
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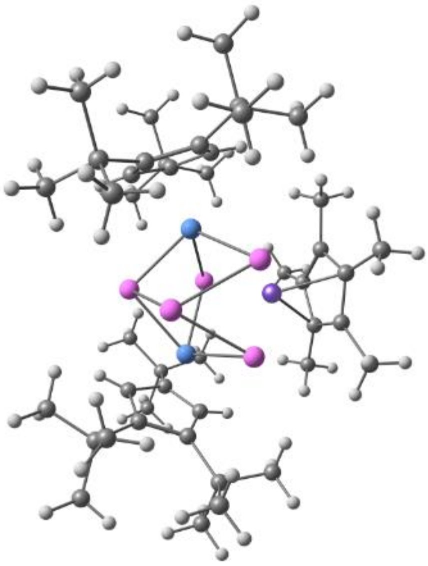
2-Cr (triplet)



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As	3.484700000	6.043000000	14.662500000
As	5.293000000	4.735300000	13.589600000
Fe	2.332600000	2.685300000	15.347400000
Cr	4.878500000	4.107900000	15.899400000
Cr	3.076400000	4.099000000	12.843700000
C	1.983100000	3.218300000	11.126200000
H	1.388900000	2.489300000	11.260800000
C	1.022600000	1.104000000	14.775400000
C	2.203200000	1.104600000	16.769100000
C	2.164300000	0.561600000	15.444400000
C	2.813700000	5.360200000	10.973900000
C	1.597600000	4.595300000	11.159800000
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C	3.134700000	0.677000000	17.866300000
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H	5.949000000	2.754700000	10.165200000
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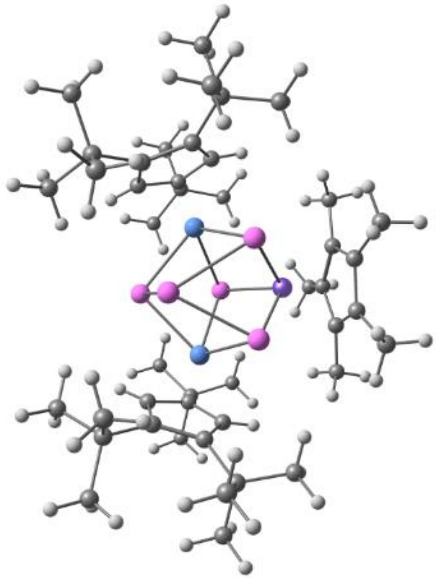
2-Cr (singlet)



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C	3.081500000	6.867100000	10.763000000
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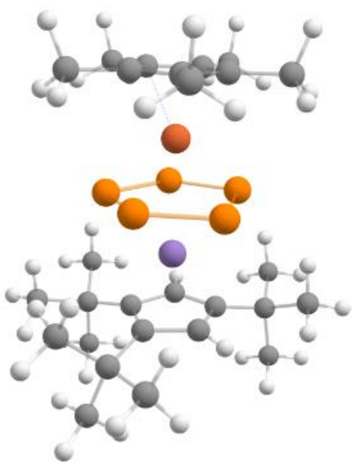
C	3.564200000	0.561800000	11.002000000
H	3.704900000	0.593100000	11.971400000
H	4.041300000	-0.207900000	10.627400000
H	2.606300000	0.475500000	10.813700000

C	7.569100000	7.310100000	18.081600000
H	8.310700000	6.673500000	18.153800000
H	7.057600000	7.311800000	18.917500000
H	7.924400000	8.207900000	17.914200000
C	8.002100000	1.981000000	14.702600000
H	7.218100000	1.987000000	14.114500000
H	8.566400000	1.209400000	14.486800000
H	8.514000000	2.806500000	14.573000000
C	5.404300000	7.819700000	16.883100000
H	5.641000000	8.699400000	17.244300000
H	4.689900000	7.425100000	17.425700000
H	5.095300000	7.918700000	15.958300000
C	-0.799300000	3.897600000	11.677000000
H	-1.740300000	4.146800000	11.564100000
H	-0.583600000	3.860100000	12.632300000
H	-0.643300000	3.018800000	11.272200000
C	8.791200000	1.829400000	17.066000000
H	9.315900000	2.649600000	16.954700000
H	9.339400000	1.055100000	16.820400000
H	8.508900000	1.746500000	18.000800000
C	3.815000000	1.788100000	8.848500000
H	2.855500000	1.657900000	8.697400000
H	4.312100000	1.041300000	8.454000000
H	4.100500000	2.627400000	8.430800000

1-Mn (singlet)

Mn	-0.849557000	0.221782000	-0.018399000
Fe	2.217497000	-0.096142000	0.001235000
P	0.680504000	0.430374000	1.789726000
P	0.925635000	1.870784000	0.203672000
P	0.610512000	-1.286160000	-1.263800000
P	0.487335000	-1.529179000	0.876321000
P	0.702285000	0.829062000	-1.681117000
C	-2.511609000	0.827274000	-1.149194000

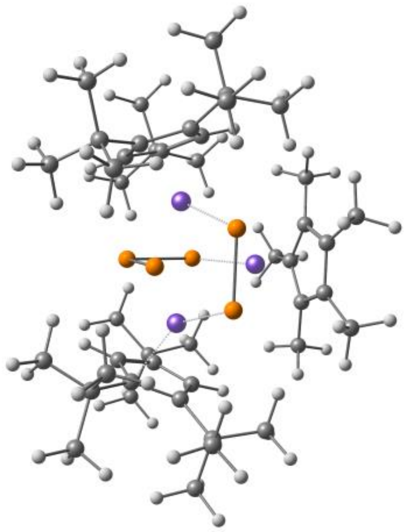


H	-2.461255000	1.163447000	-2.179238000
C	-2.503206000	0.834713000	1.120651000
H	-2.450381000	1.177235000	2.149131000
C	-2.705251000	-0.533917000	0.722291000
C	-2.401580000	1.684542000	-0.016131000
C	-2.710532000	-0.539525000	-0.740318000
C	-2.460181000	3.200814000	-0.023242000
C	3.974897000	0.627909000	0.844027000
C	3.872857000	-0.517431000	-1.180562000
C	4.003806000	0.786641000	-0.585627000
C	-2.363775000	-1.273654000	3.126954000
H	-1.280391000	-1.409094000	3.006296000
H	-2.712307000	-1.984138000	3.891714000
H	-2.540725000	-0.262665000	3.515754000
C	-1.883694000	3.795907000	1.271376000
H	-2.428893000	3.437107000	2.156656000
H	-1.966260000	4.893316000	1.250478000
H	-0.823022000	3.534245000	1.392445000
C	-3.113896000	-1.546968000	1.804426000
C	3.762601000	-1.481802000	-0.118488000
C	3.819743000	-0.773412000	1.132932000
C	-2.260458000	-2.898699000	-1.766995000
H	-1.294574000	-2.727499000	-2.260176000
H	-2.787636000	-3.685715000	-2.329685000
H	-2.050121000	-3.276636000	-0.765484000
C	4.170544000	2.074073000	-1.324917000
H	3.657360000	2.045333000	-2.295740000
H	5.237246000	2.282747000	-1.511202000
H	3.755537000	2.917618000	-0.756830000
C	4.105487000	1.721455000	1.853214000
H	3.716036000	2.672474000	1.465233000
H	5.162344000	1.875130000	2.127889000
H	3.548820000	1.486035000	2.770555000
C	3.633859000	-2.960805000	-0.283163000

H	3.052855000	-3.404076000	0.537090000
H	4.626625000	-3.440686000	-0.293763000
H	3.125659000	-3.215304000	-1.223142000
C	-4.624341000	-1.325524000	2.068520000
H	-4.812574000	-0.291776000	2.393180000
H	-4.975471000	-2.006411000	2.859996000
H	-5.223401000	-1.508102000	1.166538000
C	-1.728696000	3.796275000	-1.237260000
H	-0.650156000	3.591732000	-1.193215000
H	-1.869477000	4.887777000	-1.263072000
H	-2.114172000	3.386659000	-2.182200000
C	-3.103056000	-1.607048000	-1.776430000
C	-4.596549000	-1.948395000	-1.566178000
H	-4.766180000	-2.497170000	-0.631522000
H	-4.958859000	-2.577148000	-2.394622000
H	-5.204262000	-1.031616000	-1.536620000
C	-3.960579000	3.572877000	-0.115867000
H	-4.405434000	3.176205000	-1.040492000
H	-4.085638000	4.667187000	-0.112103000
H	-4.519350000	3.156720000	0.735508000
C	-2.967069000	-1.032649000	-3.203108000
H	-3.660780000	-0.198852000	-3.383642000
H	-3.197715000	-1.823860000	-3.932168000
H	-1.940394000	-0.686835000	-3.395119000
C	3.882034000	-0.817668000	-2.643928000
H	3.292306000	-1.716053000	-2.871127000
H	4.911276000	-0.988321000	-3.001197000
H	3.456384000	0.012466000	-3.223836000
C	3.765766000	-1.389115000	2.492999000
H	3.327589000	-0.698802000	3.226389000
H	4.777419000	-1.656658000	2.841143000
H	3.155813000	-2.302612000	2.493287000
C	-2.877351000	-3.027377000	1.478045000
H	-3.476728000	-3.376357000	0.630178000

H	-3.160279000	-3.635474000	2.351114000
H	-1.815517000	-3.220591000	1.267278000

1-Fe (singlet)



Fe	1.734153000	-0.383390000	0.160603000
Fe	-1.734264000	-0.383109000	0.160315000
Fe	0.000085000	1.728024000	-0.531418000
P	1.109775000	0.283249000	-1.861526000
P	-1.109425000	0.283258000	-1.861811000
P	-0.000268000	-1.478961000	1.278132000
P	-0.000186000	0.707178000	1.417296000
P	-0.000053000	-1.641385000	-0.889128000
C	2.931517000	-1.622166000	1.338229000
H	2.543617000	-2.398447000	1.987562000
C	3.762036000	-0.526790000	-0.521512000
C	3.626115000	0.396716000	0.578287000
H	3.893340000	1.445694000	0.537283000
C	3.160711000	-0.276018000	1.743450000
C	3.280353000	-1.818805000	-0.041624000
C	-2.932042000	-1.620857000	1.338656000
H	-2.544416000	-2.396640000	1.988744000
C	-3.161198000	-0.274381000	1.742735000
C	-3.761901000	-0.526907000	-0.522206000
C	1.163052000	3.497135000	-0.371754000
C	-0.000141000	3.589686000	0.466290000
C	3.197489000	0.218218000	3.176233000
C	-3.198401000	0.220808000	3.175178000
C	-3.626215000	0.397478000	0.576900000
H	-3.893251000	1.446468000	0.534964000
C	0.718579000	3.351462000	-1.725880000
C	-1.162583000	3.497307000	-0.372816000
C	-0.716842000	3.351455000	-1.726518000
C	-4.631522000	-0.120998000	-1.722172000
C	3.301753000	-3.235386000	-0.639298000

C	4.632096000	-0.120025000	-1.720862000
C	-3.280523000	-1.818611000	-0.041124000
C	-1.545517000	3.404435000	-2.970598000
H	-1.285634000	4.305839000	-3.550737000
H	-2.616491000	3.454724000	-2.743955000
H	-1.378467000	2.531729000	-3.619953000
C	-3.302050000	-3.235773000	-0.637486000
C	-2.953494000	1.731765000	3.254137000
H	-2.991306000	2.071144000	4.300252000
H	-3.715400000	2.293082000	2.693318000
H	-1.960065000	1.966595000	2.847545000
C	1.548290000	3.404642000	-2.969292000
H	1.384618000	2.530200000	-3.617218000
H	2.618884000	3.458679000	-2.741666000
H	1.286144000	4.304105000	-3.551374000
C	2.562464000	3.755926000	0.075036000
H	2.746547000	3.350669000	1.076366000
H	2.748872000	4.843349000	0.118091000
H	3.294607000	3.321827000	-0.614013000
C	6.099991000	-0.347715000	-1.279413000
H	6.784720000	-0.027303000	-2.080461000
H	6.301216000	-1.403133000	-1.056840000
H	6.326791000	0.236839000	-0.375666000
C	-2.562485000	3.756267000	0.072338000
H	-3.293812000	3.320870000	-0.616771000
H	-2.749369000	4.843678000	0.113548000
H	-2.747388000	3.352416000	1.074086000
C	2.952807000	1.729177000	3.256156000
H	3.714947000	2.290777000	2.695938000
H	2.990409000	2.067807000	4.302522000
H	1.959511000	1.964492000	2.849495000
C	2.615918000	-4.226423000	0.326869000
H	1.583523000	-3.916799000	0.548209000
H	3.165338000	-4.334215000	1.273626000

H	2.576550000	-5.217318000	-0.149505000
C	2.579645000	-3.397572000	-1.993740000
H	2.923150000	-4.321916000	-2.484585000
H	2.742187000	-2.563619000	-2.677492000
H	1.496135000	-3.478830000	-1.839822000
C	-6.099590000	-0.348220000	-1.281074000
H	-6.784009000	-0.028581000	-2.082695000
H	-6.326724000	0.237230000	-0.377988000
H	-6.300924000	-1.403412000	-1.057532000
C	-2.616715000	-4.226053000	0.329832000
H	-1.584370000	-3.916370000	0.551318000
H	-2.577300000	-5.217378000	-0.145640000
H	-3.166522000	-4.332931000	1.276467000
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C	4.777295000	-3.681783000	-0.768064000
H	5.319498000	-3.520647000	0.175977000
H	5.306705000	-3.141804000	-1.562441000
H	4.818644000	-4.755190000	-1.009753000
C	4.467195000	1.379926000	-2.022176000
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H	3.414559000	1.610315000	-2.226621000
H	5.057678000	1.645278000	-2.911471000
C	-4.777633000	-3.681996000	-0.766308000
H	-5.320131000	-3.519822000	0.177388000
H	-4.819119000	-4.755635000	-1.006947000
H	-5.306664000	-3.142704000	-1.561405000
C	4.384437000	-0.857790000	-3.044001000
H	5.047304000	-0.433633000	-3.813854000
H	3.346676000	-0.722275000	-3.380370000
H	4.603718000	-1.928402000	-2.981028000
C	-0.000581000	3.979329000	1.908562000

H	-0.886969000	3.605861000	2.434966000
H	0.001865000	5.079526000	1.998240000
H	0.883056000	3.601729000	2.436680000
C	-4.383371000	-0.859867000	-3.044597000
H	-4.603115000	-1.930342000	-2.980880000
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H	-5.045626000	-0.436088000	-3.815182000
C	-4.466439000	1.378702000	-2.024702000
H	-5.057093000	1.643416000	-2.914075000
H	-3.413799000	1.608727000	-2.229617000
H	-4.820675000	2.008723000	-1.198225000
C	4.620078000	-0.093856000	3.700670000
H	4.822254000	-1.174669000	3.664968000
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H	5.383272000	0.415520000	3.093444000
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H	1.146306000	-0.297591000	3.714542000
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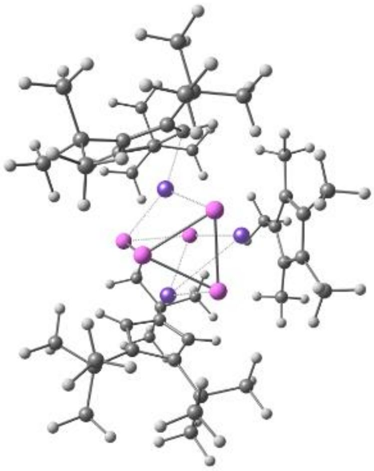

2-Fe (singlet)

As	-1.2277593	0.808852	-1.7237595
As	1.3352953	0.6063032	-1.8278881
As	-0.0599001	0.6339428	1.5351619
As	-0.1138487	-1.8001282	1.0651358
As	-0.0848937	-1.5050013	-1.3459666

Fe	-1.8614425	-0.4054765	0.1869625
Fe	1.7598029	-0.5230184	0.1887848
Fe	0.2440425	1.9818208	-0.3132016
C	0.2953427	3.6844998	0.99207
C	2.8762226	3.801839	0.7055754
H	3.0056692	3.2069833	1.6189985
H	3.1240413	4.8477175	0.9576668
H	3.6096277	3.4591587	-0.033408
C	-2.261277	3.891673	0.5764729
H	-2.9663359	3.604714	-0.2120062
H	-2.4793622	4.936576	0.8582274
H	-2.4605257	3.2625186	1.4535043
C	2.8879524	-1.9246468	1.2350879
H	2.4845967	-2.7836197	1.7590388
C	4.7882207	-0.0530018	-1.4844267
C	-3.9266984	-0.2910894	-0.4787112
C	3.8244512	-0.5985329	-0.4170593
C	-4.7637012	0.3550539	-1.59572
C	1.4813093	3.7038122	0.1817527
C	-3.1884844	-1.7048598	1.1927554
H	-2.8833497	-2.5963693	1.7288237
C	3.3110491	-1.9357323	-0.1394833
C	-0.8457262	3.7507114	0.1229351
C	-3.7019003	0.458612	0.7341747
H	-3.8802959	1.5217669	0.8441081
C	-3.5808513	-1.6790672	-0.1848668
C	3.6216502	0.1740522	0.7853794
H	3.8824481	1.2200397	0.8952019
C	3.0956443	-0.6447121	1.8258435
C	1.077178	3.7723728	-1.1881448
C	-3.2661971	-0.1055228	3.2672086
C	-0.3627223	3.7987001	-1.2281436
C	-2.234733	-0.962522	4.0176212
H	-2.390099	-2.0363746	3.8399941

H	-2.3155169	-0.7862991	5.1011948
H	-1.2146054	-0.7051993	3.701538
C	3.0799431	-0.3405795	3.3111709
C	6.2131411	-0.4011894	-0.9820291
H	6.3866922	0.0318259	0.0140316
H	6.9640087	0.0108122	-1.6744883
H	6.3694529	-1.4843831	-0.9099915
C	-3.2784008	-0.4044079	1.779713
C	-3.7207729	-2.9868547	-0.9799949
C	-4.5306302	1.877857	-1.6571342
H	-4.8180113	2.381631	-0.7251054
H	-5.1415623	2.3067448	-2.4651124
H	-3.4769431	2.1039812	-1.874916
C	-1.1678865	4.0394463	-2.4657518
H	-0.8179946	3.4248974	-3.3073407
H	-1.0914266	5.0980075	-2.7688831
H	-2.2307773	3.8149857	-2.3112806
C	1.9826529	-1.1214906	4.0504243
H	0.986818	-0.7930029	3.7235099
H	2.0653491	-0.9488881	5.1343547
H	2.0630807	-2.2041072	3.8763268
C	4.8174968	-3.7124944	-1.058405
H	5.3908886	-3.0810574	-1.7474952
H	4.8502155	-4.7425654	-1.4457807
H	5.3204919	-3.6972914	-0.0797491
C	1.9559605	3.978139	-2.3821886
H	3.0071517	3.7608891	-2.1570641
H	1.9003685	5.0271755	-2.7200037
H	1.6559214	3.3424351	-3.2277896
C	-5.2204218	-3.2802129	-1.2177857
H	-5.787799	-3.2051492	-0.2779339
H	-5.3400688	-4.3016553	-1.6114437
H	-5.6690857	-2.5919871	-1.9441274
C	-6.2463651	0.1454765	-1.1942588

H	-6.5087135	-0.9174144	-1.1335238
H	-6.9060391	0.6226766	-1.9360933
H	-6.4455877	0.5986824	-0.2120219
C	3.3457861	-3.2537872	-0.9288278
C	0.2511086	3.8176492	2.4805101
H	-0.6109033	3.2940879	2.9146222
H	0.1706349	4.8822337	2.7602866
H	1.155771	3.4179034	2.9545506
C	-2.9588221	-3.0138771	-2.3215588
H	-3.0181323	-2.0749306	-2.8753777
H	-3.3561188	-3.8197303	-2.9589999
H	-1.8940674	-3.2210846	-2.150294
C	-3.1627371	-4.1666481	-0.1544002
H	-2.1111055	-3.9969242	0.1222219
H	-3.20702	-5.0815359	-0.7639014
H	-3.7455893	-4.3466725	0.7608505
C	-4.5396109	-0.1810526	-3.016962
H	-3.489201	-0.0638266	-3.3209754
H	-5.1596043	0.3972258	-3.71916
H	-4.8237829	-1.2330261	-3.1219952
C	4.7029463	1.4828197	-1.5631802
H	3.6793515	1.807719	-1.7924121
H	5.363113	1.8472355	-2.3637909
H	5.0247853	1.9609004	-0.6289951
C	2.9026908	1.1594719	3.5760595
H	3.72119	1.7453656	3.1320794
H	2.8986926	1.3574116	4.6585191
H	1.9470234	1.5038682	3.1569536
C	2.6839544	-3.1981336	-2.3205472
H	1.5921075	-3.2648242	-2.2244362
H	3.0193556	-4.0561638	-2.9242864
H	2.9020066	-2.2821179	-2.8720754
C	4.4623459	-0.7880535	3.8467362
H	4.6144081	-1.8659717	3.6879176

H	4.5367441	-0.5828878	4.9261824
H	5.2739538	-0.250446	3.3340256
C	4.616479	-0.5809408	-2.9156272
H	4.7974706	-1.657673	-2.9943561
H	5.3458493	-0.0780981	-3.5689555
H	3.6109376	-0.3595188	-3.3013435
C	2.6024453	-4.3599364	-0.1488053
H	3.1047274	-4.6132466	0.7962461
H	2.5730869	-5.2712035	-0.764384
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C	-2.9943803	1.3788307	3.5469282
H	-3.0317606	1.5737933	4.62942
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H	-1.9952938	1.6565109	3.1815156
C	-4.6829303	-0.4612727	3.781584
H	-5.4482784	0.1370453	3.2650648
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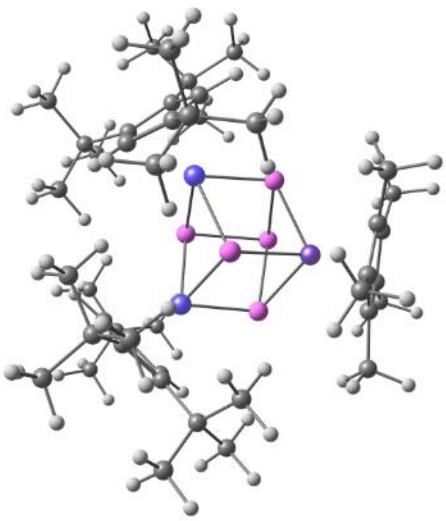
2-Ni (singlet)



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Ni	15.134566496	8.999916515	12.189441274
Ni	11.841072556	9.536119101	13.382490983
Fe	14.394589558	12.224926097	14.020032234
C	10.347456649	8.090879421	14.015256741
C	9.837167385	9.403689783	14.172096087
H	9.565130283	9.846561734	15.122816465
C	16.836911736	7.638923414	11.864522181
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H	14.128123571	7.551599705	9.856023842

C	10.280926470	9.136151379	11.907606605
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C	14.204624722	14.087833536	13.056018968
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C	13.535217639	14.155637735	14.325218942
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H	8.350297741	7.389452749	15.734512194
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C	17.931881689	7.251308636	12.867867581
C	14.486879142	13.832872114	15.349302367
C	18.557857995	5.894239478	12.478889759
H	19.425103398	5.684813557	13.123516372
H	17.859313219	5.057185377	12.585501022
H	18.905591027	5.913851043	11.435498510
C	9.210040360	11.502293833	12.804964501
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H	11.617227814	13.985593248	15.314078139
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C	10.221043845	12.529119577	12.265112064
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C	17.438441894	7.223804895	14.329218235
H	16.563804124	6.586685395	14.475037659
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C	15.629324069	4.605923250	10.739634850
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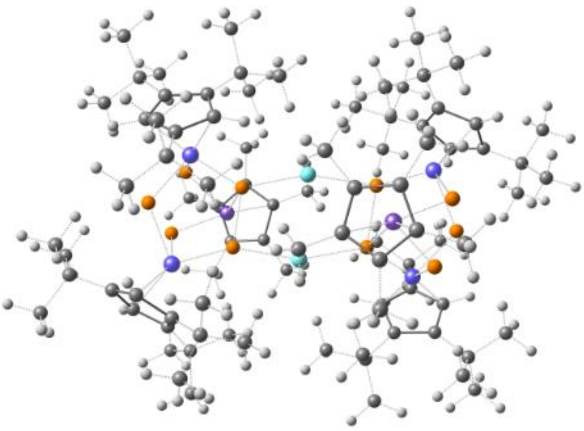
3-Ag (singlet)



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P	4.825333000	0.676535000	-1.913838000
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H	5.609721000	2.076828000	2.756518000
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H	2.006470000	-3.080796000	2.222516000
C	4.388513000	3.362352000	1.389948000
C	6.479036000	2.510606000	0.751581000
C	4.189275000	-2.707913000	2.411681000
C	5.254444000	-3.195387000	1.590347000
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C	4.690441000	3.848422000	0.018970000
C	3.346680000	3.760086000	2.434726000

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H	4.104069000	2.443652000	4.036130000
H	2.911380000	1.685900000	2.953900000
H	2.399543000	2.880637000	4.176663000
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H	2.875618000	-0.409342000	2.926346000

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C	-5.778744000	4.817383000	0.320050000
C	-3.223848000	0.285993000	4.508012000
C	-2.178481000	1.197586000	4.128192000
C	-5.284612000	5.165470000	1.732904000
H	-4.447204000	5.870059000	1.737614000
H	-6.106314000	5.637490000	2.290198000
H	-4.990206000	4.258156000	2.280260000
C	-8.083898000	-0.939246000	-1.916337000

H	-7.774153000	-1.312653000	-2.903107000
H	-9.144381000	-0.658925000	-1.987149000
H	-7.508188000	-0.032347000	-1.686979000
C	-7.039799000	3.941175000	0.507420000
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H	-7.727068000	4.443285000	1.202200000
H	-7.590017000	3.785701000	-0.429911000
C	-2.570316000	6.471381000	-0.167514000
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H	-1.734743000	7.068405000	0.226792000
H	-2.732276000	6.762199000	-1.215537000
C	-1.945912000	-4.074631000	-1.893485000
H	-1.270630000	-4.270234000	-2.739194000
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H	-1.922309000	-4.958654000	-1.249086000
C	-0.537261000	-2.109960000	3.380380000
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H	0.090650000	-2.355327000	4.252561000
H	-1.092064000	-3.012657000	3.103559000
C	-6.201341000	6.110812000	-0.419264000
H	-6.617850000	5.875822000	-1.409484000
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H	-5.356338000	6.796534000	-0.561940000
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H	0.937553000	0.940234000	4.085582000
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C	-5.518268000	0.939801000	-3.605625000
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C	-8.761898000	-3.241107000	-1.176779000
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H	-8.454840000	-3.673614000	-2.140113000
C	-4.443976000	2.836514000	-4.864664000
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H	-3.193717000	-6.216129000	-0.627794000
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H	-4.862534000	-6.573887000	-0.134339000
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C	-3.493710000	-2.305604000	4.614982000
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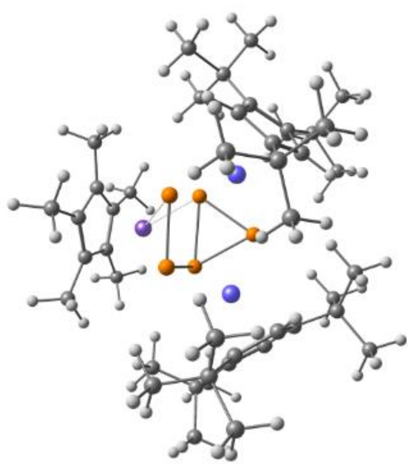
H	-3.344733000	-2.521106000	5.685571000
H	-4.576467000	-2.216343000	4.448455000
C	-4.525320000	0.657203000	5.141059000
H	-5.317881000	-0.061621000	4.892140000
H	-4.426694000	0.676673000	6.238426000
H	-4.862137000	1.652571000	4.820865000

1-Ni (singlet)

Fe	-0.111186000	2.543867000	-0.135982000
Ni	-1.765875000	-0.731756000	-0.318212000
Ni	1.904215000	-0.466625000	0.222781000
P	-1.282612000	0.967540000	1.082916000
P	0.847564000	1.129662000	1.389275000
P	1.307431000	1.182940000	-1.161852000
P	-1.059204000	1.049784000	-1.451415000



P	0.266877000	-0.882465000	-1.241913000
C	-2.613722000	-2.551117000	0.461594000
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C	3.444366000	-0.699279000	1.654511000
H	3.563404000	-0.009536000	2.481031000
C	-3.506563000	-1.454937000	0.719249000
C	-2.448667000	-2.727153000	-0.941779000
C	2.613569000	-1.860231000	1.695462000
C	2.716010000	-2.437649000	0.403701000
H	2.196020000	-3.334078000	0.084608000
C	1.854103000	-2.407075000	2.886628000
C	-1.336364000	4.213294000	0.311421000
C	4.104687000	-0.573022000	0.378775000
C	-3.919954000	-0.933478000	-0.596951000
C	-4.019636000	-1.245027000	2.151546000
C	5.399522000	1.291384000	1.477206000
H	5.784710000	0.616240000	2.255433000
H	6.151273000	2.075682000	1.305007000
H	4.490218000	1.781398000	1.854877000
C	-3.255206000	-1.733383000	-1.571477000
H	-3.312697000	-1.581949000	-2.642556000
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C	-5.182278000	-2.248323000	2.351120000
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C	-0.931147000	4.256610000	-1.067354000
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C	0.504633000	4.300028000	-1.107454000
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C	2.884808000	-3.130702000	-2.364616000
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H	2.331552000	3.947150000	-2.196340000

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