

Supporting information for the manuscript

Metal–Metal vs Metal–Ligand Cooperation in Iron-Mediated Activation and Catalytic Reduction of Nitrous Oxide and Nitrobenzene

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A. Experimental section

General Considerations Unless otherwise noted, all manipulations were carried out at ambient temperature under an inert nitrogen atmosphere using Schlenk techniques and an MBraun glovebox equipped with a purifier unit. The water and oxygen levels were always kept at less than 0.1 ppm. Glassware was dried overnight at 120°C before use.

NMR experiments were carried out using borosilicate glass NMR tubes adapted with J-Young valves. NMR spectra were recorded on Solution NMR spectra were recorded with Bruker AVANCE NEO-300, AVANCE NEO-400, AVANCE III-400, and AVANCE NEO-500 spectrometers. Spectra were referenced to external SiMe₄ (δ : 0 ppm) by using the residual proton solvent peaks as internal standards (¹H NMR experiments), or the characteristic resonances of the solvent nuclei (¹³C NMR experiments), while ³¹P was referenced to H₃PO₄ and ¹¹B to BF₃·OEt₂. For the latter, BPh₃ was generally used as internal standard for catalytic studies, and the spectra were processed using automatic phase correction and automatic baseline correction (Whittaker Smoother) as implemented in MestReNova (version 14.3.1). Peaks were integrated manually and did not change (<1%) when using other phase/baseline corrections implemented in MestReNova. Reference spectrum from the glass borosilicate were not subtracted, nor deconvolution/FID shifting were applied.

Elemental analyses were performed under nitrogen using a LECO TruSpec CHN Organic Elemental Analyzer at the Instituto de Investigaciones Químicas (IIQ).

FT-IR spectra were recorded with a Bruker Tensor 27 FTIR spectrophotometer.

X-band EPR spectroscopy was performed on a Bruker EMX nano system standard VT spectrometer at 77 K. Simulation of the EPR spectra were performed by iteration of the isotropic g-values, hyperfine couplings and line width using EasySpin¹ via the cwEPR 3.2 GUI.²

Due to the limitations of our equipment, EPR spectra could not be recorded at liquid He temperatures. As such, we cannot completely rule out the formation of any S > ½ species.

Starting materials Unless otherwise noted, reagents were purchased from commercial suppliers and used without further purification. Nitrosobenzene (C_6H_5NO) was purified by sublimation. All solvents were dried, stored over 4 Å molecular sieves, and degassed prior to use. d_8 -THF, d_8 -toluene and C_6D_6 were dried over CaH_2 , distilled under inert atmosphere and stored under 3 Å molecular sieves. All other reagents were used as received from commercial suppliers. $LiCp^*$ was prepared according to the published procedure.³

Syntheses and reactivity

Synthesis of $[Fe(tmeda)(Cp^*)Cl]$, **A.** A yellow solution was formed by suspending pink-orange solid $FeCl_2$ (1070 mg, 7.85 mmol, 1 equiv.) in a mixture of 18.0 mL of THF and 6.5 mL of TMEDA upon 1 h under stirring at 25°C. To the cold (-80 °C) suspension of $[FeCl_2(tmeda)_x]$, off-white solid $LiCp^*$ (1116 mg, 7.85 mmol, 1 equiv) was added neat, and left to react for 24 h at -80°C under vigorous stirring, followed by 3 h at 25°C. The reaction mixture was filtered through a 4-porosity glass frit with celite, obtaining a green-yellow solution. The solution was concentrated to 70% of its volume and stored at -35°C for 16 h, to yield 1608 mg of **A** as a pure light green-yellow microcrystalline powder (57% yield). Spectroscopic characterization of **A** was consistent with the previously reported data.⁴

Reactivity with $NaCp^$ gave more complicated reaction mixtures, poorer yields and the presence of $[Fe(Cp^*)_2]$ as impurity.*

Synthesis of $[Fe(depe)(Cp^*)Cl]$, **1.** A cold (-80°C) colorless solution of 1,2-bis(diethylphosphino)-ethane (228 mg, 1.11 mmol, 1.05 equiv) in THF (3.5 mL) was added to a cold (-80°C) green-yellow solution of **A** (377 mg, 1.05 mmol, 1 equiv) in THF (8.5 mL) resulting in the immediate change of color to dark violet. The reaction mixture was stirred at -80°C for 4 h. After, all volatiles were removed under vacuum, yielding a dark violet oily solid, which was further dried under vacuum at 25°C yielding a more powdery solid. 15.0 mL of pentane were added to the crude, yielding a dark violet solution with some grey powder remaining insoluble. It was then filtered through a 4-porosity glass frit containing celite, to obtain a dark violet solution. This was stored at -35°C for 20 h, yielding **1** as dark violet needles in 82% yield (425 mg).

Anal. Calcd. for $C_{20}H_{39}P_2ClFe$: C: 55.51%; H: 9.08%. **Found:** C: 55.53%; H: 9.24%.

$^{31}P\{^1H\}$ NMR (C_6D_6 , 161.98 MHz, 298 K): $\delta = 83.8$

1H NMR (C_6D_6 , 400 MHz, 298 K): $\delta = 2.3-1.8$ (m, 10 H), 1.59 (s, 15H, C_5Me_5), 1.32-1.18 (m, 14 H). (**Figure S2**)

$^{13}C\{^1H\}$ NMR (C_6D_6 , 100.61 MHz, 298 K): $\delta = 81.8$ (C_5Me_5), 22.0 (t, $J_{CP} = 19$ Hz), 20.7 (br), 18.4 (t, $J_{CP} = 11$ Hz), 10.9, 9.6, 8.3. (**Figure S3**)

The synthesis of complex **1** by reaction of $FeCl_2$ with $LiCp^*$,⁵⁻⁷ followed by addition of 1,2-bis(diethylphosphino)-ethane, resulted in mixtures of **1**, $[Fe(Cp^*)_2]$ and $[Fe(depe)_2Cl_2]$, even by performing the addition at $-80^\circ C$.

Synthesis of $[Fe(depe)(Cp^*)N_2][BAR^F]$, **2.** A dark violet solution of **1** (354 mg, 0.79 mmol, 1 equiv) in Et_2O (20.0 mL) was added to white solid $NaBAR^F$ (736 mg, 0.83 mmol, 1.05 equiv) inside a 50.0 mL ampoule and left to react under stirring with a N_2 atmosphere at $25^\circ C$. After 3 h, the reaction mixture had an orange color with a lot of solid in suspension. The reaction mixture was filtered through a 4-porosity glass frit containing celite, to obtain an orange solution. This was stored at $-35^\circ C$ for 18 h, yielding **2** as orange needles in 92% yield (930 mg). *Good-quality X-ray quality crystals can be grown from a vapor diffusion of pentane into a diluted Et_2O solution of **2**.*

Anal. Calcd. for $C_{52}H_{51}P_2N_2BF_{24}Fe$: C: 48.47%; H: 3.99%; N: 2.17%. **Found:** C: 48.16%; H: 4.26%; N: 2.12%.

$^{31}P\{^1H\}$ NMR (d_8 -THF, 202.46 MHz, 298 K): $\delta = 79.3$ (s) (**Figure S4**)

1H NMR (d_8 -THF, 500 MHz, 298 K): $\delta = 7.83$ (t, 8H, BAR^F), 7.61 (br, 4H, BAR^F), 2.22 (m, 2H), 2.09 (m, 4H), 1.99 (m, 2H), 1.78 (s, 15H, C_5Me_5), 1.69 (m, 4H), 1.24 (m, 12H). (**Figure S5**)

$^{13}C\{^1H\}$ NMR (d_8 -THF, 125.76 MHz, 298 K): $\delta = 161.63$ (dd, $^1J_{CF} = 50$ Hz, BAR^F), 134.61 (bs, BAR^F), 129.13 (dddd, BAR^F), 127.28 (BAR^F), 125.62 (BAR^F), 123.45 (BAR^F), 121.29 (BAR^F), 117.18 (m, BAR^F), 91.19, 20.67 (dd, $J_{CP} = 19$ Hz), 18.81 (dd, $J_{CP} = 9$ Hz), 18.08 (dd, $J_{CP} = 11$ Hz), 9.00, 7.88, 6.68 (t, $J_{CP} = 5$ Hz). (**Figure S6**)

ATR-IR spectrum: $\nu(N\equiv N) = 2106\text{ cm}^{-1}$ (**Figure S75**)

Reaction of complex **2** with N₂O

a) in d₈-THF: A light-orange-yellow solution of complex **2** (11.3 mg, 0.0089 mmol) in d₈-THF (0.6 mL) was transferred into a J-Young adapted NMR tube and connected to a Schlenk line. The solution was degassed by three cycles of freeze-pump-thawing and 1 bar of N₂O was added to the reaction mixture, which turned darker orange-brown over the course of 30 minutes. The ³¹P{¹H} NMR spectrum of the reaction mixture at 25°C shows the slow consumption of the starting material over the course of 36 h, with no new resonances appearing (**Figure S7**). The ¹H NMR spectrum of the reaction mixture shows the appearance of several new resonances over the course of the reaction (**Figure S8**), but we were unable to isolate this species or identify their nature. By the end of the reaction, the solution had a dark orange-red color.

Multinuclear NMR spectroscopic analysis of the reaction mixture suggests the formation of paramagnetic species, which is further supported by the variable temperature ¹H NMR spectrum (**Figure S9**). Unfortunately, no resonances could be observed in the ³¹P{¹H} NMR spectrum down to temperatures as low as -80°C.

b) in Et₂O

i) NMR scale: A light-orange-yellow solution of complex **2** (5.5 mg, 0.0060 mmol) in Et₂O (0.6 mL) was transferred into a J-Young adapted NMR tube and connected to a Schlenk line. The solution was degassed by three cycles of freeze-pump-thawing and 1 bar of N₂O was added to the reaction mixture, which turned darker orange-brown over the course of 30 minutes. The ³¹P{¹H} NMR spectrum of the reaction mixture at 25°C shows the slow consumption of the starting material over the course of 24 h, with no new resonances appearing (**Figure S11**).

Good quality X-ray single crystals could be grown by vapour diffusion of pentane into the Et₂O solution over the course of 2 days. Two different complexes, [Fe^{III}(depe)(Cp*)(OH)][BAr^F] (**3**) and [Fe^{III}(depe)(η⁵,κ¹O-C₅Me₄CH₂N(NH₂)O)][BAr^F] (**4**), were repeatedly identified from these reaction mixtures from different experiments. The two products could not be separated completely, since they co-crystallize and the EPR spectra of different batches and/or different experiments always showed the presence of both Fe(III) complexes (Figure 2 in the main text).

ii) preparative scale: A light-orange-yellow solution of complex **2** (33.5 mg, 0.0263 mmol) in Et₂O (6.5 mL) was transferred into a J-Young adapted 50.0 mL ampoule and connected to a Schlenk line. The solution was degassed by three cycles of freeze-pump-thawing and 1 bar of N₂O was added to the reaction mixture, which turned darker orange-brown over the course of 30 minutes. The reaction mixture was left to react under stirring for 24 h at 25°C, obtaining a dark orange-red solution. 10.5 mg of red microcrystalline powder containing a mixture of **3** and **4** (as confirmed by EPR spectroscopy at 77 K) could be recovered by layering pentane into the Et₂O solution after two days at -35°C.

c) in toluene

i) NMR scale: A pale yellow suspension of complex **2** (2.8 mg, 0.0022 mmol) in d₈-toluene (0.4 mL) was transferred into a J-Young adapted NMR tube and connected to a Schlenk line. The solution was degassed by three cycles of freeze-pump-thawing and 1 bar of N₂O was added to the reaction mixture, which turned pale salmon-pink over the course of 30 minutes. The ³¹P{¹H} NMR spectrum of the reaction mixture at 25°C shows the consumption of the starting material over the course of 2 h, with no new resonances appearing (**Figure S12**). The reaction was left for 24 h under stirring at 25°C to ensure completion, due to the low solubility of the reactant and product(s) in the solvent. ¹H NMR monitoring of the reaction mixture clearly shows the formation of new species over the course of 24 h (**Figure S13**). All volatiles were removed under vacuum, obtaining a salmon-red oily solid, which was further dried at 25°C for 30 min. The solid was dissolved in 0.5 mL of Et₂O, obtaining a pink salmon solution. Crystals were grown by vapor diffusion of pentane into the Et₂O solution. The first time crystals were grown, two different complexes were found co-crystallized in the unit cell, [Fe(depe)(Cp*)(OH)][BAR^F] (**3**) and another complex, [Fe^{II}(κ²P:κ²C-depe')(Cp*)][BAR^F] (**5**), where depe' denotes a diphosphine ligand in which one of the ethyl arms has been dehydrogenated towards a vinyl group, that in turn coordinates to Fe(II) in a κ²-fashion. Single crystals of **5**, independently crystallized from **3**, could be analyzed by mounting multiple crystals from the same batch. EPR analyses of the solids obtained from this method also show recurrently the presence of complex **4**, which prevented us from isolating these species as analytically pure samples.

ii) preparative scale: An orange suspension of complex **2** (95.1 mg, 0.0746 mmol) in toluene (10.0 mL) was transferred into a J-Young adapted 100 mL ampoule and connected to a Schlenk line. The solution was degassed by three cycles of freeze-

pump-thawing and 1 bar of N₂O was added to the reaction mixture, which turned darker orange-brown over the course of 30 minutes. The reaction mixture was left to react under stirring for 24 h at 25°C, obtaining a dark red-salmon suspension. The toluene soluble fraction was separated, and all volatiles were removed under vacuum to yield an oily red solid, which was further dried under vacuum for 30 min. Afterwards, it was dissolved in Et₂O (0.6 mL) and placed inside a bigger vial for vapor diffusion of pentane into it. A few crystals of a mixture of complexes **3**, **4** and **5** were obtained and identified by means of single crystal XRD and/or EPR spectroscopy at 77 K.

The remaining red solid in the ampoule was dissolved in 15.0 mL of Et₂O, obtaining a red-dark orange solution. 9.0 mL of pentane were carefully layered on top of it and stored at -35°C for 2 days, after when 32.0 mg of red microcrystalline solid could be obtained. EPR analysis at 77 K of the solid showed the presence of **3** and **4**.

Reaction of complex 1 with LiHBEt₃ for in situ generation of [Fe(depe)(Cp*)H].

22.0 μL of a colorless 1.0 M solution of LiHBEt₃ in THF (2.3 mg, 0.022 mmol, 1.1 equiv) was added to a dark violet solution of complex **1** (9.3 mg, 0.021 mmol, 1 equiv) in C₆D₆ (0.6 mL) in a J-Young adapted NMR tube, resulting in the immediate change of color to yellow and the formation of an off-white precipitate. The ³¹P{¹H} NMR spectrum shows only one signal at 103.97 ppm (**Figure S14**), which compares well with the previously Fe(II) hydride analogue reported by Valerga and collaborators, [Fe^{II}(dippe)(Cp*)H] (dippe = 1,2-bis(di-isopropylphosphino)-ethane).⁸ The ¹H NMR spectrum shows the presence of a triplet assigned to the hydride, at a -17.77 ppm (³J_{HP} = 69.6 Hz). (**Figure S15**) This independent synthesis of the neutral Fe^{II}-hydride allowed us to identify its spectroscopic signature and therefore to discard its formation during our catalytic studies (*vide infra*).

Reaction of complex 2 with H₂. A light orange-yellow solution of **2** (10.9 mg, 0.00855 mmol) in d₈-THF (0.5 mL) was prepared in a J-Young adapted NMR tube. The solution was degassed by three cycles freeze-pump-thawing and then 1 atm of H₂ was added. Multinuclear NMR spectroscopy shows the consumption of the starting material **2** and the formation of only one diamagnetic species, together with other paramagnetic(s) species over the course of 3 h. The ³¹P{¹H} NMR spectrum of the reaction mixture shows only one signal, at 91.12 ppm (**Figure S16**). The ¹H NMR spectrum of the

reaction mixture shows a triplet resonance centered at -9.21 ppm ($J_{\text{HP}} = 67.4$ Hz), (**Figure S17**) reminiscent of the Fe(IV) hydride reported for Valerga's analogue system, $[\text{Fe}^{\text{IV}}(\text{H})_2(\text{dippe})(\text{Cp}^*)][\text{BAr}^{\text{F}}]$.⁵⁻⁷ The multinuclear NMR spectroscopy data (**Figure S17-Figure S24**), together with the single crystal-XRD data (**Figure S74**) support the formation of $[\text{Fe}^{\text{IV}}(\text{H})_2(\text{depe})(\text{Cp}^*)][\text{BAr}^{\text{F}}]$ (**7**)

In-situ characterization of **7**:

$^{31}\text{P}\{^1\text{H}\}$ NMR (d_8 -THF, 161.98 MHz, 298 K): $\delta = 91.12$ (s) (**Figure S16**)

^1H NMR (d_8 -THF, 400 MHz, 298 K): $\delta = 7.82$ (br, s, 6H, BAr^{F}), 7.61 (br, 6H, BAr^{F}), 2.11-1.96 (m, 4H), 1.95 (s, 15 H, C_5Me_5), 1.85-1.72 (m, 4H), 1.52 (d, 4H, $^1J_{\text{HP}} = 7.9$ Hz), 1.28-1.12 (m, 12H), -9.21 (t, 2H, $^3J_{\text{HP}} = 67.4$ Hz). (**Figure S17**)

$^1\text{H}\{^{31}\text{P}\}$ NMR (d_8 -THF, 400 MHz, 253 K): $\delta = 7.82$ (br, s, BAr^{F}), 7.61 (br, BAr^{F}), 2.00 (dt, $J = 14.8, 7.4$ Hz), 1.95 (s, C_5Me_5), 1.84-1.75 (m), 1.49 (s), 1.14 (t, $^3J_{\text{HP}} = 7.5$ Hz), -9.32 (s). (**Figure S18**)

$^{13}\text{C}\{^1\text{H}\}$ NMR (d_8 -THF, 400 MHz, 298 K): $\delta = 161.82$ (dd, $^1J_{\text{CF}} = 1000, 50$ Hz, BAr^{F}), 134.61 (bs), 129.04 (dddd, BAr^{F}), 127.28 (BAr^{F}), 125.88 (BAr^{F}), 123.17 (BAr^{F}), 120.47 (BAr^{F}), 117.20 (BAr^{F}), 94.01, 22.79-22.39 (m), 9.79, 7.82. (**Figure S20**)

The 2D experiments show that some ^{13}C and ^1H resonances are hidden under the solvent peaks.

The reaction with H_2 was also performed in C_6D_6 and Et_2O , resulting in the same resonances, confirming the formation of the same species in all the solvents used for the catalytic experiments.

Furthermore, EPR analysis of the frozen reaction mixture at 77 K (**Figure S76**) confirmed the concomitant formation of a paramagnetic species. A very similar EPR spectrum was reported by Peters and collaborators for $[\text{Fe}^{\text{III}}(\text{dppe})(\text{Cp}^*)\text{H}][\text{BAr}^{\text{F}}]$ (dppe = 1,2-bis(diphenylphosphino)-ethane).⁹ They also observed only coupling to the P atoms of the phosphine ligand in a $S=1/2$ system, supporting the formation of $[\text{Fe}^{\text{III}}(\text{depe})(\text{Cp}^*)\text{H}][\text{BAr}^{\text{F}}]$ in the reaction of **2** with 1 bar of H_2 .

Reaction of complex 2 with nitrobenzene (C₆H₅NO₂). A light orange-yellow suspension of **2** (6.2 mg, 0.0049 mmol, 1 equiv) in C₆D₆ (0.5 mL) was prepared in a J-Young adapted NMR tube. To this, 4.0 μL of nitrobenzene (4.5 mg, 0.00364 mmol, 7.5 equiv) were added without any significant change of color. The reaction proceeds slowly at 25°C, and only after 19 h at 25°C, a pale green solution is observed, with a lot of light orange solid **2** still unreacted. However, the reaction can be completed by warming up the tube at 50°C for 24 h, observing a color change to deep blue, with the concomitant formation of a blue oil. The ³¹P{¹H} NMR spectrum of the reaction mixture shows two resonances at 89.1(minor) and 81.1 ppm (major). (**Figure S25**) The ¹H NMR spectrum of the reaction mixture shows the presence of nitrobenzene, as expected from the addition of excess of this reagent (**Figure S26**). The EPR spectrum (**Figure S77**) of a frozen solution (THF:Et₂O 1:1) of the reaction mixture at 77 K shows an anisotropic signal attributed to compound **3** (g_x = 2.387; g_y = 2.072; g_z = 2.002), since it closely resembles one of the two products obtained and characterized for the reaction of **2** with N₂O.

All volatiles were removed under vacuum and the oily solid was further dried at 25°C for 15 min. The crude was dissolved in 0.5 mL of Et₂O, obtaining a deep blue-green solution and crystals were grown from vapor diffusion of pentane into this Et₂O solution over the course of 2 days. Two types of crystals were grown together, as can be seen in the following picture (Picture S1). The green-blue plates correspond to the formation of [[Fe^{II}(depe)(Cp*)(κ¹N-C₆H₅NO)][BAR^F]] (**6-N**) and the red-orange blocks to [Fe(depe)(Cp*)(OH)][BAR^F]] (**3**), as confirmed by cell check and preliminary resolution of the data. However, the small size of the crystals and their instability did not allowed us to separate them in sufficient amount by hand picking.



Picture S1: Crystals grown from a vapor diffusion of pentane into the reaction mixture of **2** with nitrobenzene in Et₂O.

Reaction of complex 2 with nitrosobenzene (C₆H₅NO). A light orange-yellow suspension of **2** (9.3 mg, 0.0073 mmol, 1 equiv) in C₆D₆ (0.5 mL) was prepared in a J-Young adapted NMR tube. To this, white solid nitrosobenzene (1.2 mg, 0.02 mmol, mmol, 1.5 equiv) was added, resulting in the change of color first to green and then to deep blue, as observed after reaction with nitrobenzene (or during the catalysis in presence of HBPin). A lot of deep blue oil can also be seen on the walls of the tube. The ³¹P{¹H} NMR spectrum of the reaction mixture shows six resonances at 89.2, 89.1, 81.4, 81.1, 78.4 and 78.3 ppm, suggesting the formation of multiple species upon coordination of nitrosobenzene (**Figure S27**). The ¹H NMR spectrum of the reaction mixture shows a complicated pattern of signals, further supporting the formation of multiple species (**Figure S28**).

All volatiles were removed under vacuum and the oily solid was further dried at 25°C for 15 min. Reaction mixture was dissolved in 0.5 mL of Et₂O, obtaining a deep blue-green solution and crystals were grown from vapor diffusion of pentane into this Et₂O solution over the course of 2 days. Green-blue rods crystals of [Fe(depe)(Cp*)(κ¹O-C₆H₅NO)][BAR^F] (**6-O**, Figure 2 in manuscript) were mounted and measured by single-crystal XRD, showing the formation of a nitrosobenzene adduct that consists in a different isomer to the previously identified from the reactivity with nitrobenzene.

Catalytic experiments

General procedure for the reaction of complex **2 with 20 equiv. of HBPin in the presence of 1 bar of N₂O.** In a glovebox, **2** (5.0 mg, 0.0039 mmol, 1 equiv.) and HBPin (11.4 μL, 0.078 mmol, 20 equiv.) were placed in a J-Young NMR tube and 0.5 mL of solvent were added. The contents of the tube were thoroughly mixed, resulting in no evident color change. ³¹P{¹H} and ¹¹B NMR spectroscopy showed that no reaction happened between the two reactants (**Figure S30** and **Figure S31**). The solution was degassed by two freeze-pump-thawing cycles and then 1 atm of N₂O was added and the evolution of the reaction was followed by multinuclear NMR spectroscopy. The ³¹P{¹H} NMR of the reaction mixture shows the slow consumption of **2** and the formation of [Fe^{IV}(H)₂(depe)(Cp^{*})] [BAr^F], which is attributed to an off-cycle species, as explained in the main text (see **Figure S34** and **Figure S35**). No other Fe-containing species intermediates could be detected by NMR monitoring. Furthermore, the formation of the Fe(IV) bis-hydride is supported by the appearance of a triplet resonance at -9.2 ppm in the ¹H NMR spectrum (**Figure S36**), in perfect agreement to what was observed by direct reaction of **2** with H₂ (**Figure S17**). The conversion of HBPin to O(OBpin)₂ was followed by ¹¹B{¹H} NMR spectroscopy (**Figure S37** and **Figure S39**).

Crystals of O(Bpin)₂ were obtained by vapor diffusion of pentane into Et₂O or THF solutions of the reaction mixtures, as confirmed by sc-XRD and comparison with the reported unit cell.

*The reaction in CH₂Cl₂ showed no transformation of HBPin to O(Bpin)₂ (**Figure S40**), which is consistent with precatalyst **2** decomposing in this solvent.*

*The catalytic conversion of HBPin to O(Bpin)₂ is much slower in toluene suspension, not reaching 100% over the course of 20 h at 25°C (89% conversion, **Figure S39**). This could be explained by the low solubility of **2** and the species formed during the reaction in toluene.*

Reaction of complex **2 with 34 equiv. of HBPin in the presence of 1 bar of N₂O, and further addition of N₂O.** In a glovebox, **2** (4.3 mg, 0.0034 mmol, 1 equiv.) and HBPin (16.5 μL, 0.114 mmol, 34 equiv.) were placed in a J-Young NMR tube and 0.5 mL of Et₂O were added. The contents of the tube were thoroughly mixed, resulting in no evident color change, ³¹P{¹H} and ¹¹B{¹H} NMR spectroscopy showed that no

reaction occurred between the two reactants (**Figure S41a** and **Figure S42a**). The solution was degassed by two freeze-pump-thawing cycles and then 1 atm of N₂O was added and the evolution of the reaction was followed by multinuclear NMR spectroscopy. The ³¹P{¹H} NMR of the reaction mixture shows the slow consumption of **2** and the formation of [Fe^{IV}(depe)(Cp*)(H)₂][BAr^F] (**7**) (**Figure S41**), as in the prior case. Furthermore, the formation of the Fe(IV) bis-hydride is supported by the appearance of a triplet resonance at -9.2 ppm in the ¹H NMR spectrum (**Figure S43**), in perfect agreement to what was observed by direct reaction of **2** with H₂ (**Figure S17**).

The conversion of HBpin to O(OBpin)₂ was followed by ¹¹B{¹H} NMR spectroscopy, observing that after 30 h some HBpin was still present, (**Figure S42**). To see if the reaction could proceed to completion, the solution was again degassed by two freeze-pump-thawing cycles and again 1 bar of N₂O was added. The evolution of the reaction mixture was followed by multinuclear NMR spectroscopy, as before, showing the slow consumption of the bis-hydride and the formation of a dark red-orange solution over the course of 36 h (**Figure S44** and **Figure S45**). Moreover, ¹¹B{¹H} NMR monitoring of the reaction mixture (**Figure S46**) shows the consumption of HBpin and the concomitant formation of O(Bpin)₂.

General procedure for the reaction of complex 2 with 200 equiv. of HBPin in the presence of 1 bar of N₂O. In a glovebox, **2** (3.5 mg, 0.0027 mmol, 1 equiv.) and HBpin (80.0 μL, 0.5512 mmol, 200 equiv.) were placed in a 50.0 mL ampoule and 3.5 mL of solvent were added. The contents of the ampoule were thoroughly mixed, resulting in no evident color change. The solution was degassed by two freeze-pump-thawing cycles and then 1 atm of N₂O was added. The reaction mixture was placed inside an oil bath to react for 24 h at a controlled temperature. The conversion of HBpin to O(Bpin)₂ was monitored by ¹¹B{¹H} NMR spectroscopy at the end of the reaction, and corroborated by using BPh₃ as internal standard.

Table S1. Conversion of HBpin to O(Bpin)₂ from the mixture of 2 (0.5 mol %) and N₂O (1 bar) over the course of 24 h at different temperatures.

Entry	Solvent	Temperature	%Conversion
1	THF	25°C	62
2		50°C	52
3		80°C	36
4		50°C	31

5	Toluene	80°C	62
6		100°C	36

General procedure for the reaction of complex 2 with 100 equiv. of HBPin and 20 equiv. of nitrobenzene (C₆H₅NO₂). In a glovebox, **2** (3.0 mg, 0.0024 mmol, 1 equiv.), HBpin (34.2 μL, 0.238 mmol, 100 equiv.) and nitrobenzene (4.9 μL, 0.0477 mmol, 20 equiv.) were placed inside a J-Young NMR tube and 0.5 mL of solvent were added. The contents of the NMR tube were thoroughly mixed, and the reaction mixture was placed inside an oil bath to react at a controlled temperature. The evolution of the reaction mixture was checked over time by multinuclear NMR spectroscopy. The conversion proceeds slowly at 25°C in C₆D₆ not being completed even after 4 days of reaction (**Figure S58**). Although the formation of H₂ is observed during the reaction in the ¹H NMR spectrum (**Figure S59**), the formation of the Fe(IV) hydride **7** is not observed. At 80°C, the catalysis is finished over the course of 30 min (**Figure S62**). In Et₂O the conversion is faster at 25°C, with the reaction being finished over the course of 30 h (**Figure S64**), most likely due to the higher solubility of the complexes. THF was not investigated due to poorer results of the previous catalysis.

In all the cases the reaction mixture goes from a light orange-yellow color, to first a green, followed by deep blue and again yellow-orange after finishing.

Table S2. Time required for the complete conversion of HBpin (100 equiv.) to O(Bpin)₂ from the mixture of 2 (5 mol %) and nitrobenzene (20 equiv) in C₆D₆ at different temperatures.

Entry	Temperature	Time
1	25°C	4 days
2	50°C	5 h
3	80°C	30 min

Reaction of complex 2 with 500 equiv. of HBPin and 100 equiv. of nitrobenzene (C₆H₅NO₂) in C₆D₆ at 80°C. In a glovebox, **2** (1.2 mg, 0.00094 mmol, 1 equiv.), HBpin (68.5 μL, 0.472 mmol, 500 equiv.) and nitrobenzene (9.7 μL, 0.00945 mmol, 1000 equiv.) were placed inside a J-Young NMR tube and 0.5 mL of C₆D₆ were added. The contents of the NMR tube were thoroughly mixed, and the reaction mixture was placed inside an oil bath to react at 80°C. The evolution of the reaction mixture was checked over time by multinuclear NMR spectroscopy, showing that is finished over the course of 30 min (**Figure S66**).

Reaction of complex 2 with 5000 equiv. of HBPin and 1000 equiv. of nitrobenzene (C₆H₅NO₂) in C₆D₆ at 80°C. In a glovebox, **2** (1.0 mg, 0.00078 mmol, 1 equiv.), HBPin (568.9 μL, 3.920 mmol, 5026 equiv.) and nitrobenzene (80.5 μL, 0.00945 mmol, 1005 equiv.) were placed inside a J-Young NMR tube and 0.5 mL of C₆D₆ were added. The contents of the NMR tube were thoroughly mixed, and the reaction mixture was placed inside an oil bath to react at 80°C. The evolution of the reaction mixture was checked over time by multinuclear NMR spectroscopy, showing that is finished over the course of 4 h (**Figure S68**). After this time, the reaction mixture was diluted by adding 1.5 mL of dry Et₂O. Afterwards, 1.5 mL of a 2.0 M solution of HCl in Et₂O was added, resulting in the immediate precipitation of a white solid. The crude was filtered through a 4-porosity glass frit, obtaining an off-white solid, which was washed with Et₂O (2 x 0.3 mL) and then pentane (2 x 1.5 mL), before drying under vacuum.¹⁰ 95.0 mg of anilinium chloride were recovered, for a 94% yield.

B. NMR spectroscopic data

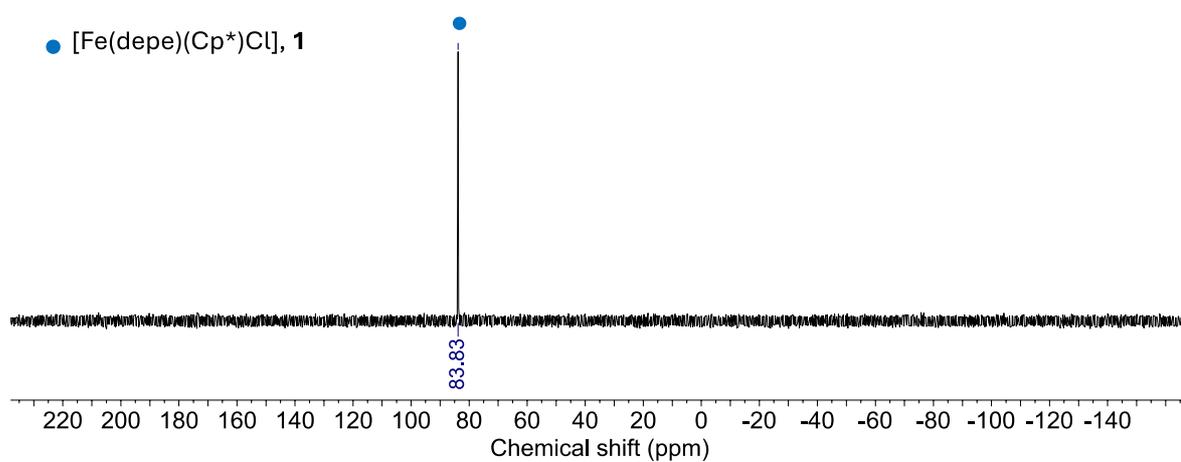


Figure S1: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (161.98 MHz, C_6D_6 , 298 K) of isolated **1**.

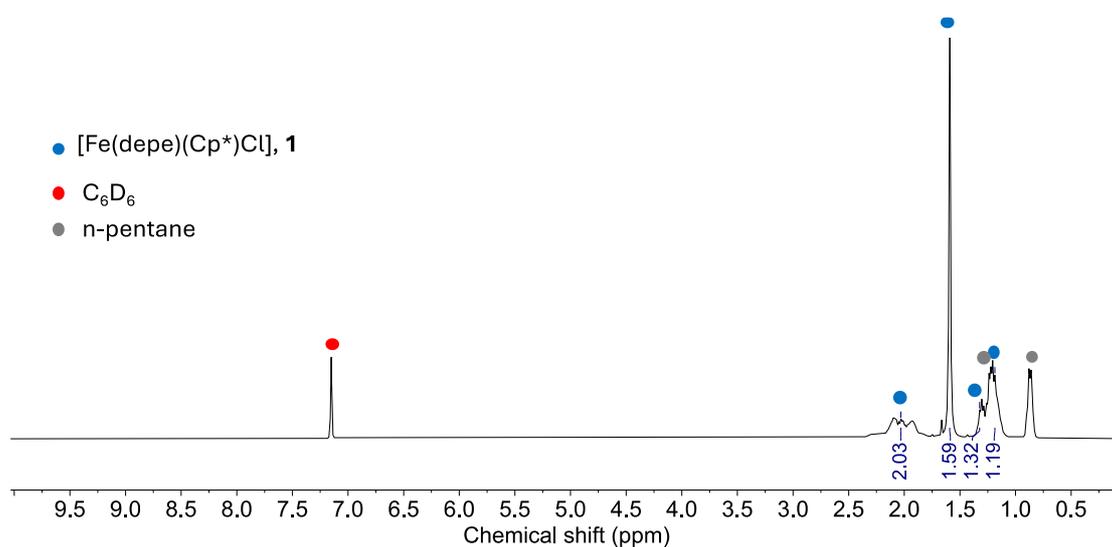


Figure S2: ^1H NMR spectrum (400 MHz, C_6D_6 , 298 K) of isolated **1**.

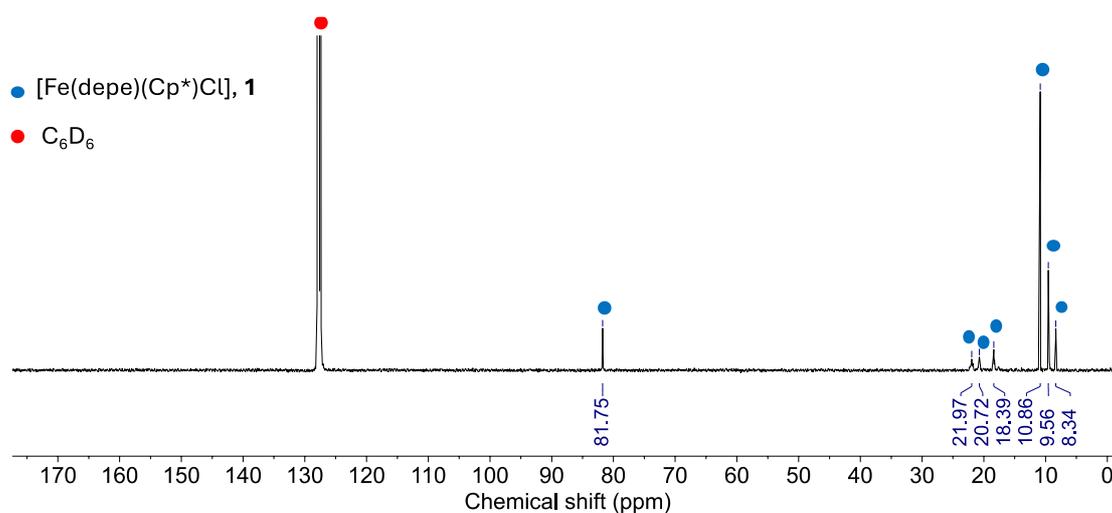


Figure S3: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (100.61 MHz, C_6D_6 , 298 K) of isolated **1**.

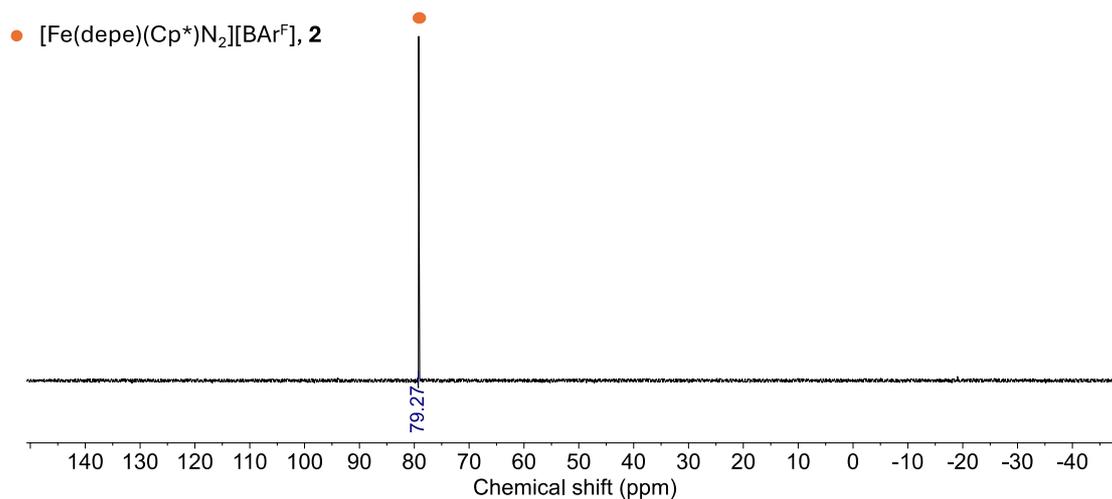


Figure S4: ³¹P{¹H} NMR spectrum (202.46 MHz, d₈-THF, 298 K) of isolated **2**.

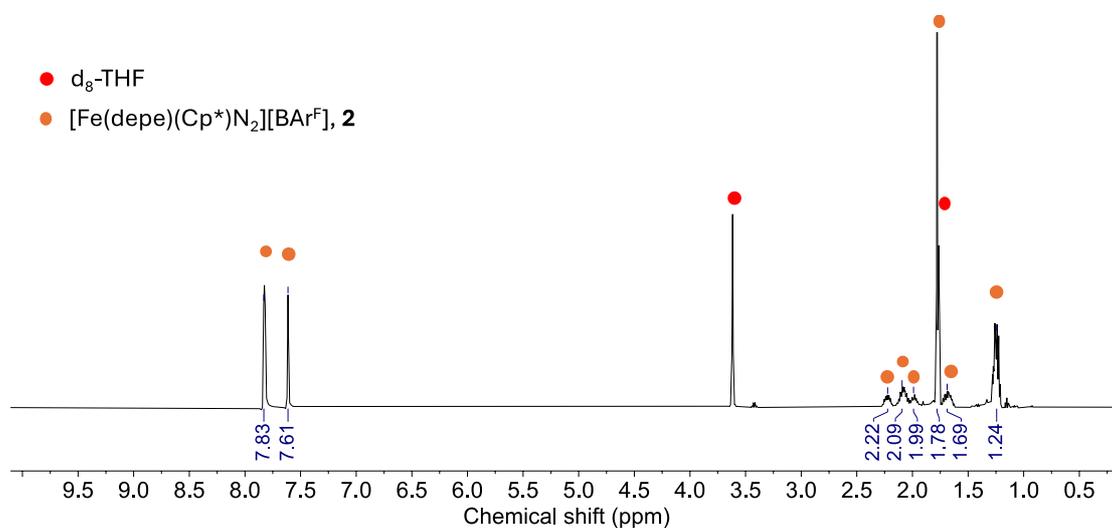


Figure S5: ¹H NMR spectrum (500 MHz, d₈-THF, 298 K) of isolated **2**.

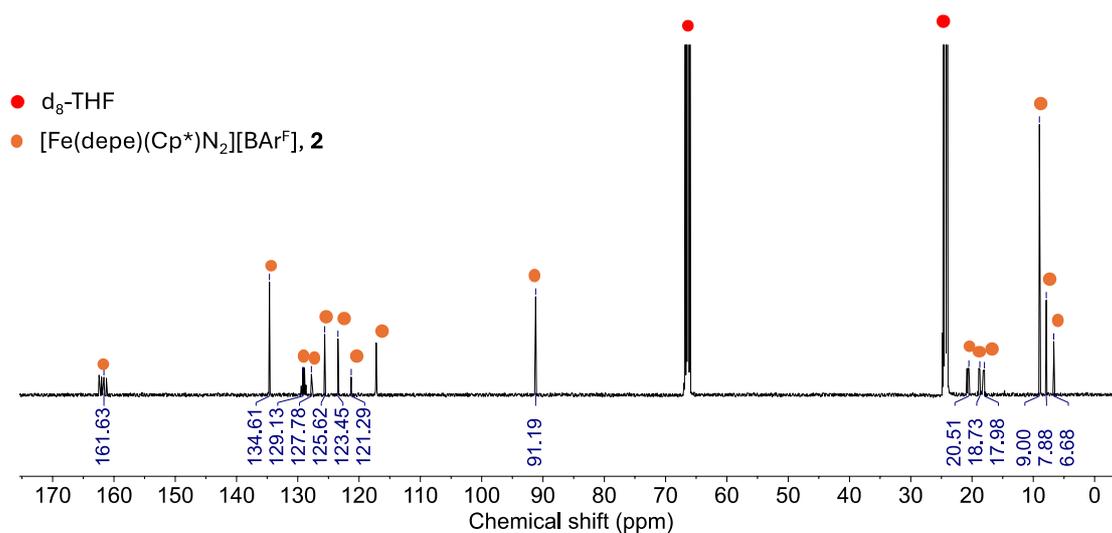


Figure S6: ¹³C{¹H} NMR spectrum (125.76 MHz, d₈-THF, 298 K) of isolated **2**.

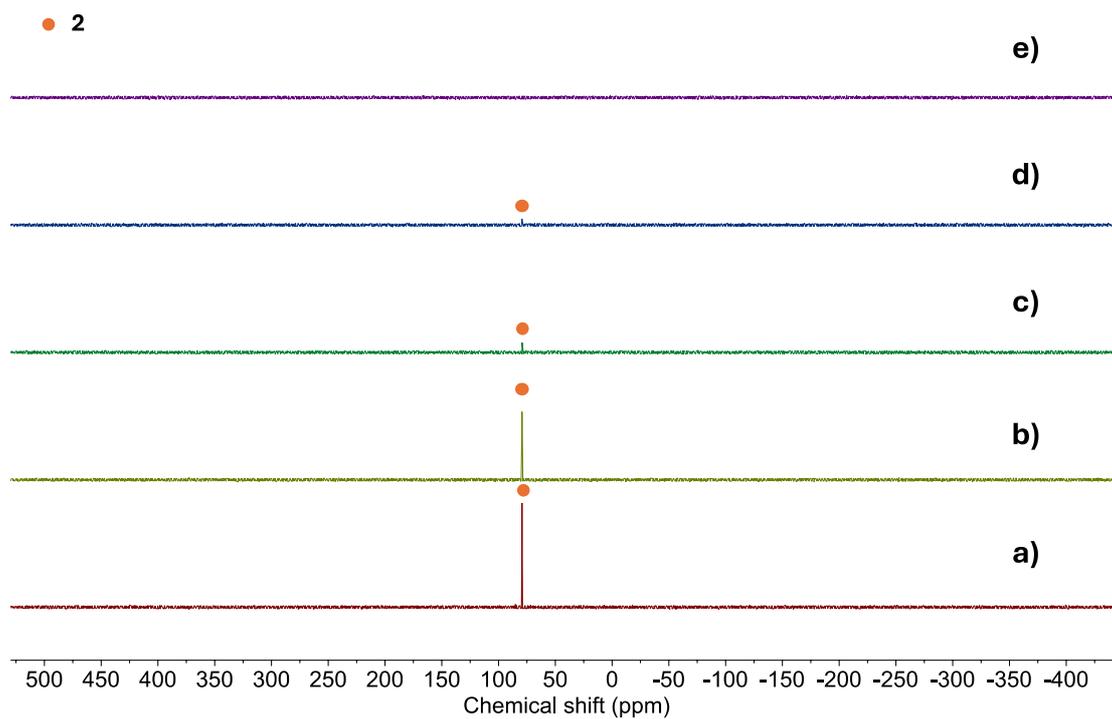


Figure S7: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (121.50 MHz, $\text{d}_8\text{-THF}$, 298 K) monitoring of the reaction mixture obtained by adding 1 bar of N_2O to a THF solution of **2** a) 40 min after, b) 2.5 h after, c) 17 h after, d) 24 h after and, e) 36 h after.

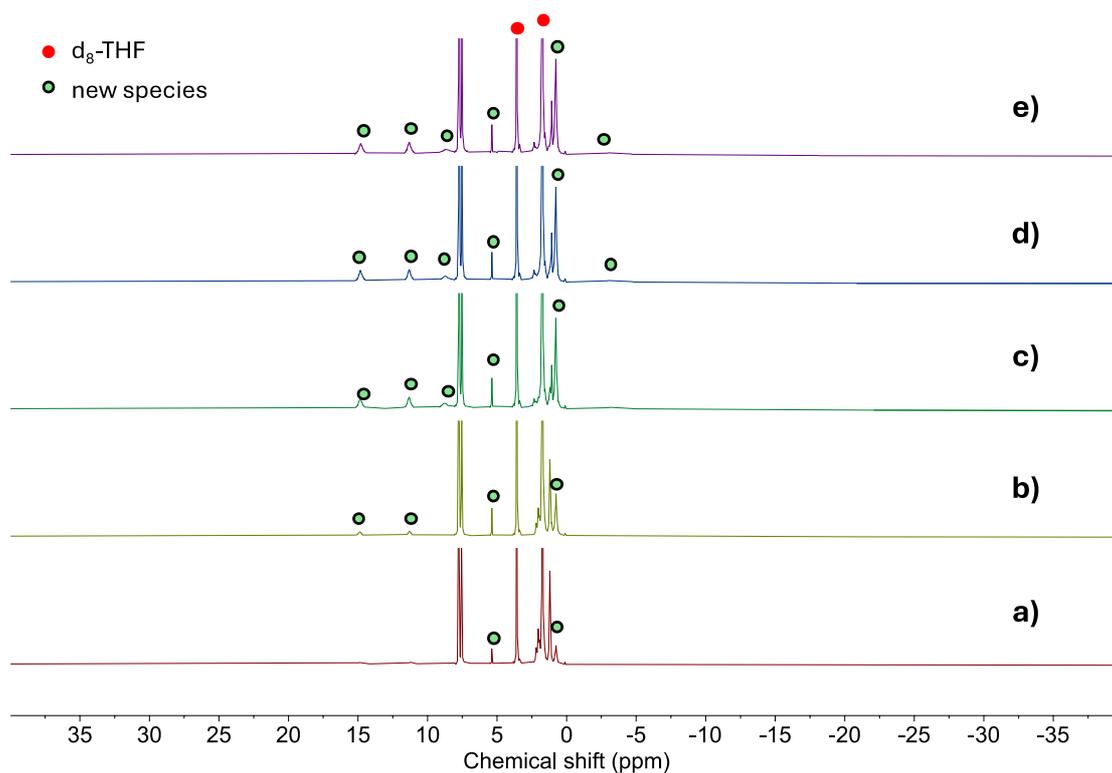


Figure S8: ^1H NMR spectrum (300 MHz, d_8 -THF, 298 K) monitoring of the reaction mixture obtained by adding 1 bar of N_2O to a THF solution of **2** a) 40 min after, b) 2.5 h after, c) 17 h after, d) 24 h after and, e) 36 h after. Green dots highlight resonances for a new appearing species whose nature we were unable to identify.

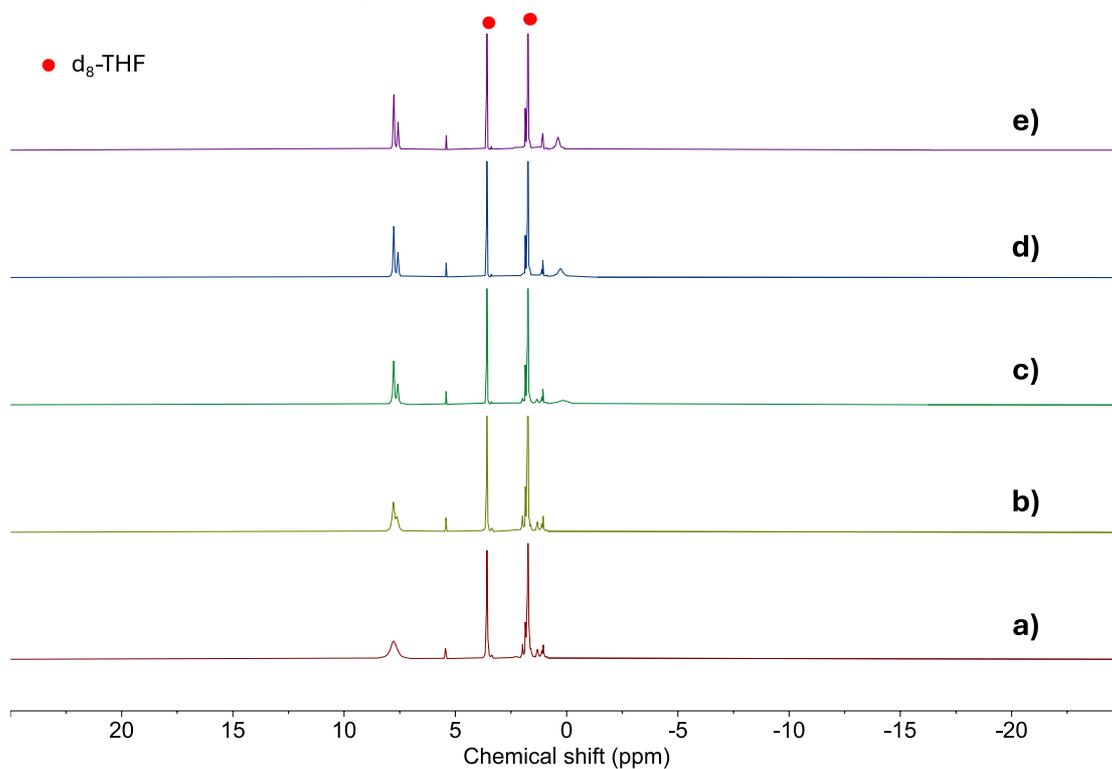


Figure S9: Variable temperature ^1H NMR spectra (400 MHz, $\text{d}_8\text{-THF}$) of the reaction mixture obtained 36 h after addition of 1 bar of N_2O to a THF solution of **2** a) 193 K, b) 213 K, c) 233 K, d) 243 K and, e) 253 K.

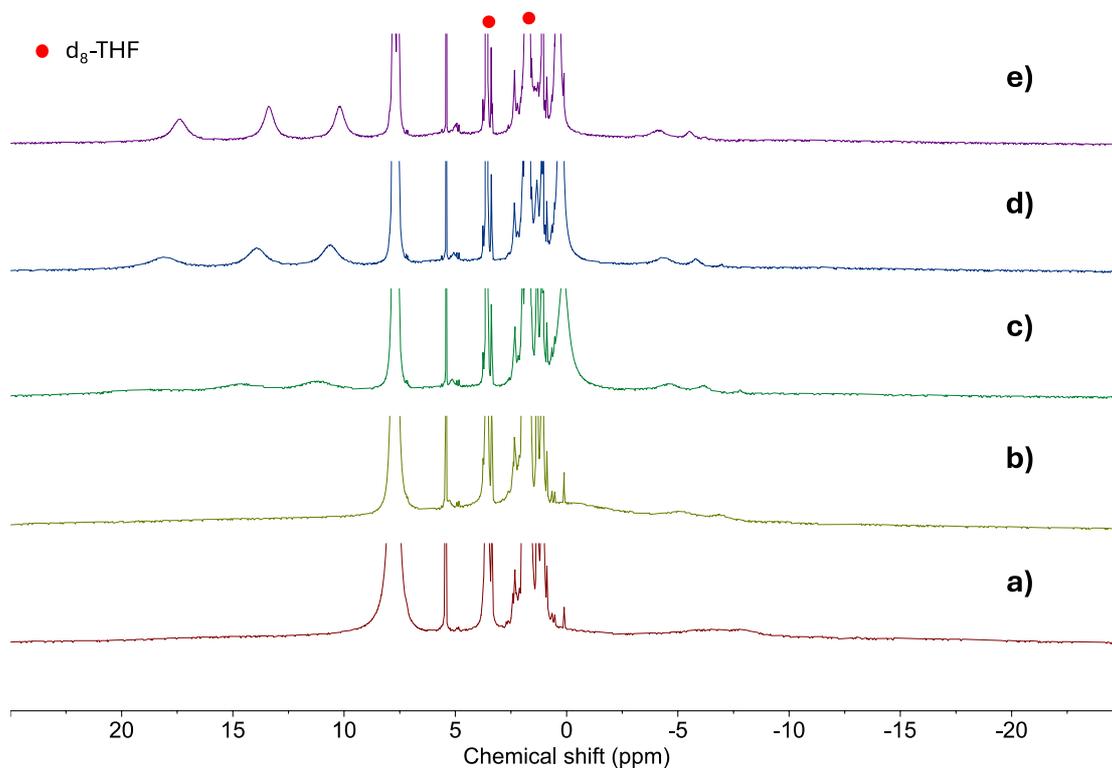


Figure S10: Variable temperature ^1H NMR spectra (400 MHz, $\text{d}_8\text{-THF}$) of the reaction mixture obtained 36 h after addition of 1 bar of N_2O to a THF solution of **2** a) 193 K, b) 213 K, c) 233 K, d) 243 K and, e) 253 K. (*Increased intensity*)

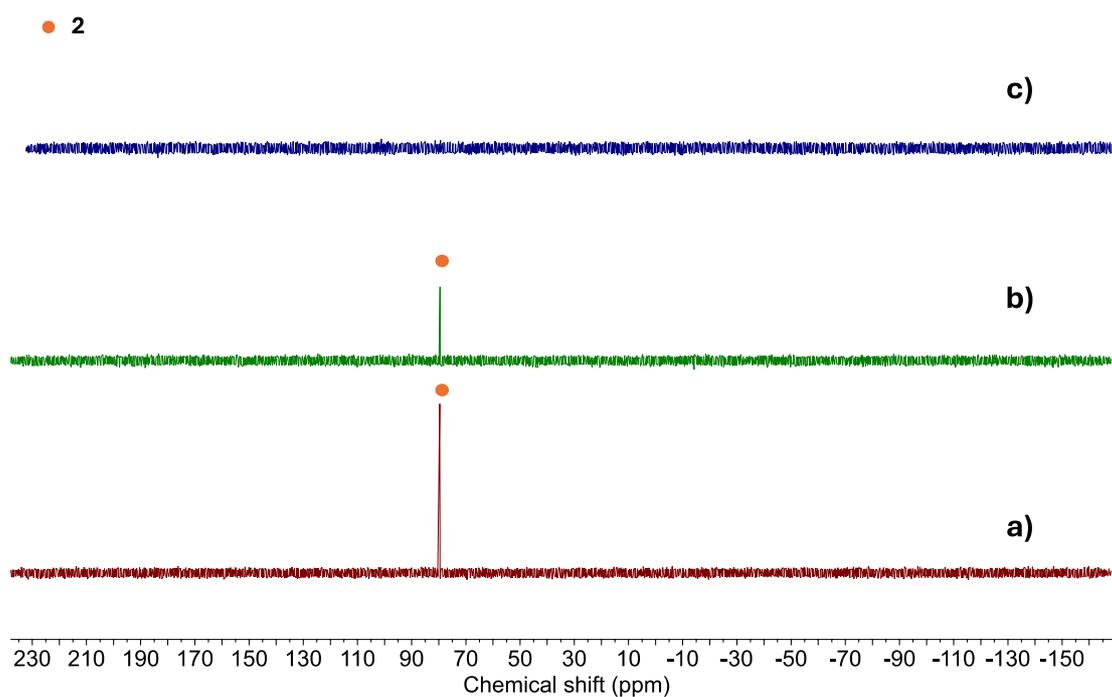


Figure S11: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (202.46 MHz, Et_2O , 298 K) monitoring of the reaction mixture obtained by adding 1 bar of N_2O to a Et_2O solution of **2** a) 15 min after, b) 2 h after and, c) 24 h after.

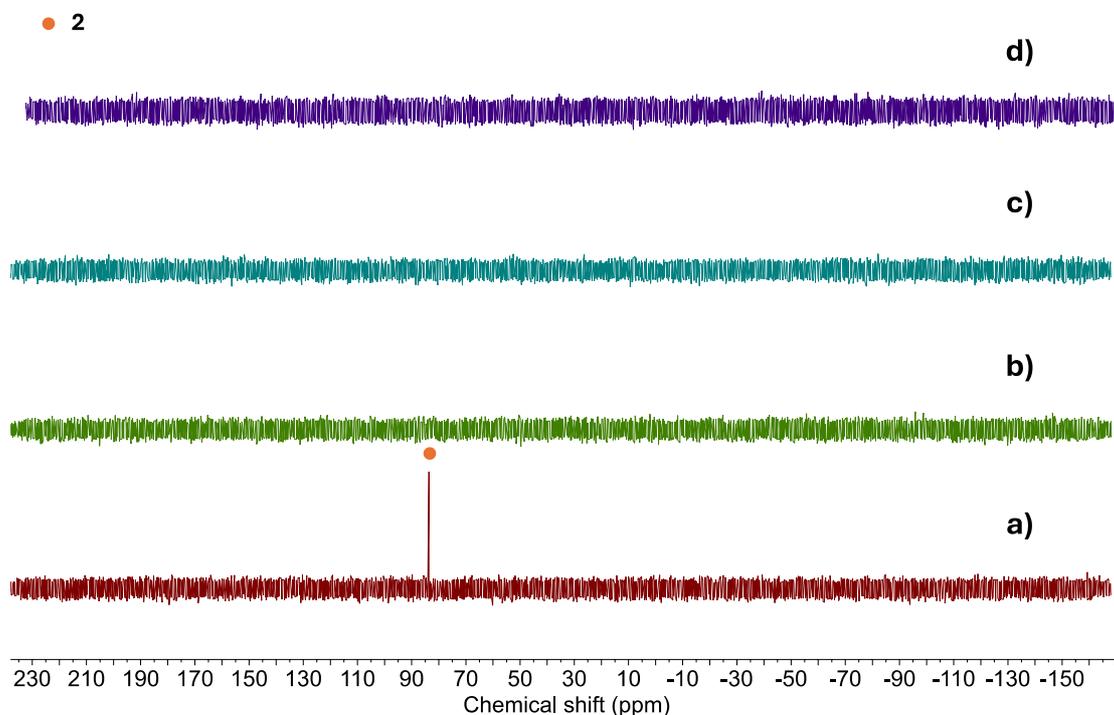


Figure S12: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (202.46 MHz, d_8 -Toluene, 298 K) monitoring of the reaction mixture obtained by adding 1 bar of N_2O to a toluene suspension of **2** a) 10 min after, b) 2 h after c) 5.5 h after and, d) 24 h after.

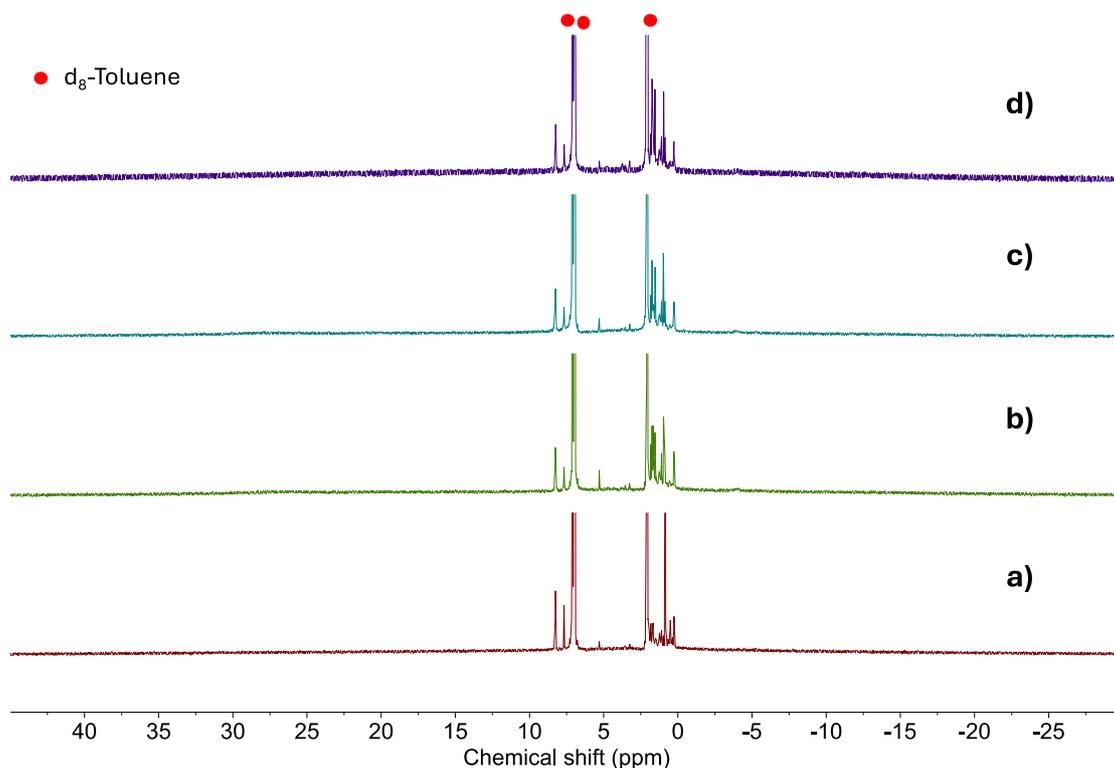


Figure S13: ^1H NMR spectrum (500 MHz, d_8 -Toluene, 298 K) monitoring of the reaction mixture obtained by adding 1 bar of N_2O to a toluene suspension of **2** a) 10 min after, b) 2 h after c) 5.5 h after and, d) 24 h after.

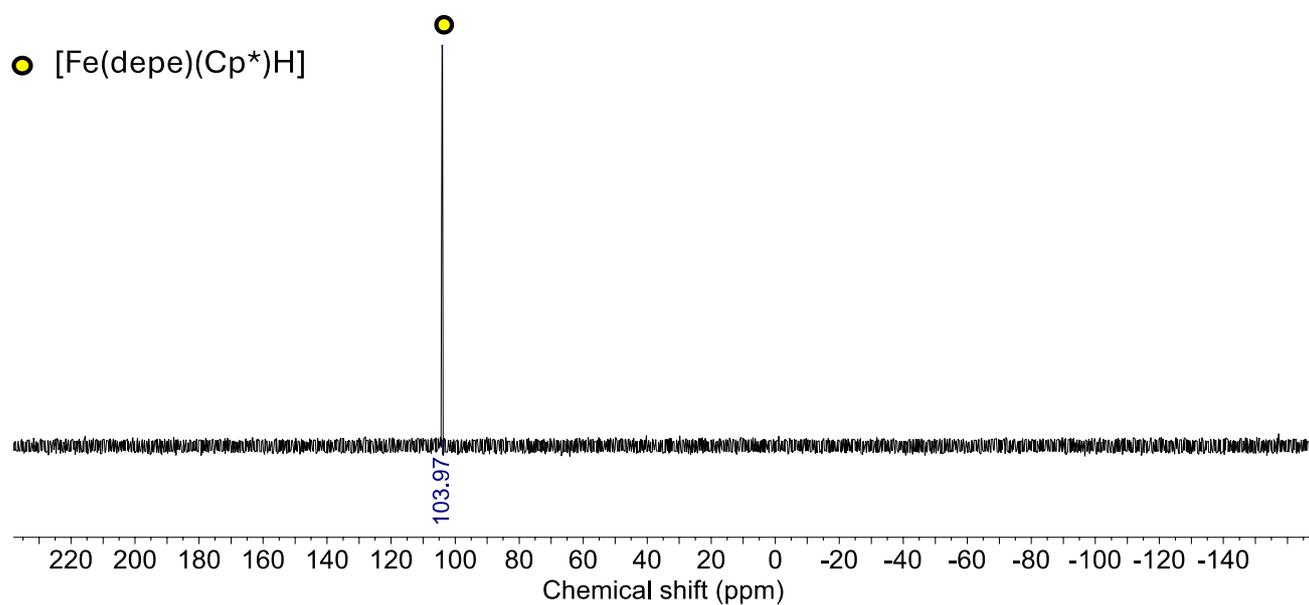


Figure S14: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (261.98 MHz, C_6D_6 , 298 K) of the reaction mixture obtained after addition of 1 equiv. of LiHBEt_3 to a C_6D_6 solution of **1**.

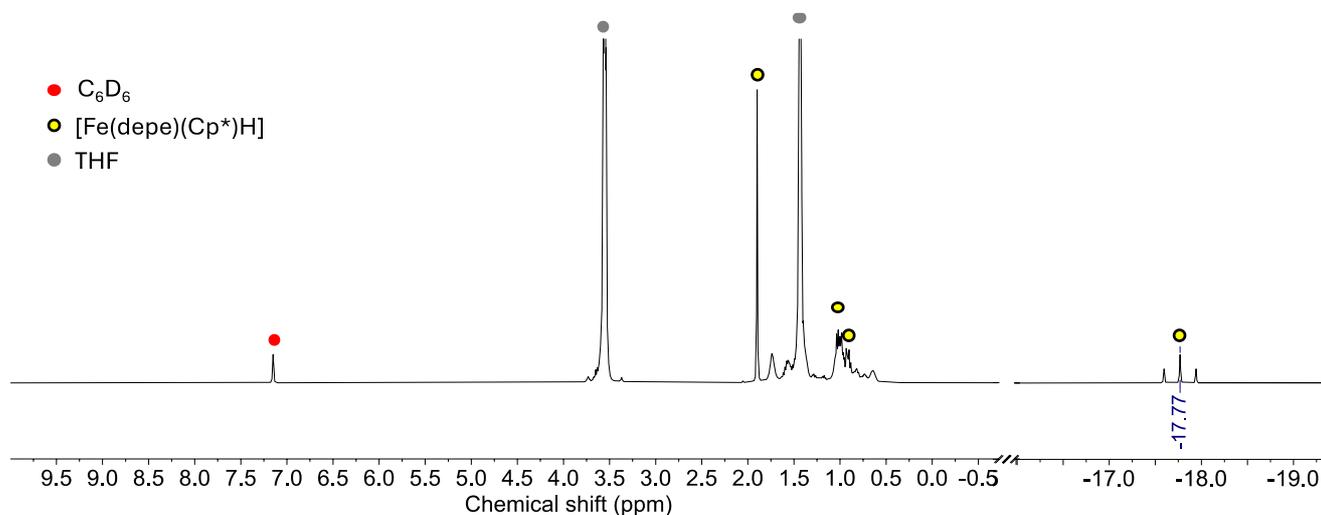


Figure S15: ^1H NMR spectrum (400MHz, C_6D_6 , 298 K) of the reaction mixture obtained after addition of 1 equiv. of LiHBEt_3 to a C_6D_6 solution of **1**.

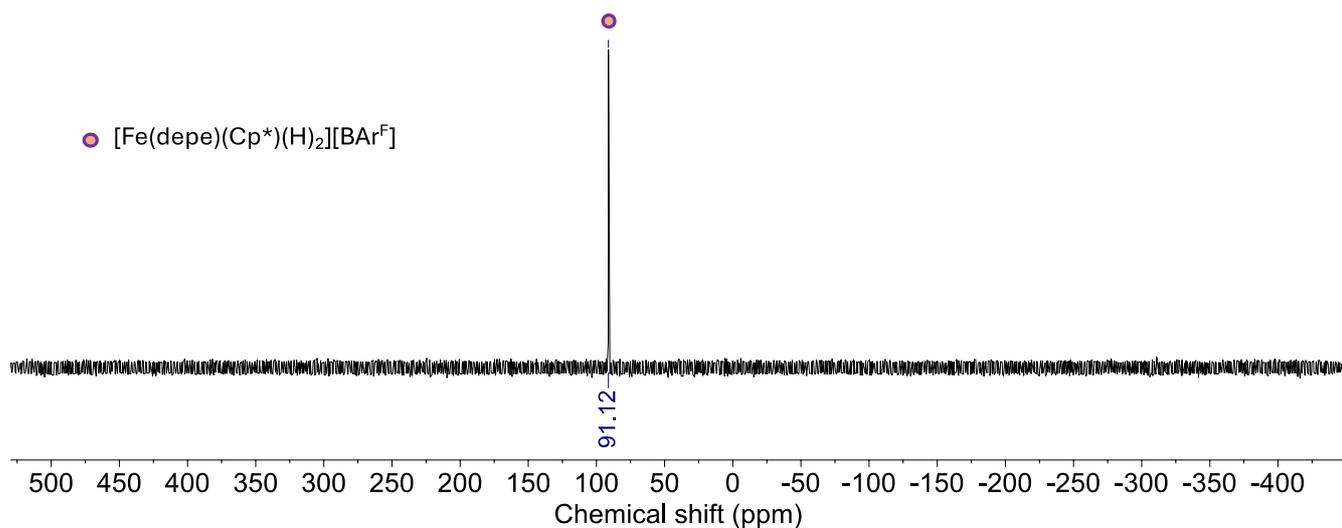


Figure S16: ³¹P{¹H} NMR spectrum (121.50 MHz, d₈-THF, 298 K) of the reaction mixture obtained after addition of 1 bar of H₂ to a d₈-THF solution of **2**.

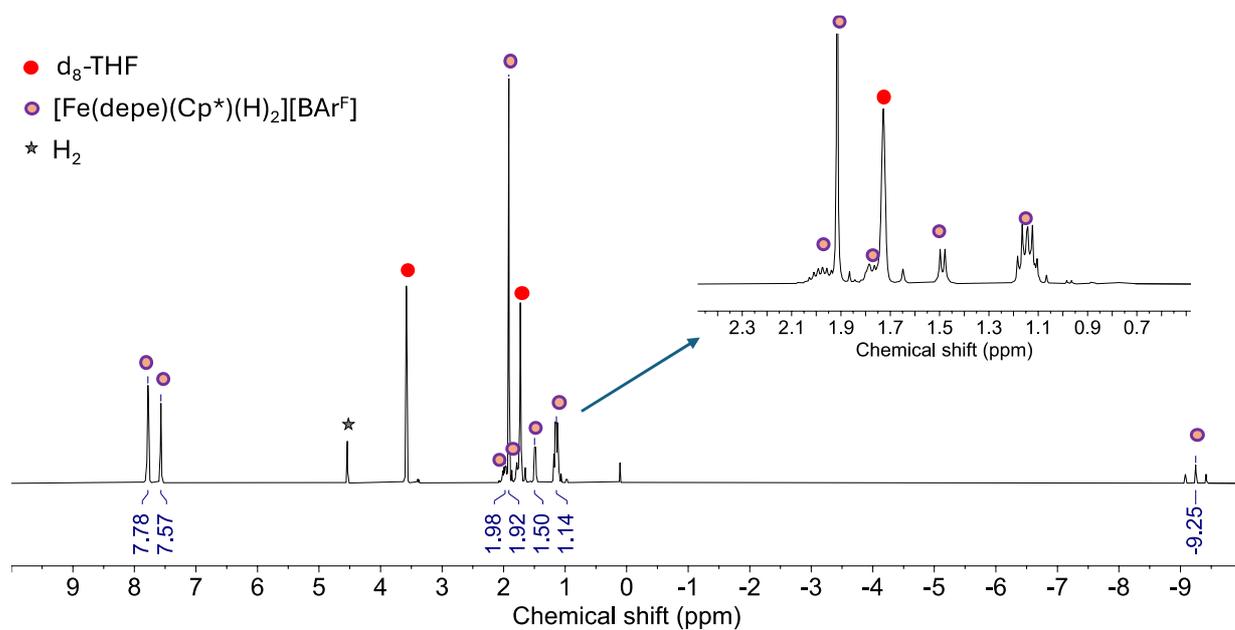


Figure S17: ¹H NMR spectrum (400 MHz, d₈-THF, 298 K) of the reaction mixture obtained after addition of 1 bar of H₂ to a d₈-THF solution of **2**.

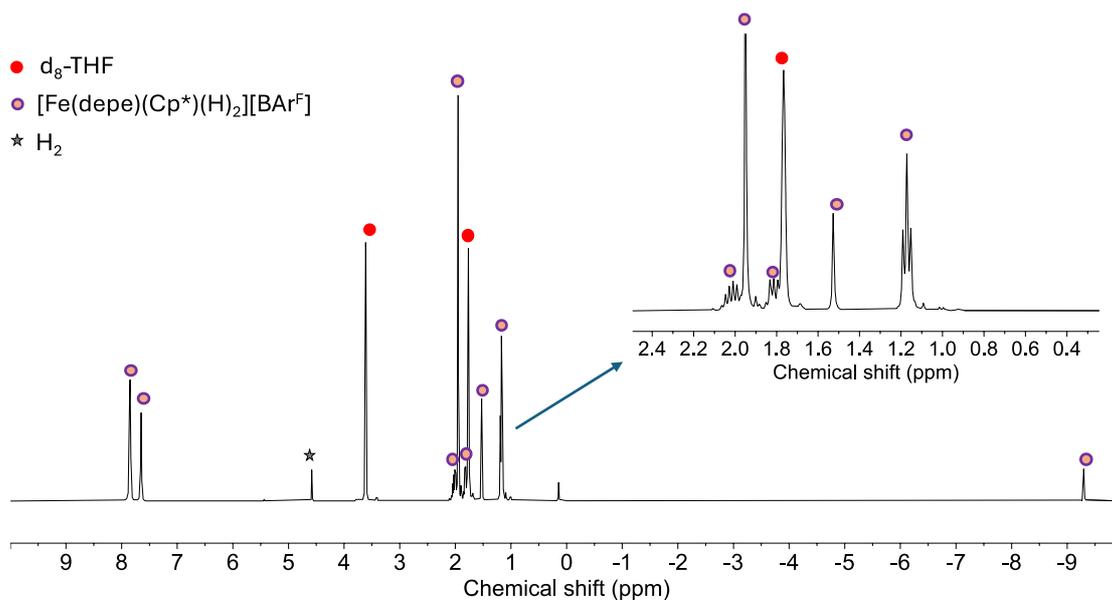


Figure S18: $^1\text{H}\{^{31}\text{P}\}$ NMR spectrum (400 MHz, d_8 -THF, 298 K) of the reaction mixture obtained after addition of 1 bar of H_2 to a d_8 -THF solution of **2**.

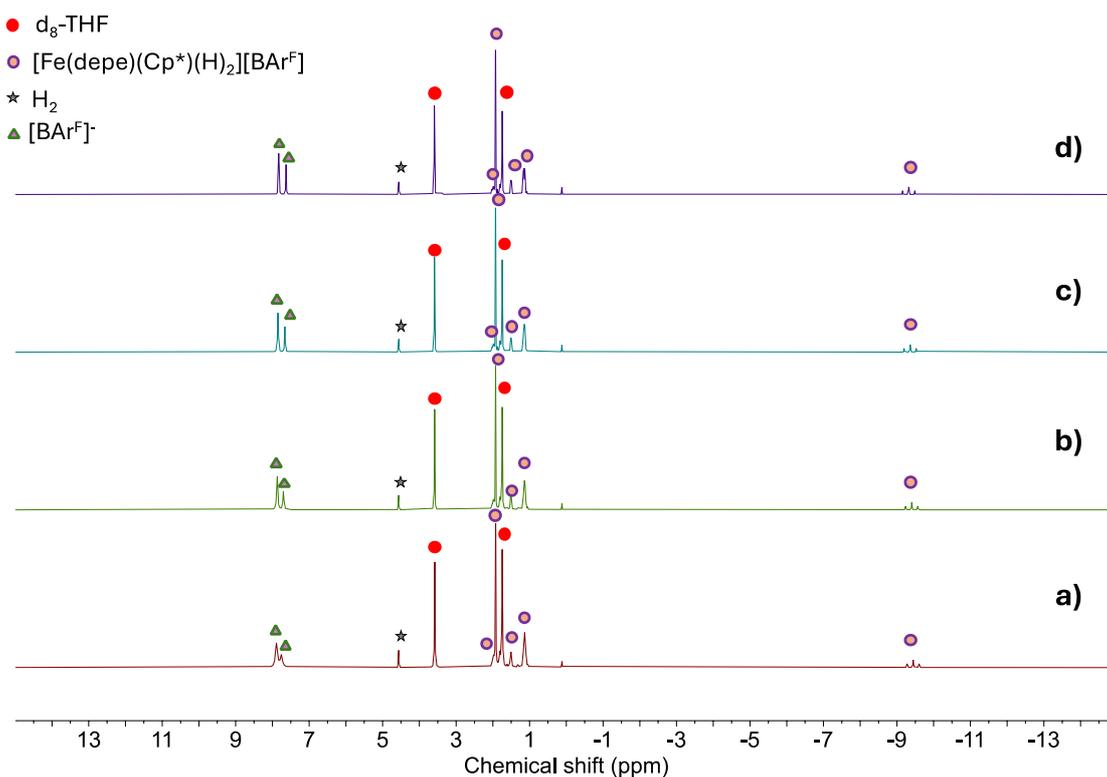


Figure S19: Variable temperature ^1H NMR spectrum (400 MHz, d_8 -THF) of the reaction mixture obtained after addition of 1 bar of H_2 to a d_8 -THF solution of **2** a) at 193 K, b) at 213 K, c) at 233 K, and d) at 253 K.

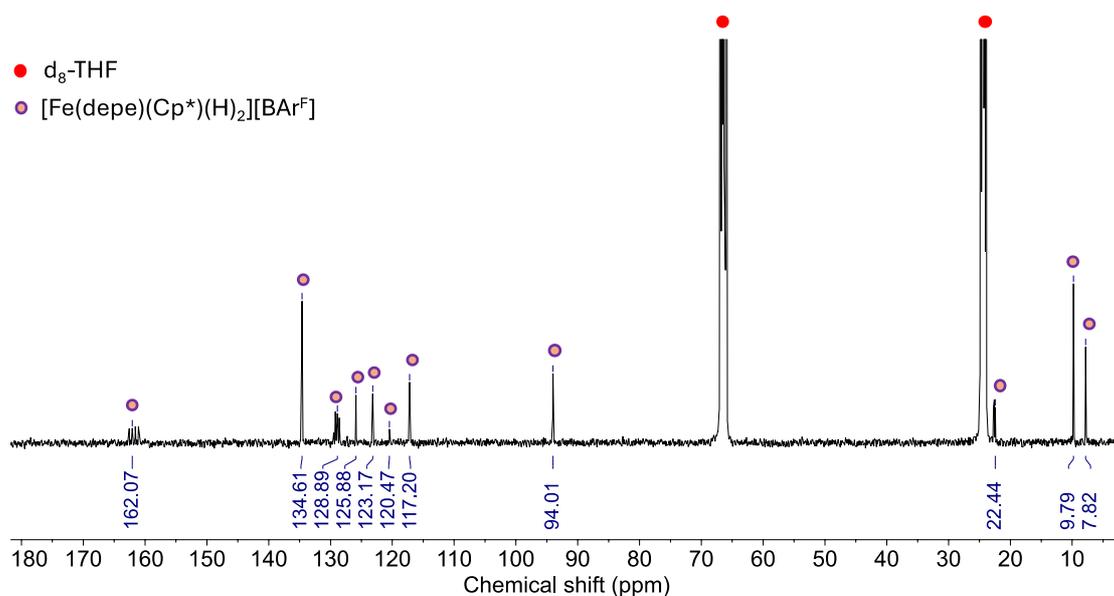


Figure S20: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (100 MHz, d_8 -THF, 298 K) of the reaction mixture obtained after addition of 1 bar of H_2 to a d_8 -THF solution of **2**.

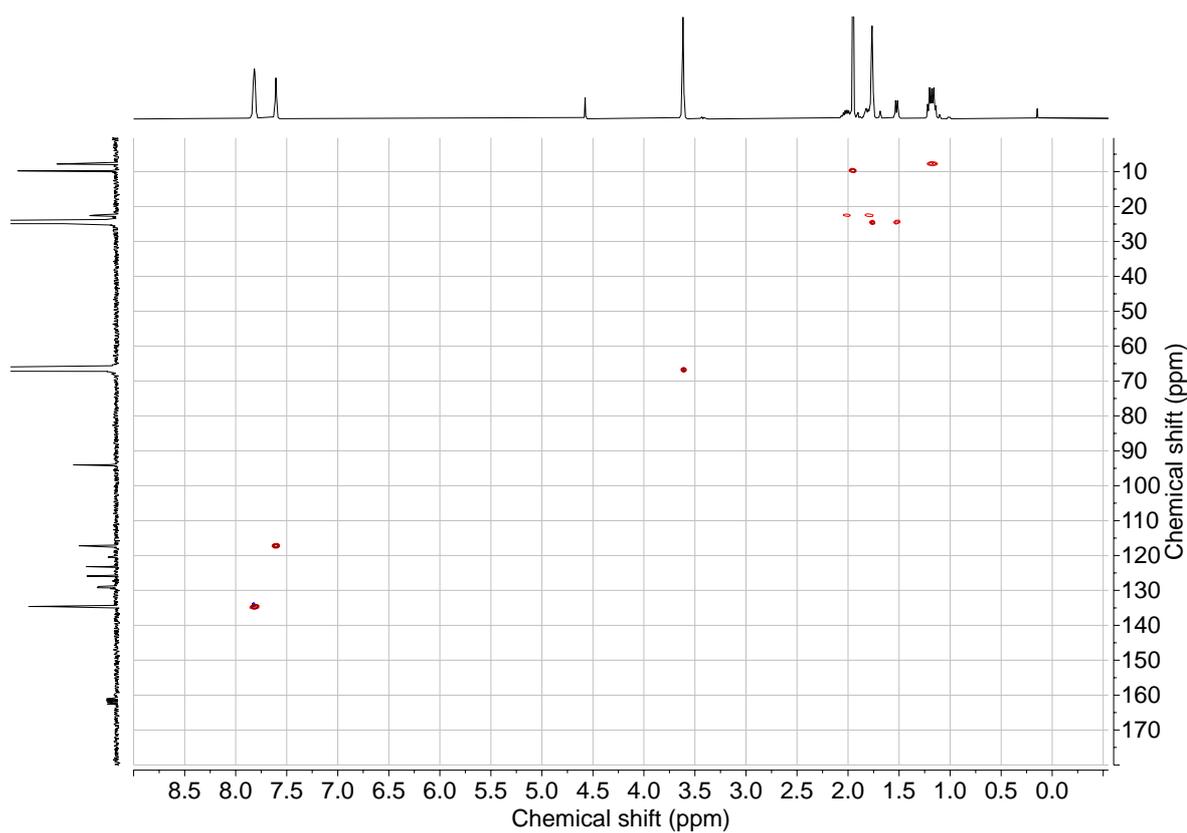


Figure S21: ^1H - ^{13}C HSQC NMR spectrum (d_8 -THF, 298 K) of the reaction mixture obtained after addition of 1 bar of H_2 to a d_8 -THF solution of **2**.

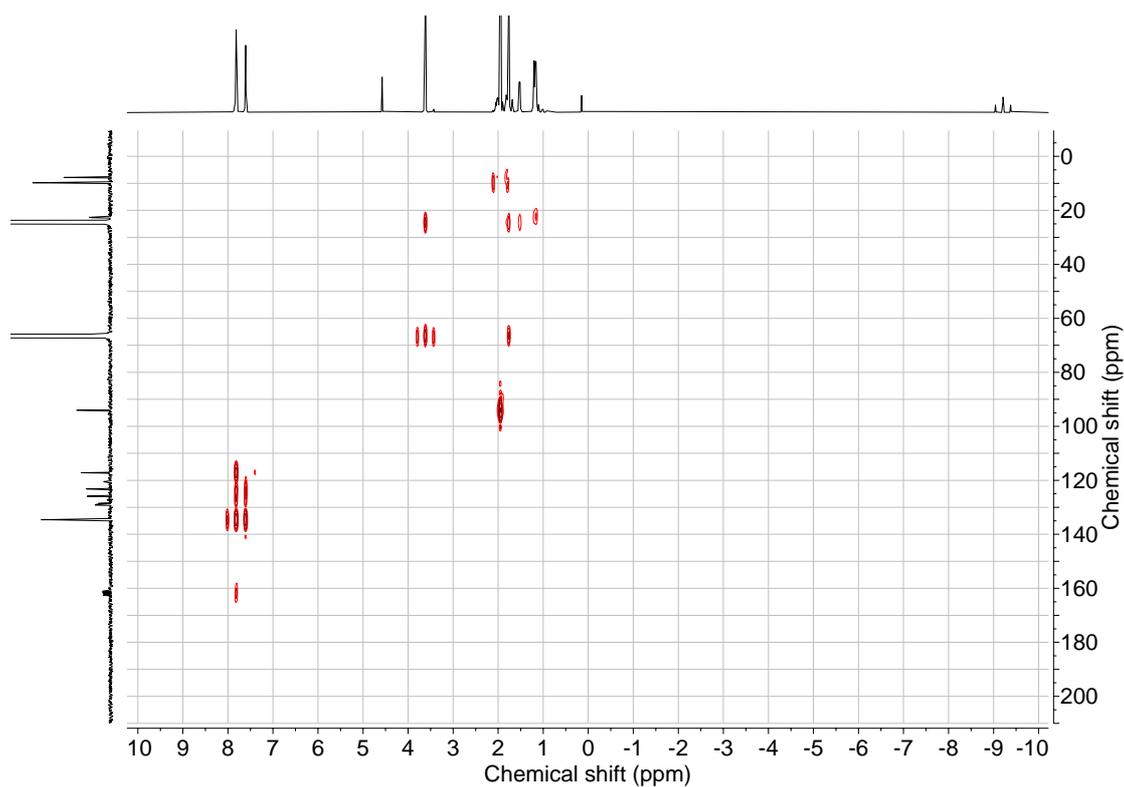


Figure S22: ^1H - ^{13}C HMBC NMR spectrum (d_8 -THF, 298 K) of the reaction mixture obtained after addition of 1 bar of H_2 to a d_8 -THF solution of **2**.

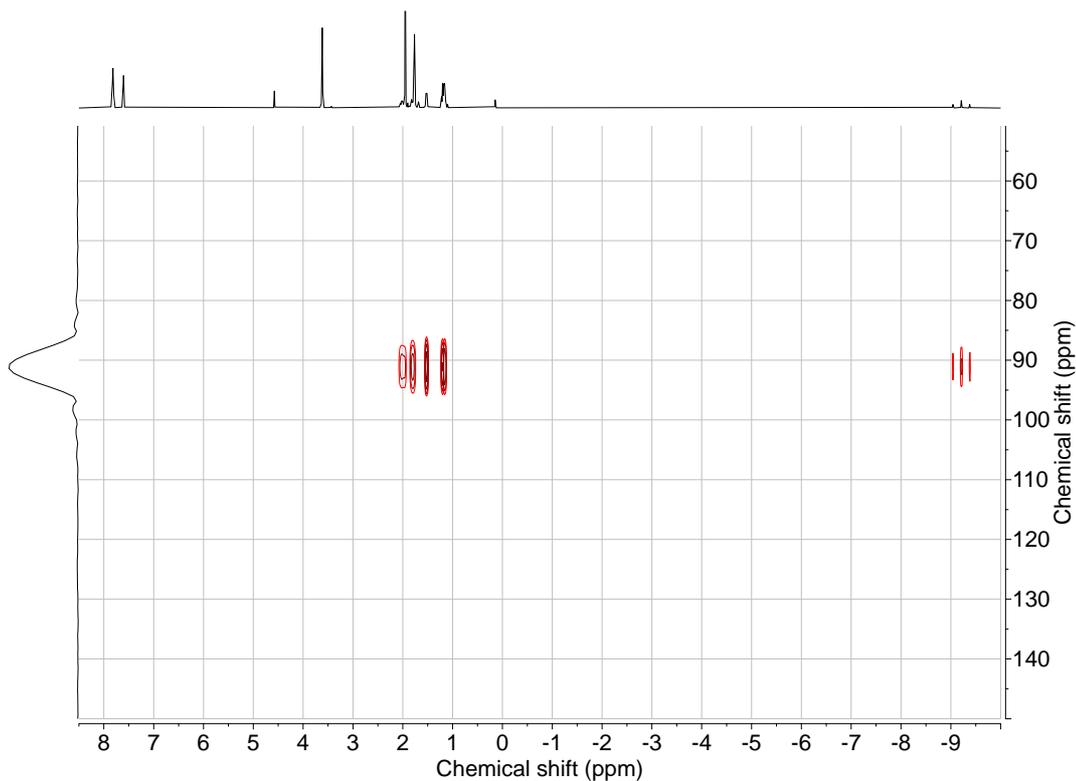


Figure S23: ^1H - ^{31}P HMBC NMR spectrum (d_8 -THF, 298 K) of the reaction mixture obtained after addition of 1 bar of H_2 to a d_8 -THF solution of **2**.



Figure S24: ^1H - ^1H NOESY NMR spectrum (d_8 -THF, 298 K) of the reaction mixture obtained after addition of 1 bar of H_2 to a d_8 -THF solution of **2**.

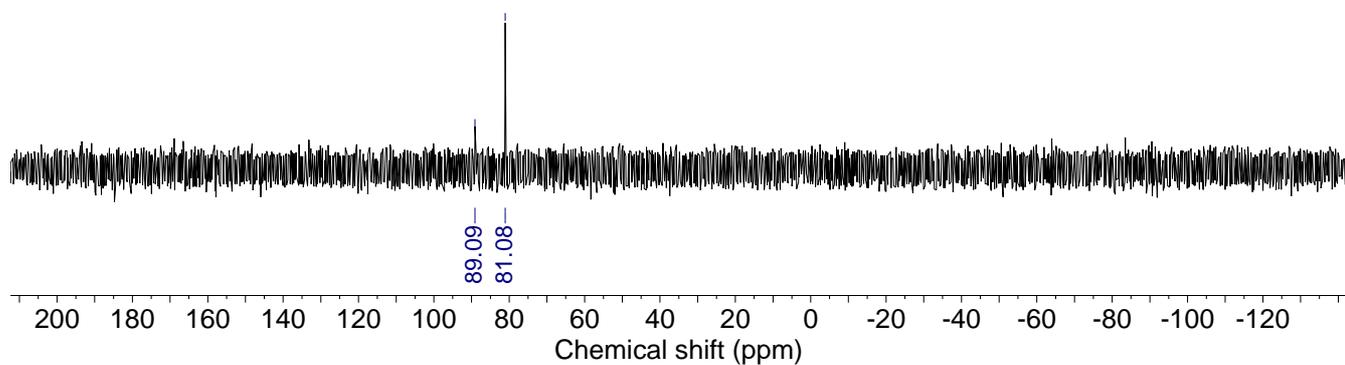


Figure S25: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (121.50 MHz, C_6D_6 , 298 K) of the reaction mixture obtained after addition of 7 equiv. of $\text{C}_6\text{H}_5\text{NO}_2$ to a C_6D_6 solution of **2** and warming up for 24 h at 50°C .

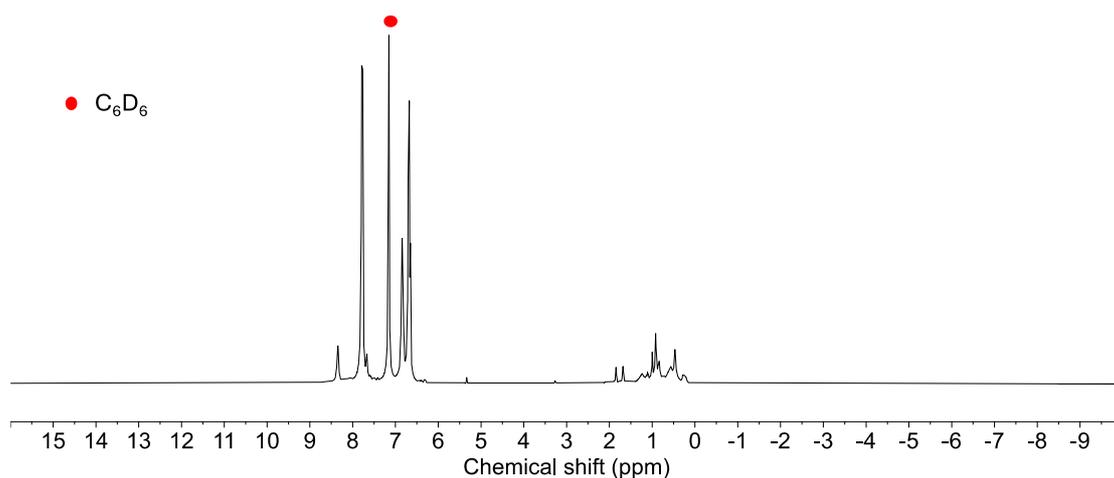


Figure S26: ^1H NMR spectrum (300 MHz, C_6D_6 , 298 K) of the reaction mixture obtained after addition of 7 equiv. of $\text{C}_6\text{H}_5\text{NO}_2$ to a C_6D_6 solution of **2** and warming up for 24 h at 50°C .

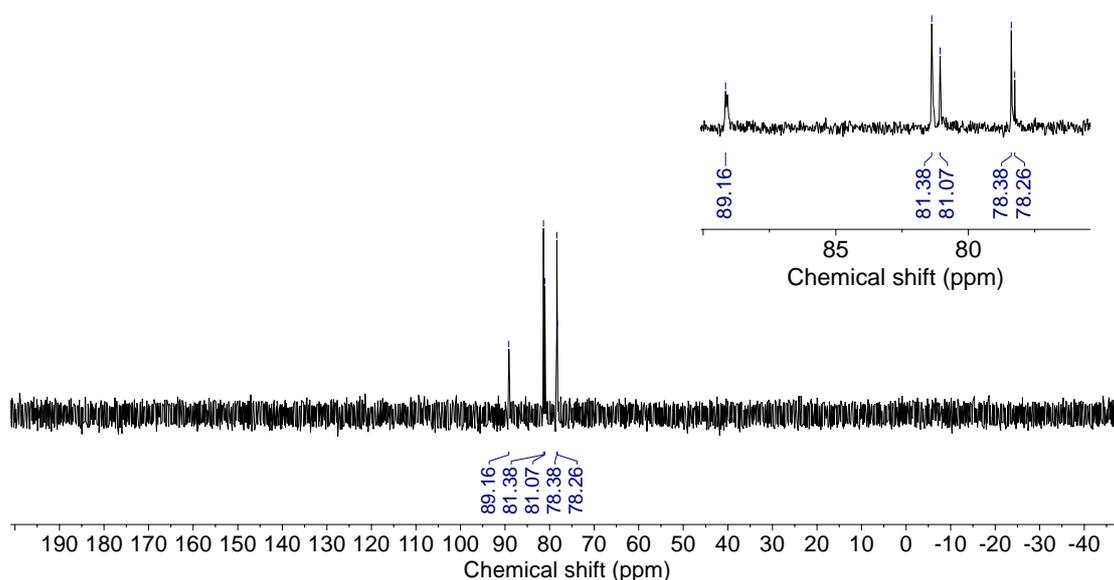


Figure S27: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (121.50 MHz, C_6D_6 , 298 K) of the reaction mixture obtained after addition of 1.5 equiv. of $\text{C}_6\text{H}_5\text{NO}$ to a C_6D_6 solution of **2** at 25°C .

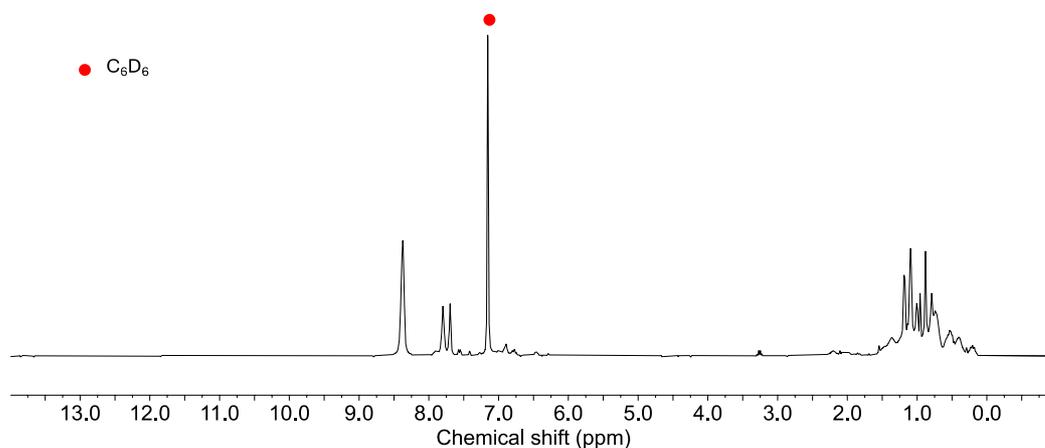


Figure S28: ^1H NMR spectrum (300 MHz, C_6D_6 , 298 K) of the reaction mixture obtained after addition of 1.5 equiv. of $\text{C}_6\text{H}_5\text{NO}$ to a C_6D_6 solution of **2** at 25°C .

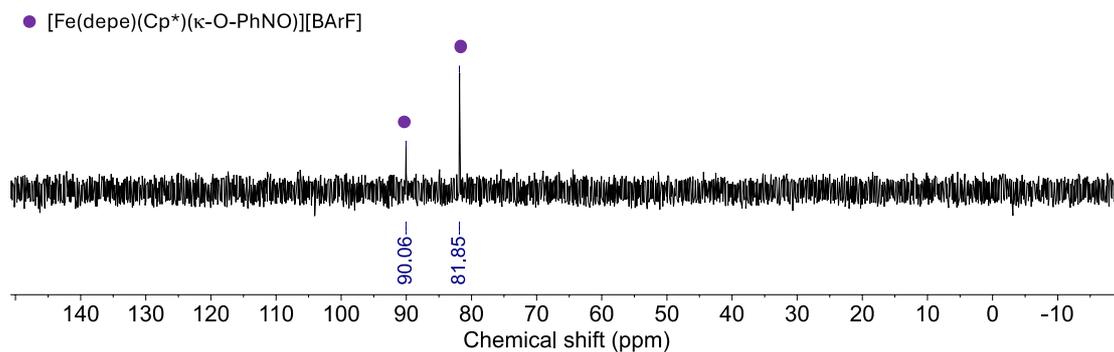


Figure S29: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (121.50 MHz, d_8 -THF, 298 K) of crystals of [Fe(depe)(Cp*)(κ^1 O-PhNO)][BAR^F] at 25°C.

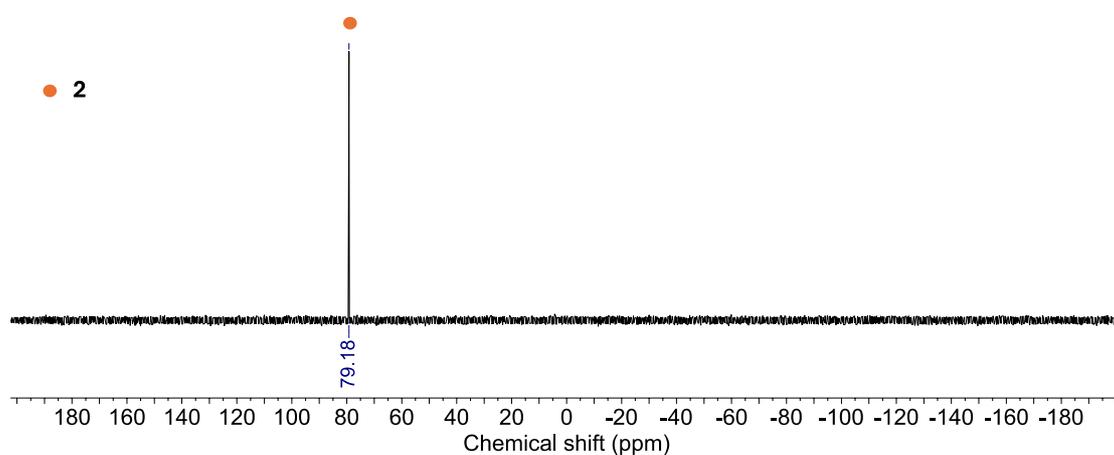


Figure S30: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (202.46 MHz, THF, 298 K) of the reaction mixture obtained after addition of 20 equiv. of HBPin to a THF solution of **2** at 25°C.

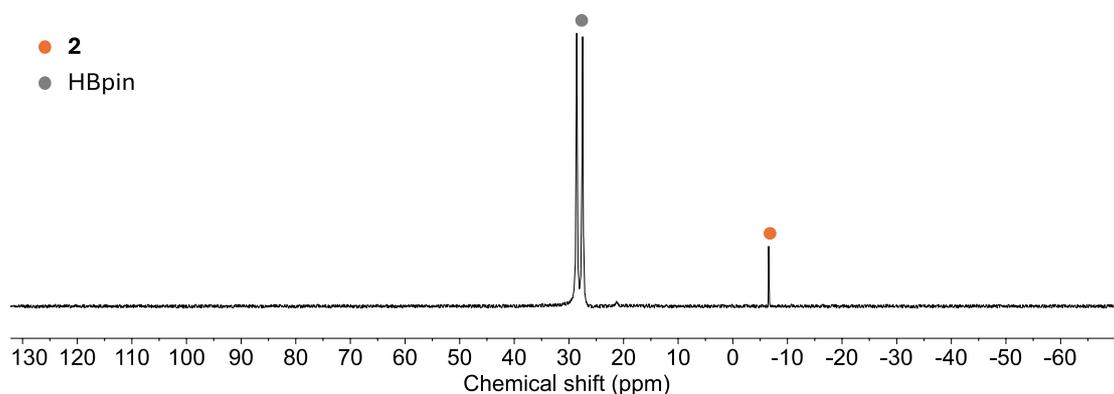


Figure S31: ^{11}B NMR spectrum (160.46 MHz, THF, 298 K) of the reaction mixture obtained after addition of 20 equiv. of HBPin to a THF solution of **2** at 25°C.

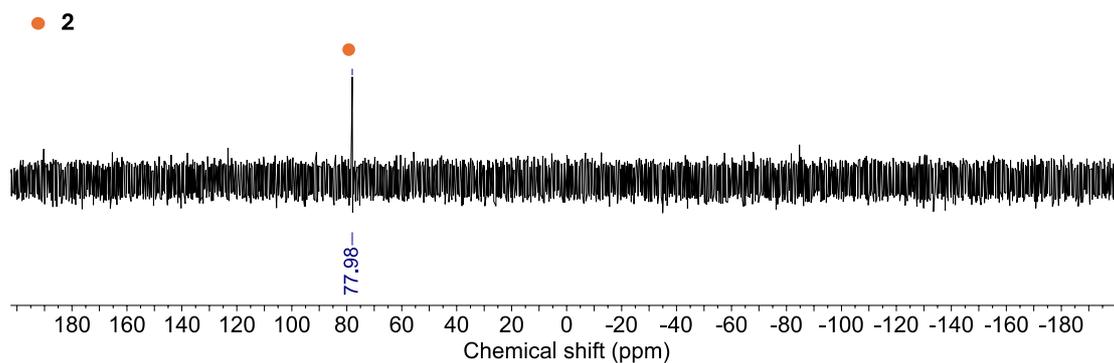


Figure S32: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (202.46 MHz, Toluene, 298 K) of the reaction mixture obtained after addition of 20 equiv. of HBPin to a toluene solution of **2** at 25°C.

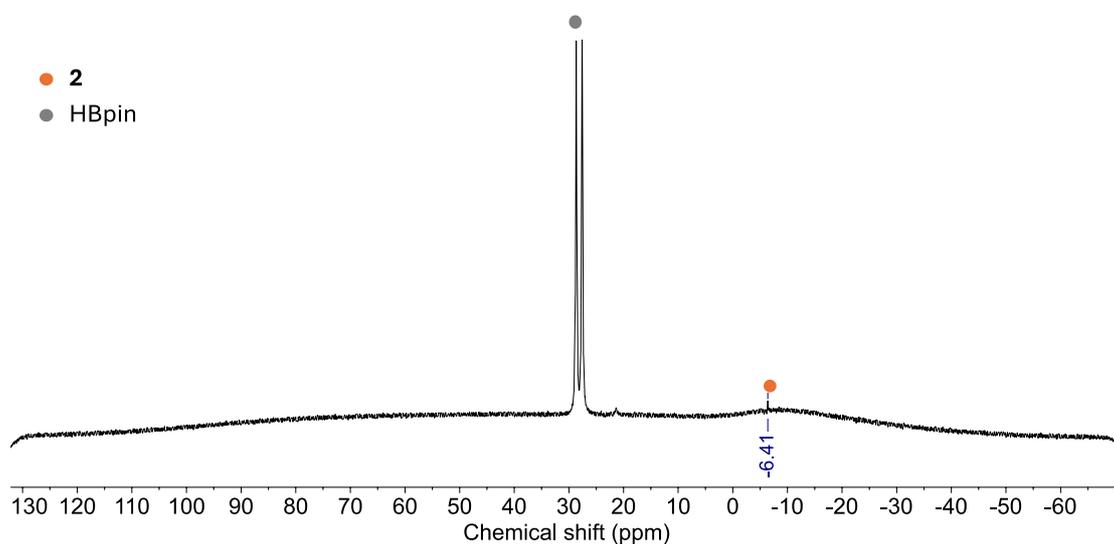


Figure S33: ^{11}B NMR spectrum (160.46 MHz, Toluene, 298 K) of the reaction mixture obtained after addition of 20 equiv. of HBPin to a toluene solution of **2** at 25°C.

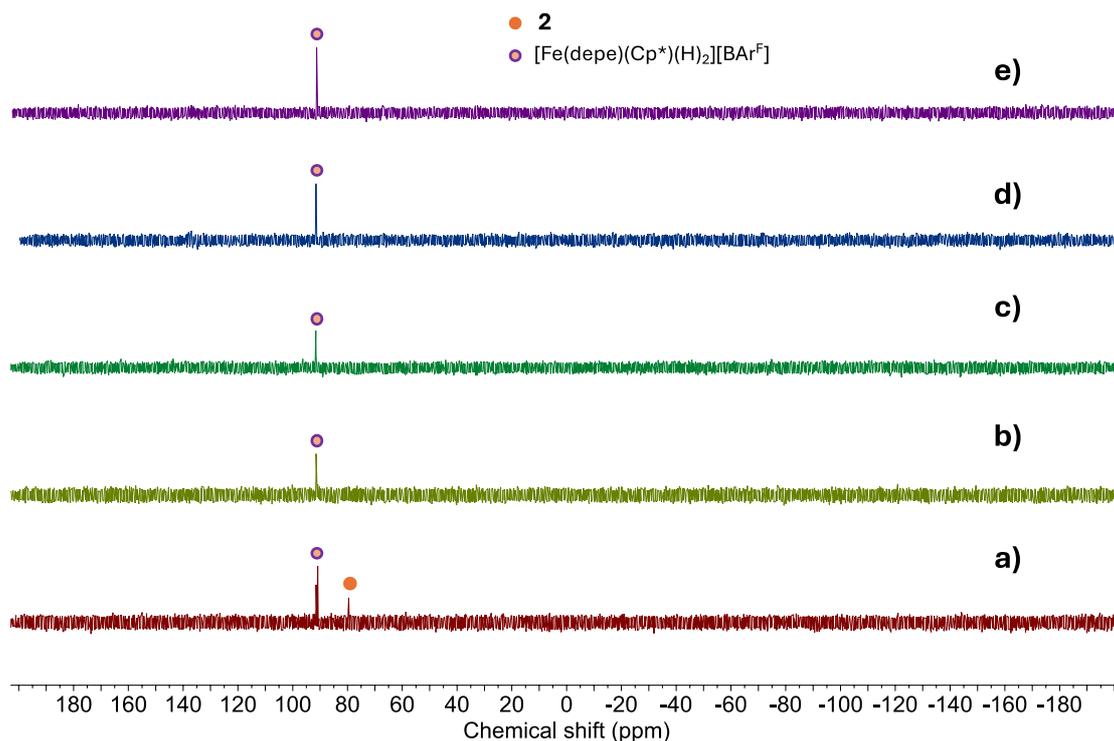


Figure S34: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (161.98 MHz, THF, 298 K) monitoring of the reaction mixture obtained by adding 1 bar of N_2O to a mixture of **2** and 20 equiv. of HBPIn in THF solution a) 15 min after, b) 1.5 h after c) 4 h after and, d) 17 h after and, e) 20 h after.

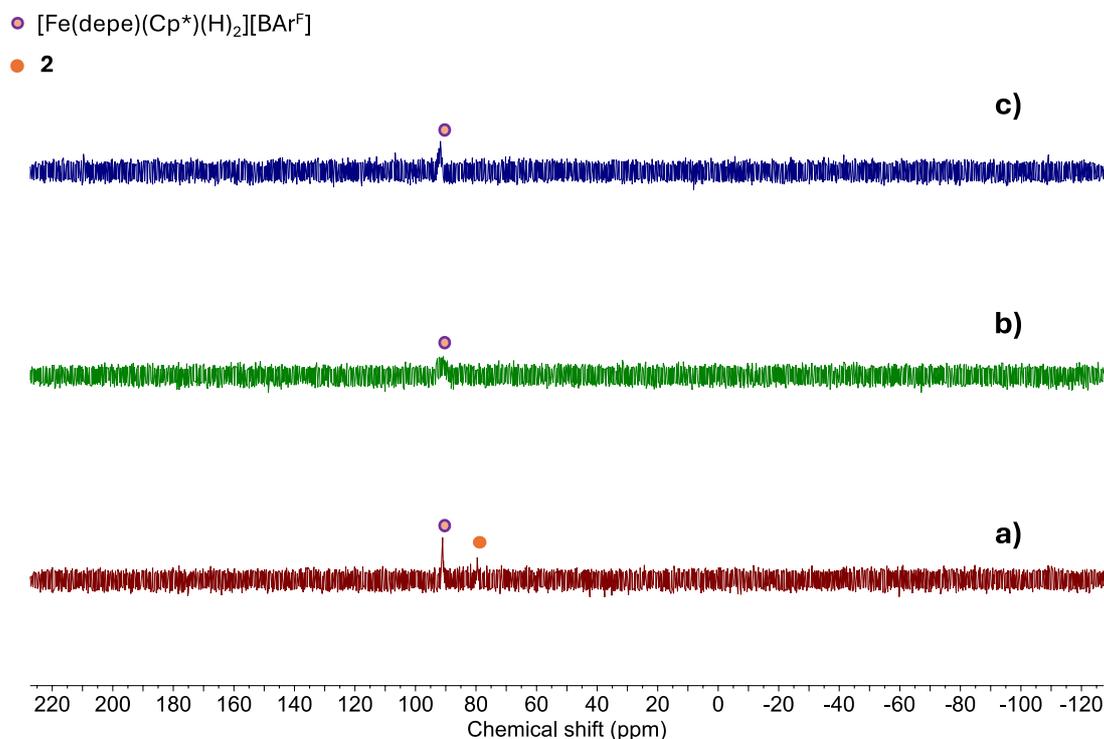


Figure S35: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (121.50 MHz, Et_2O , 298 K) monitoring of the reaction mixture obtained by adding 1 bar of N_2O to a mixture of **2** and 10 equiv. of HBPIn in THF solution a) 15 min after, b) 3 h after and, c) 19 h after.

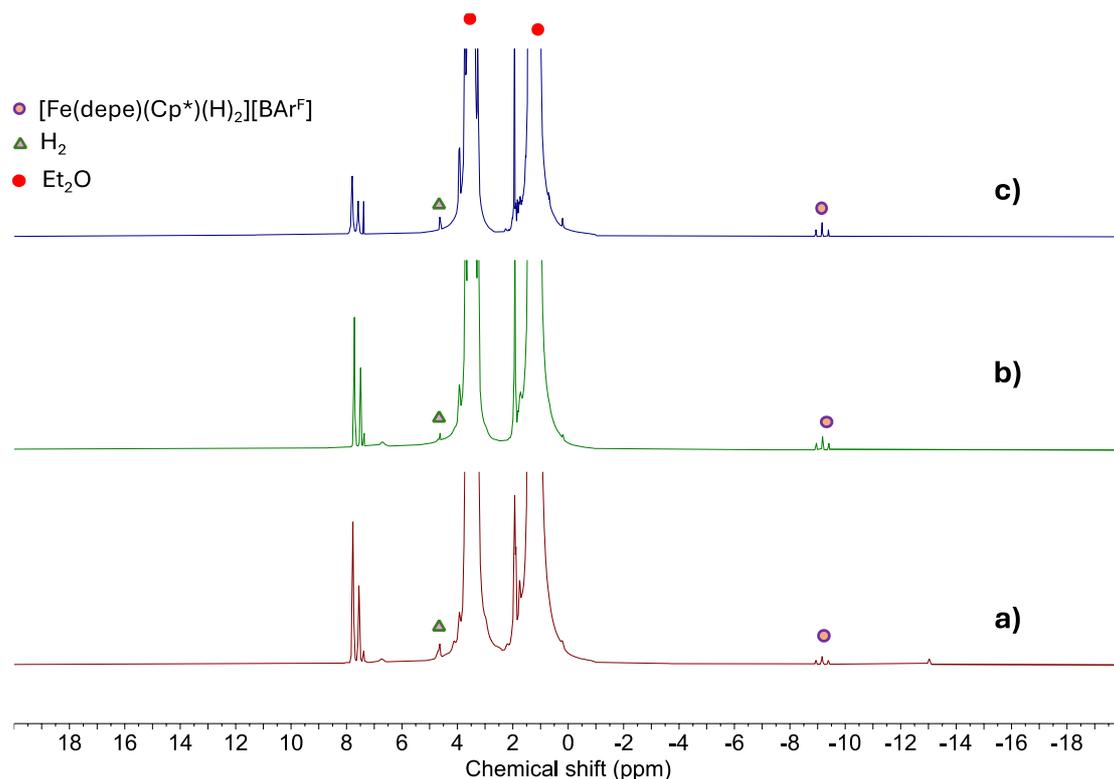


Figure S36: ¹H NMR spectrum (300 MHz, Et₂O, 298 K) monitoring of the reaction mixture obtained by adding 1 bar of N₂O to a mixture of **2** and 10 equiv. of HBPin in THF solution a) 15 min after, b) 3 h after and, c) 19 h after.

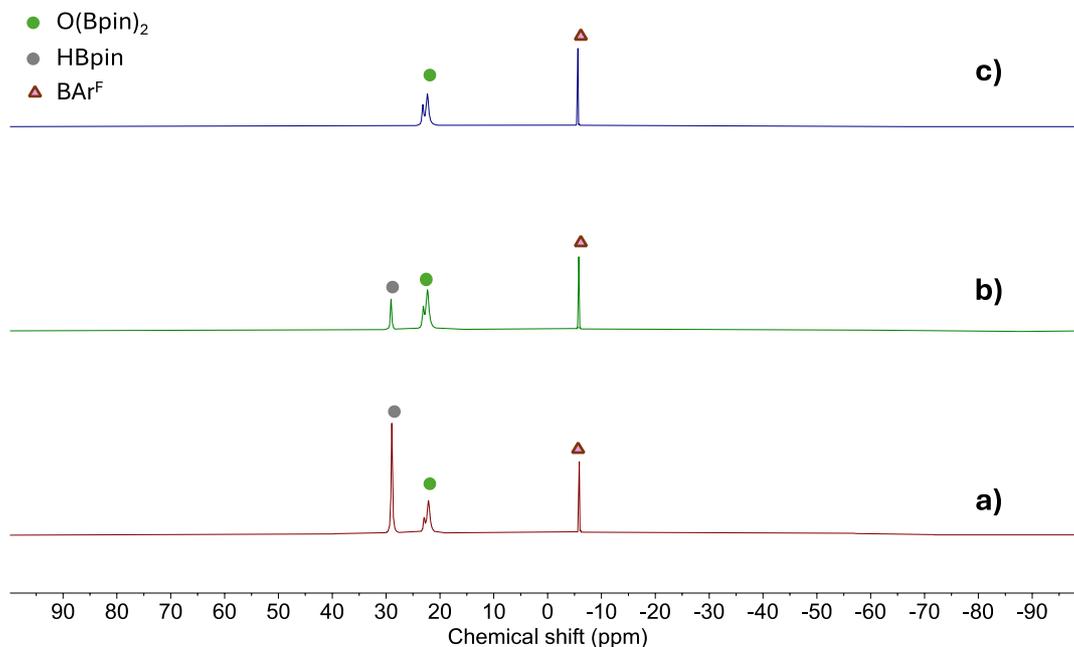


Figure S37: ¹¹B{¹H} NMR spectrum (96.29 MHz, Et₂O, 298 K) monitoring of the reaction mixture obtained by adding 1 bar of N₂O to a mixture of **2** and 10 equiv. of HBPin in THF solution a) 15 min after, b) 3 h after and, c) 19 h after.

● 2

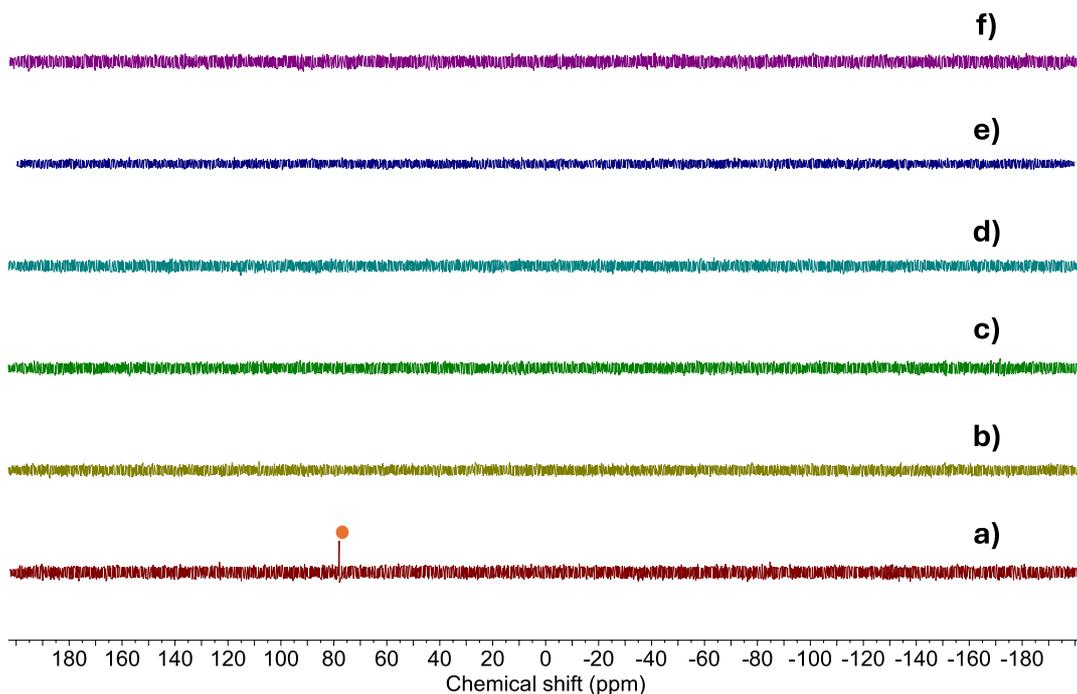


Figure S38: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (161.98 MHz, Toluene, 298 K) monitoring of the reaction mixture obtained by adding 1 bar of N_2O to a mixture of **2** and 20 equiv. of HBPin in toluene suspension a) before N_2O , b) 15 min after, c) 1.5 h after, d) 4 h after, e) 17 h after, and f) 20 h after.

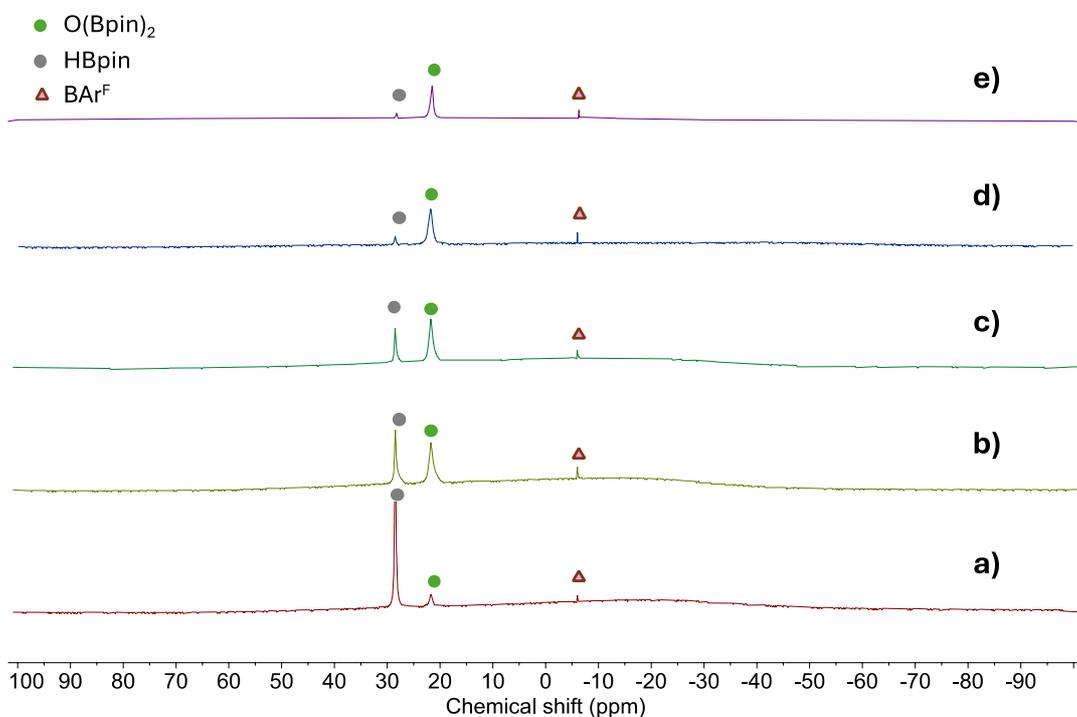


Figure S39: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (161.98 MHz, Toluene, 298 K) monitoring of the reaction mixture obtained by adding 1 bar of N_2O to a mixture of **2** and 20 equiv. of HBPin in toluene suspension a) 15 min after, b) 1.5 h after, c) 4 h after, d) 17 h after, and e) 20 h after.

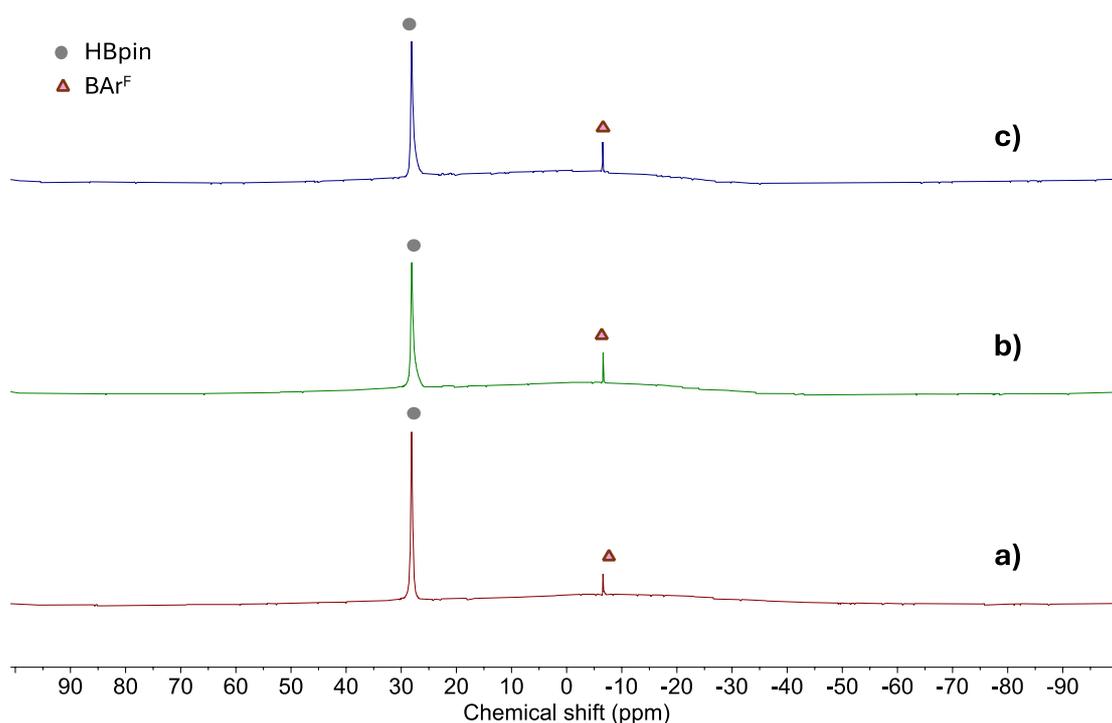


Figure S40: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (161.98 MHz, CH_2Cl_2 , 298 K) monitoring of the reaction mixture obtained by adding 1 bar of N_2O to a mixture of **2** and 20 equiv. of HBPin in dichloromethane solution a) 15 min after, b) 1.5 h after, and c) 4 h after.

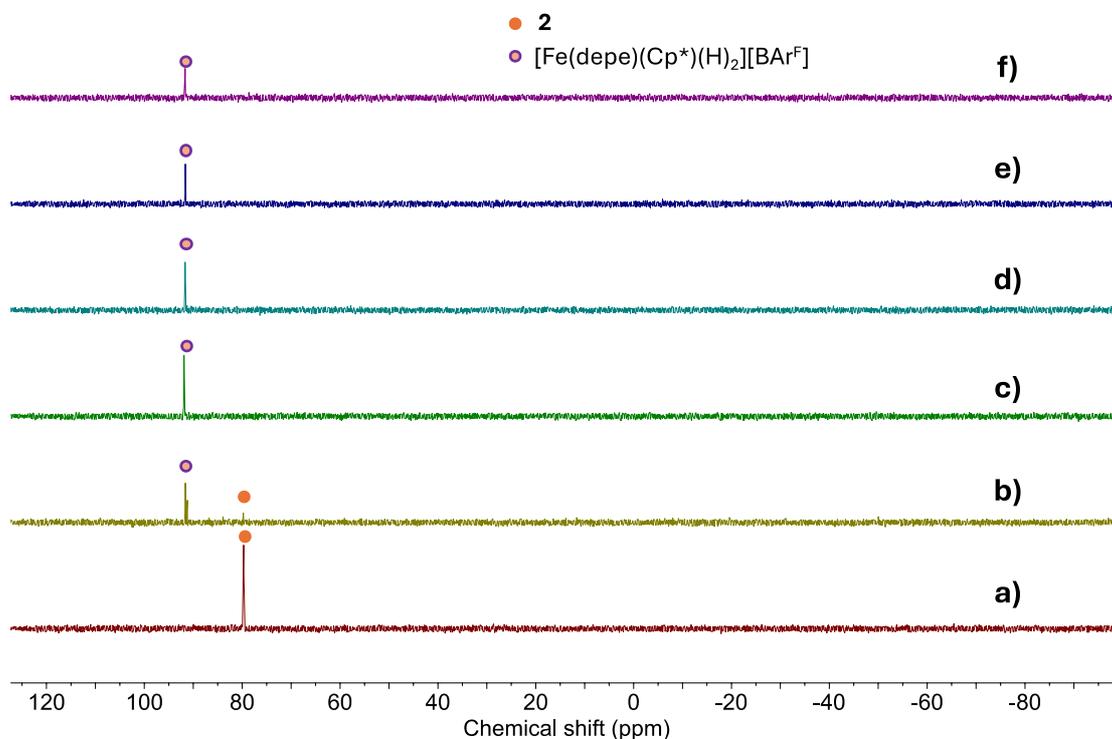


Figure S41: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (121.50 MHz, Et_2O , 298 K) monitoring of the reaction mixture obtained by adding 1 bar of N_2O to a mixture of **2** and 34 equiv. of HBPin in Et_2O suspension a) before N_2O , b) 15 min after, c) 4 h after, d) 8 h after, e) 21 h after, and f) 30 h after.

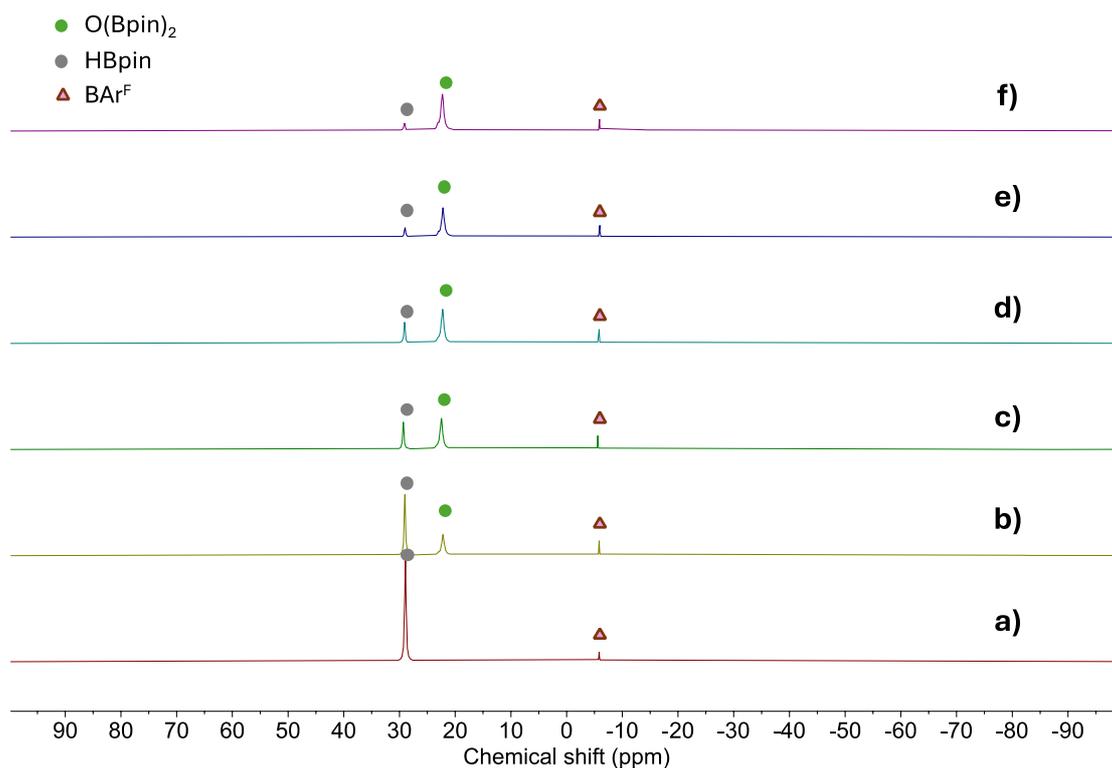


Figure S42: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (96.29 MHz, Et_2O , 298 K) monitoring of the reaction mixture obtained by adding 1 bar of N_2O to a mixture of **2** and 34 equiv. of HBPin in Et_2O solution a) before N_2O , b) 15 min after, c) 4 h after, d) 8 h after, e) 21 h after, and f) 30 h after.

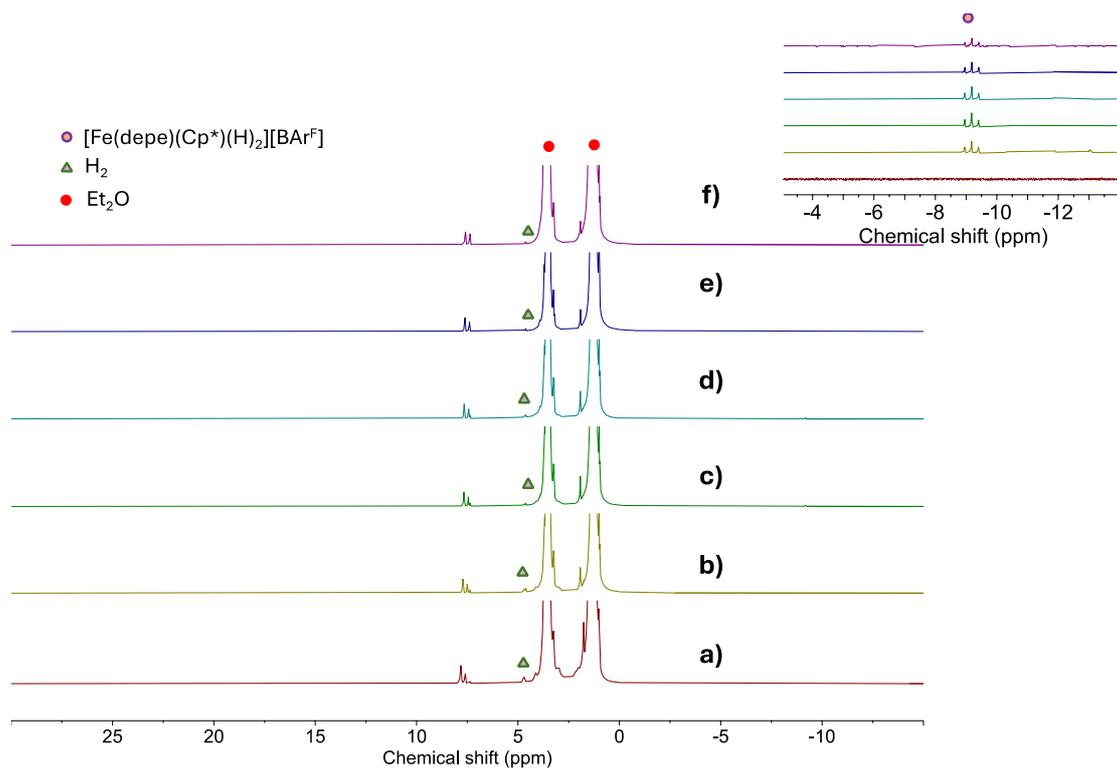


Figure S43: ¹H NMR spectrum (300 MHz, Et₂O, 298 K) monitoring of the reaction mixture obtained by adding 1 bar of N₂O to a mixture of **2** and 34 equiv. of HBPIn in Et₂O solution a) before N₂O, b) 15 min after, c) 4 h after, d) 8 h after, e) 21 h after, and f) 30 h after.

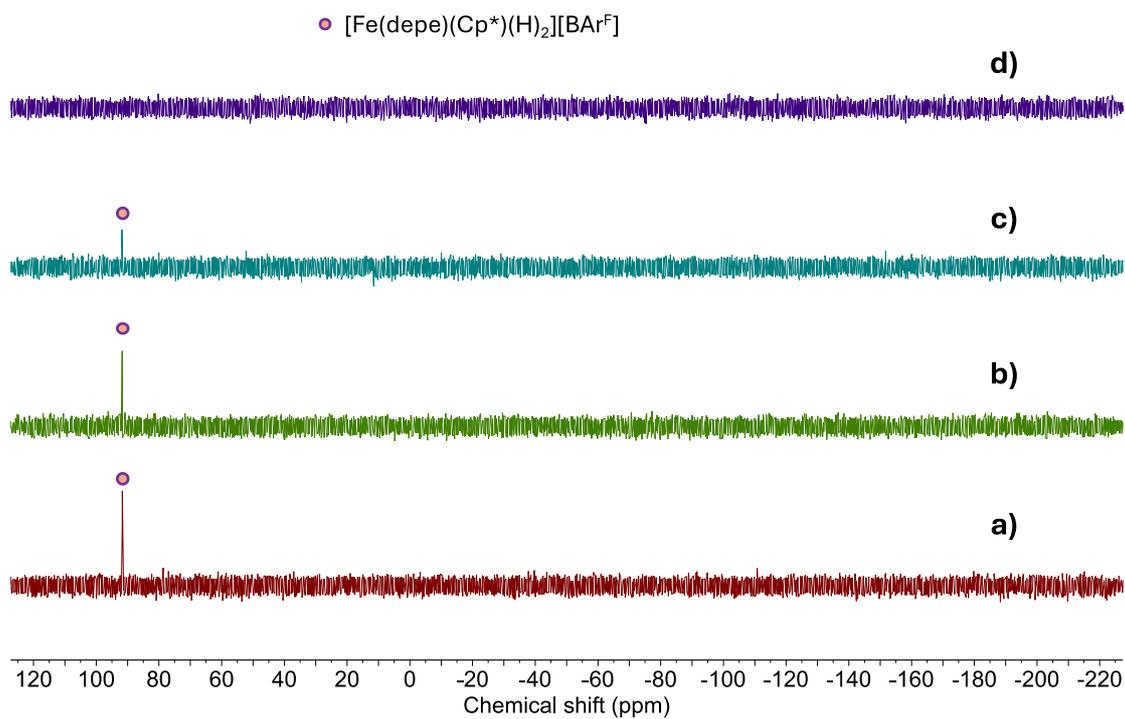


Figure S44: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (121.50 MHz, Et_2O , 298 K) monitoring of the reaction mixture obtained a) before, b) 1 h after, c) 16 h after, and d) 19 h after re-addition of 1 bar of N_2O to the previous mixture of **2** and 34 equiv. of HBPIn in Et_2O solution.

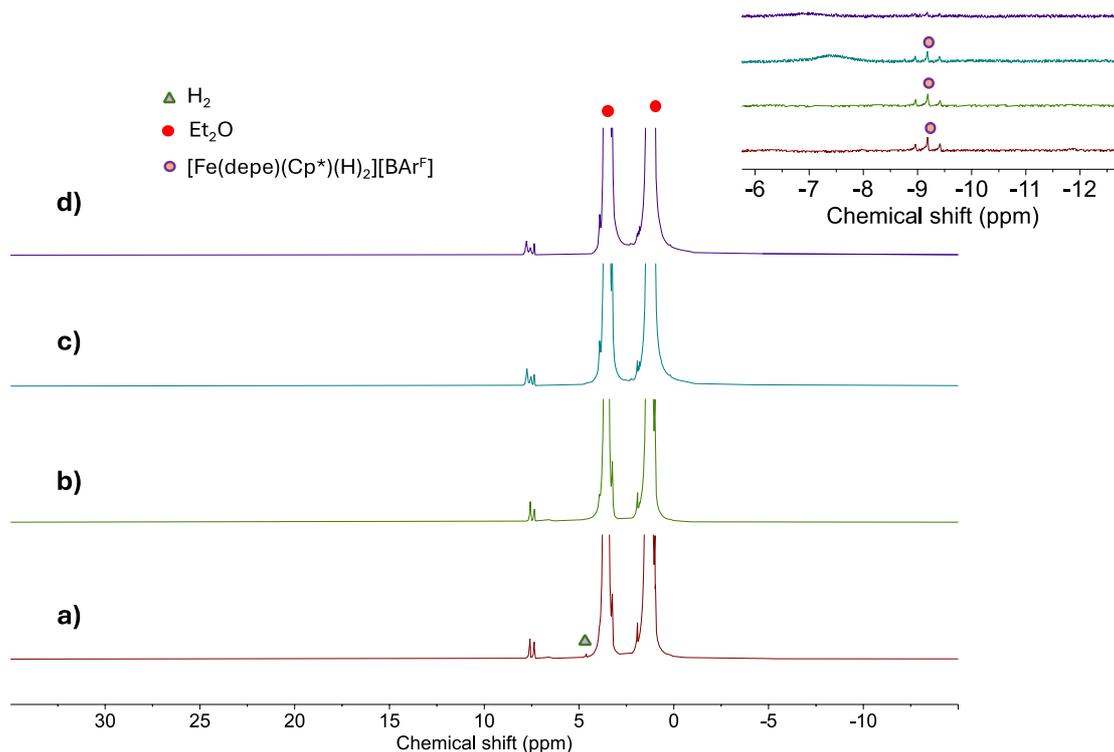


Figure S45: ^1H NMR spectrum (300 MHz, Et_2O , 298 K) monitoring of the reaction mixture obtained a) before, b) 1 h after, c) 16 h after, and d) 19 h after re-addition of 1 bar of N_2O to the previous mixture of **2** and 34 equiv. of HBPin in Et_2O solution.

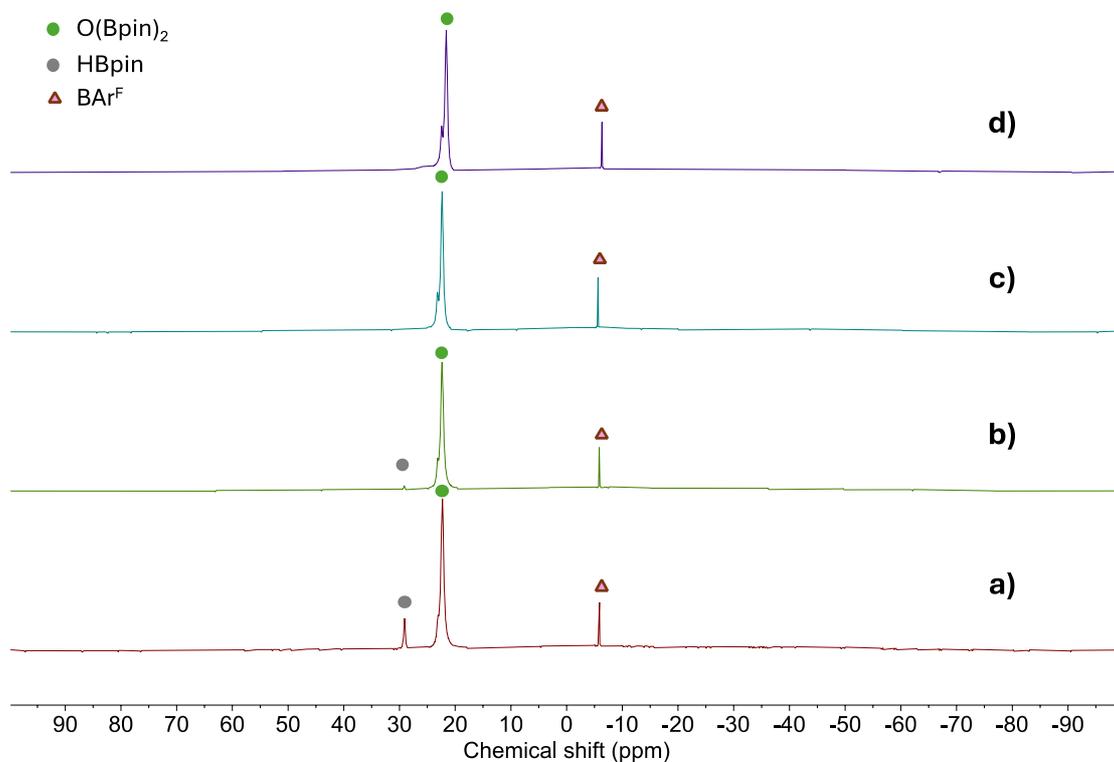


Figure S46: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (96.29 MHz, Et_2O , 298 K) monitoring of the reaction mixture obtained a) before, b) 1 h after, c) 16 h after, and d) 19 h after re-addition of 1 bar of N_2O to the previous mixture of **2** and 34 equiv. of HBPin in Et_2O solution.

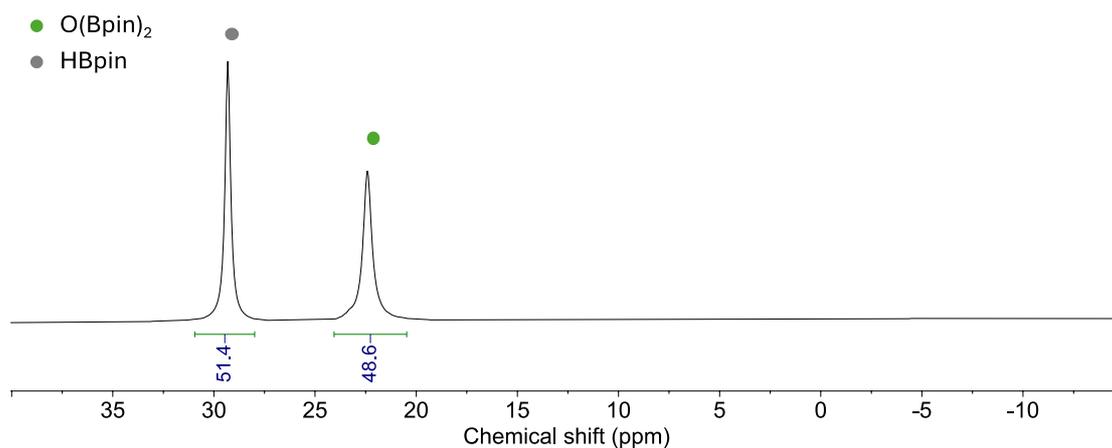


Figure S47: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (128.38 MHz, Et_2O , 298 K) of the reaction mixture obtained after addition of 1 bar of N_2O to the mixture of **2** and 200 equiv. of HBPin in Et_2O solution and reacting for 24 h at 25°C in a 50 mL ampoule.

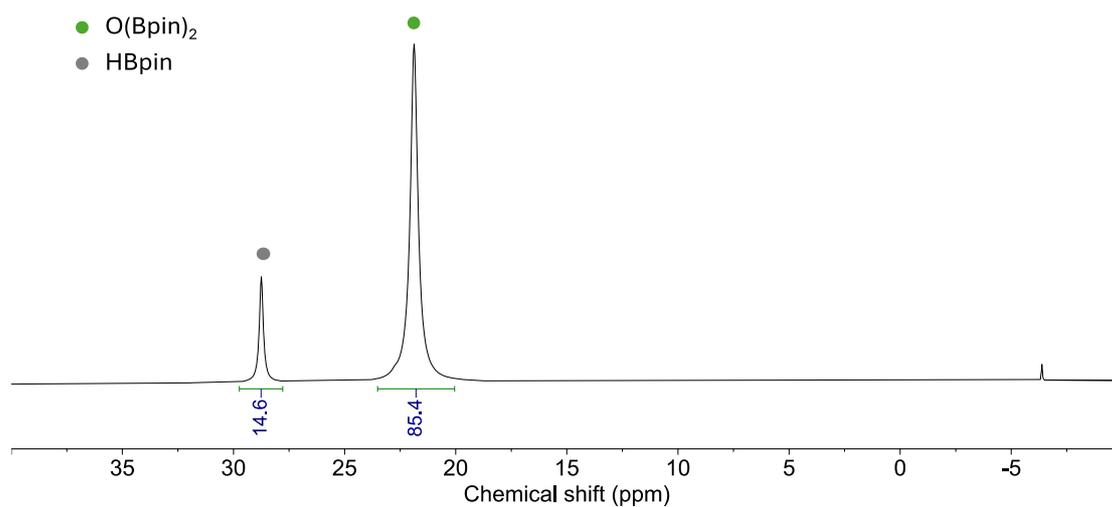


Figure S48: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (128.38 MHz, Et_2O , 298 K) of the reaction mixture obtained after addition of 1 bar of N_2O to the mixture of **2** and 200 equiv. of HBPin in Et_2O solution and reacting for 24 h at 50°C in a 50 mL ampoule.

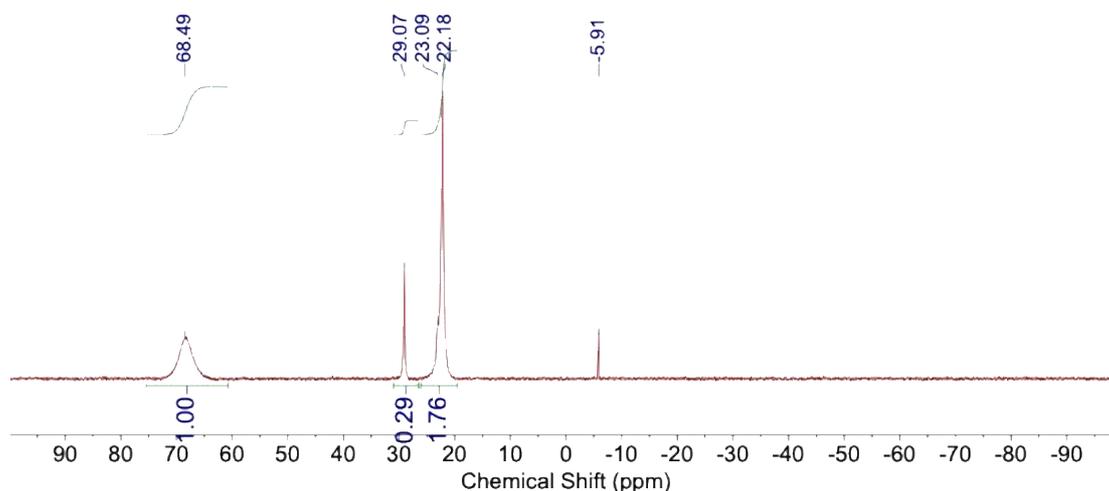


Figure S49: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (96.29 MHz, Et_2O , 298 K) of the reaction mixture obtained after addition of 1 bar of N_2O to mixture of **2** and 200 equiv. of HBPin in Et_2O solution and reacting for 24 h at 50°C in a 50 mL ampoule, with BPh_3 (20 mg, 0.083 mmol, 75 equiv.) as internal standard.

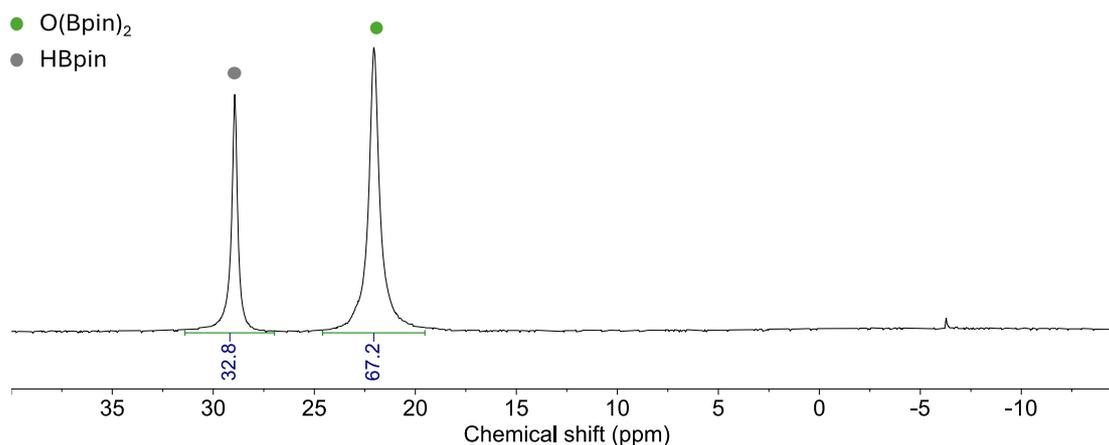


Figure S50: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (96.29 MHz, Et_2O , 298 K) of the reaction mixture obtained after addition of 1 bar of N_2O to mixture of **2** and 200 equiv. of HBPin in Et_2O solution and reacting for 24 h at 80°C in a 50 mL ampoule.

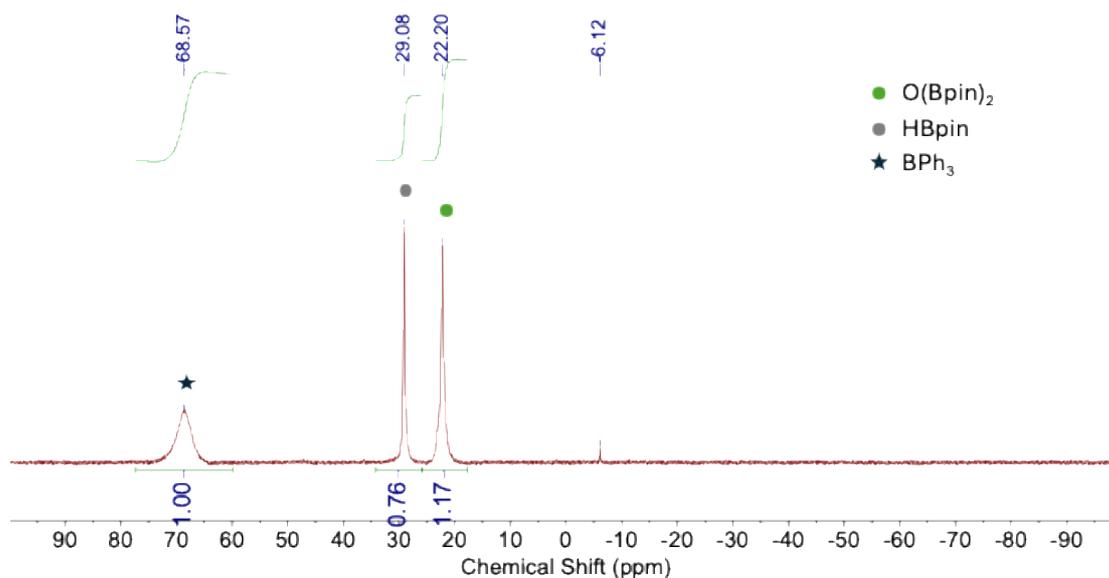


Figure S51: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (96.29 MHz, Et_2O , 298 K) of the reaction mixture obtained after addition of 1 bar of N_2O to mixture of **2** and 200 equiv. of HBPin in Et_2O solution and reacting for 24 h at 80°C in a 50 mL ampoule, with BPh_3 (20 mg, 0.083 mmol, 75 equiv.) as internal standard.

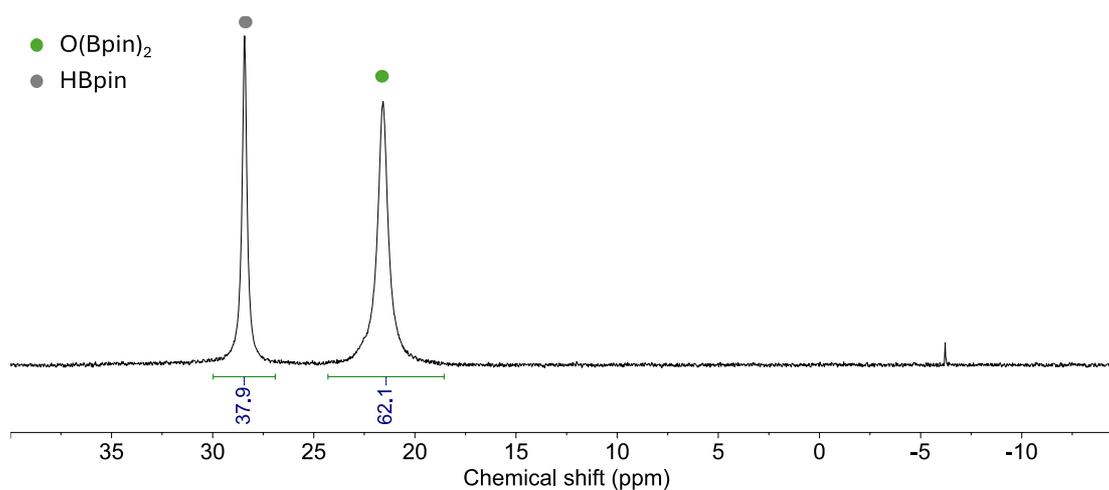


Figure S52: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (96.29 MHz, THF, 298 K) of the reaction mixture obtained after addition of 1 bar of N_2O to mixture of **2** and 200 equiv. of HBPin in THF solution and reacting for 24 h at 25°C in a 50 mL ampoule.

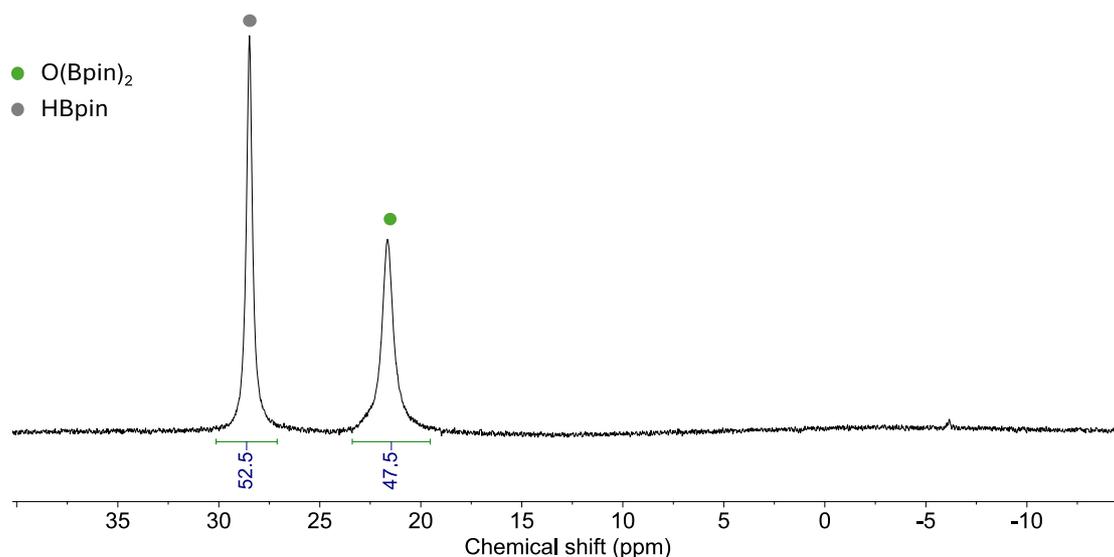


Figure S53: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (96.29 MHz, THF, 298 K) of the reaction mixture obtained after addition of 1 bar of N_2O to mixture of **2** and 200 equiv. of HBPin in THF solution and reacting for 24 h at 50°C in a 50 mL ampoule.

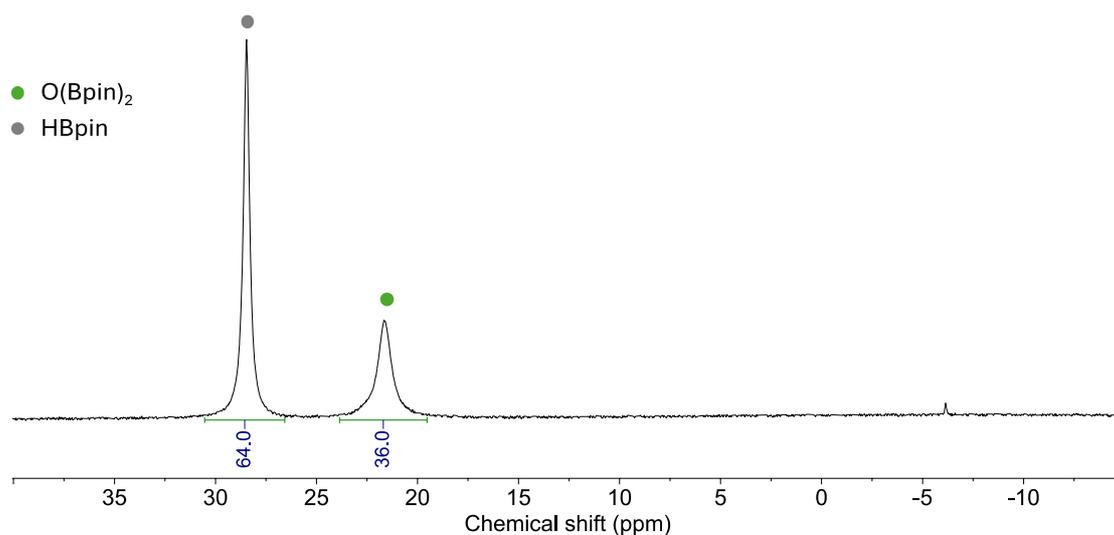


Figure S54: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (96.29 MHz, THF, 298 K) of the reaction mixture obtained after addition of 1 bar of N_2O to mixture of **2** and 200 equiv. of HBPin in THF solution and reacting for 24 h at 80°C in a 50 mL ampoule.

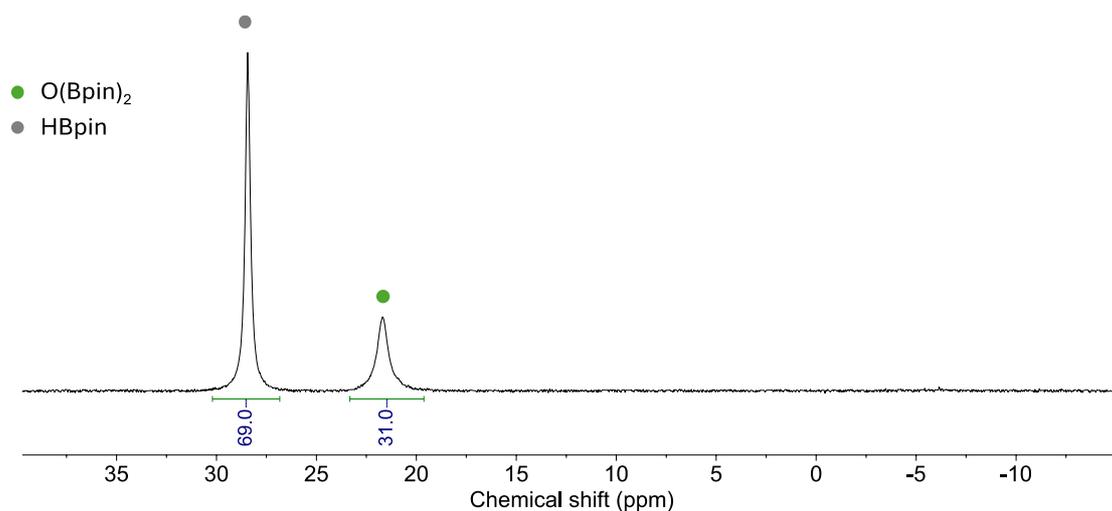


Figure S55: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (128.38 MHz, Toluene, 298 K) of the reaction mixture obtained after addition of 1 bar of N_2O to the mixture of **2** and 200 equiv. of HBPin in toluene suspension and reacting for 24 h at 50°C in a 50 mL ampoule.

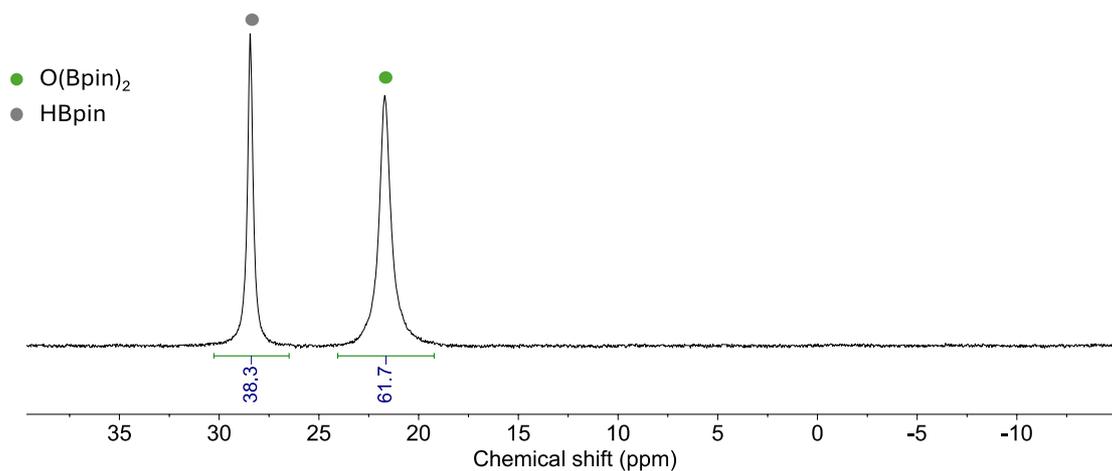


Figure S56: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (128.38 MHz, Toluene, 298 K) of the reaction mixture obtained after addition of 1 bar of N_2O to the mixture of **2** and 200 equiv. of HBPin in toluene suspension and reacting for 24 h at 80°C in a 50 mL ampoule.

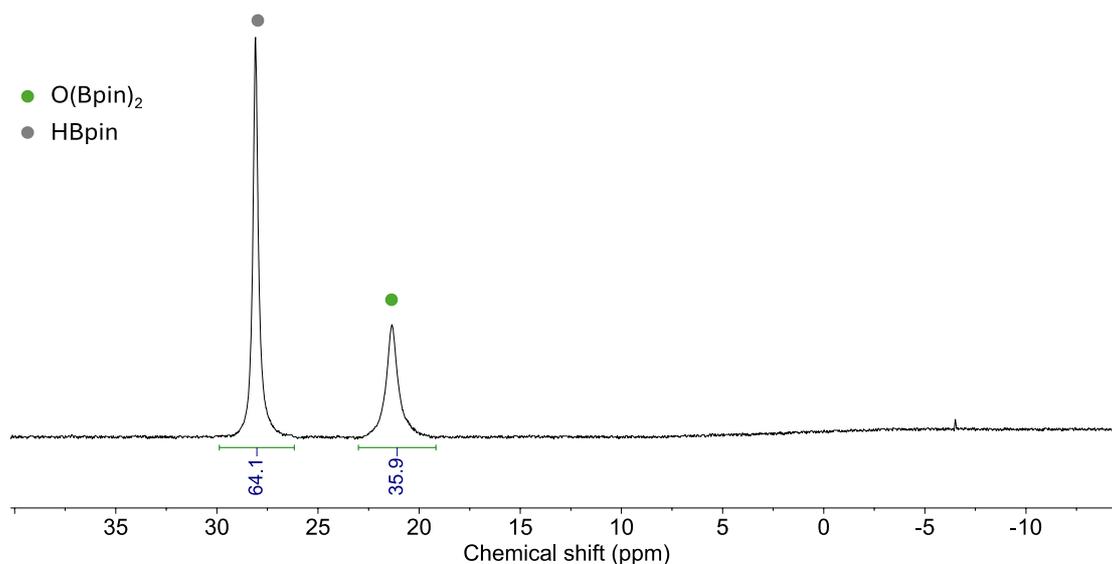


Figure S57: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (128.38 MHz, Toluene, 298 K) of the reaction mixture obtained after addition of 1 bar of N_2O to the mixture of **2** and 200 equiv. of HBPin in toluene suspension and reacting for 24 h at 100°C in a 50 mL ampoule.

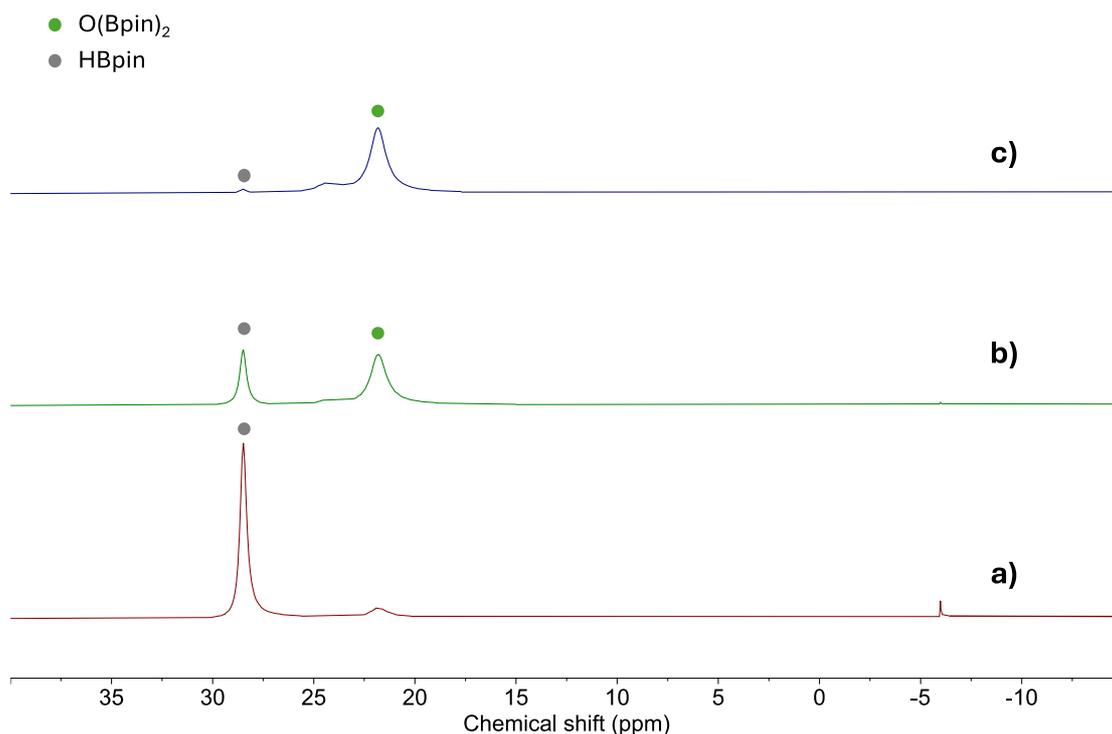


Figure S58: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (96.29 MHz, C_6D_6 , 298 K) monitoring of the reaction mixture obtained by reacting **2** with 100 equiv. of HBpin and 20 equiv. of nitrobenzene in C_6D_6 suspension at 25°C a) 15 min after, b) 20 h after, and c) 4 days after.

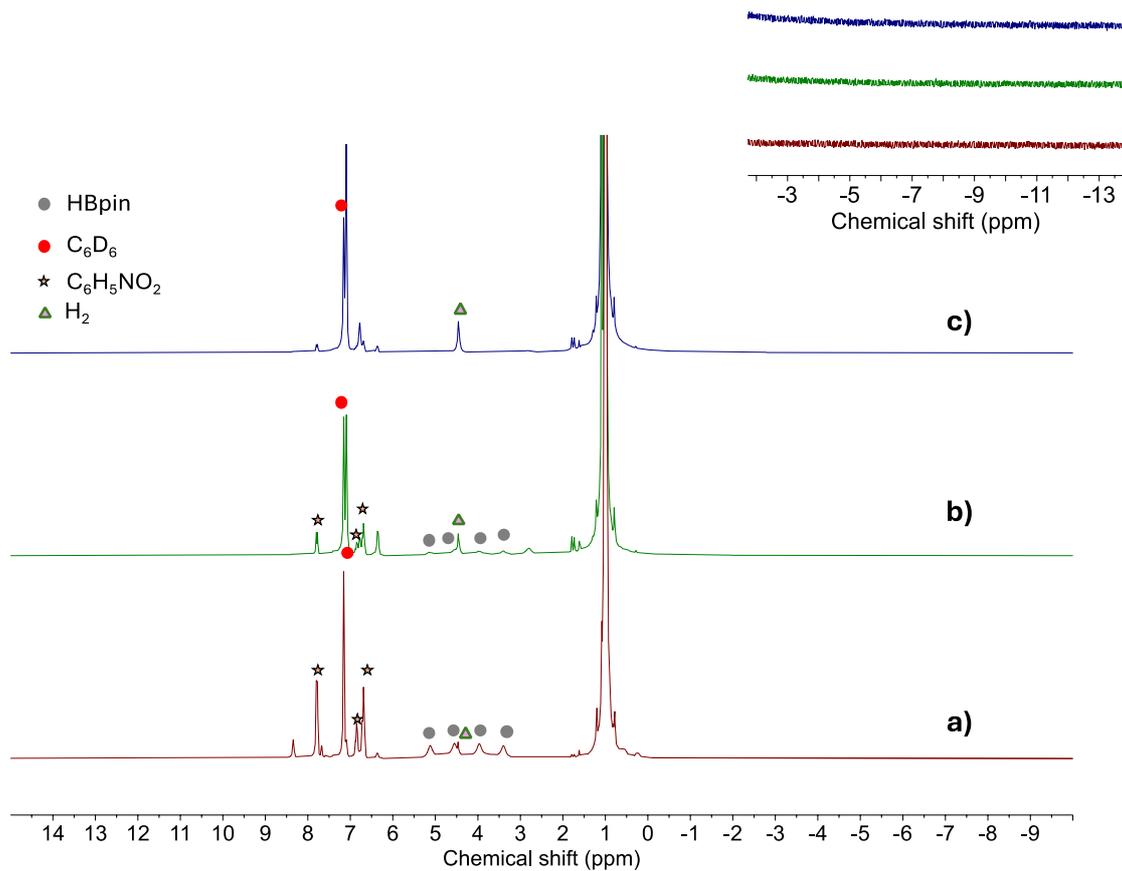


Figure S59: ¹H NMR spectrum (300 MHz, C₆D₆, 298 K) monitoring of the reaction mixture obtained by reacting **2** with 100 equiv. of HBpin and 20 equiv. of nitrobenzene in C₆D₆ suspension at 25°C a) 15 min after, b) 20 h after, and c) 4 days after.

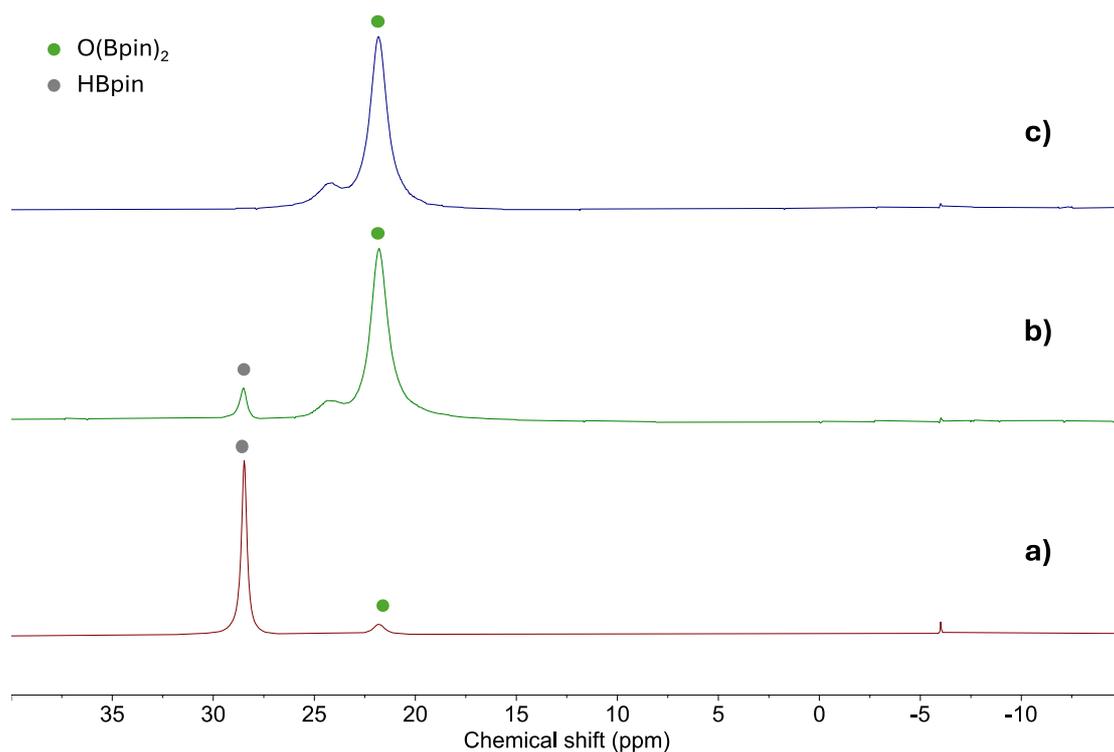


Figure S60: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (96.29 MHz, C_6D_6 , 298 K) monitoring of the reaction mixture obtained by reacting **2** with 100 equiv. of HBpin and 20 equiv. of nitrobenzene in C_6D_6 suspension at 50°C a) 15 min after, b) 2 h after, and c) 5 h after.

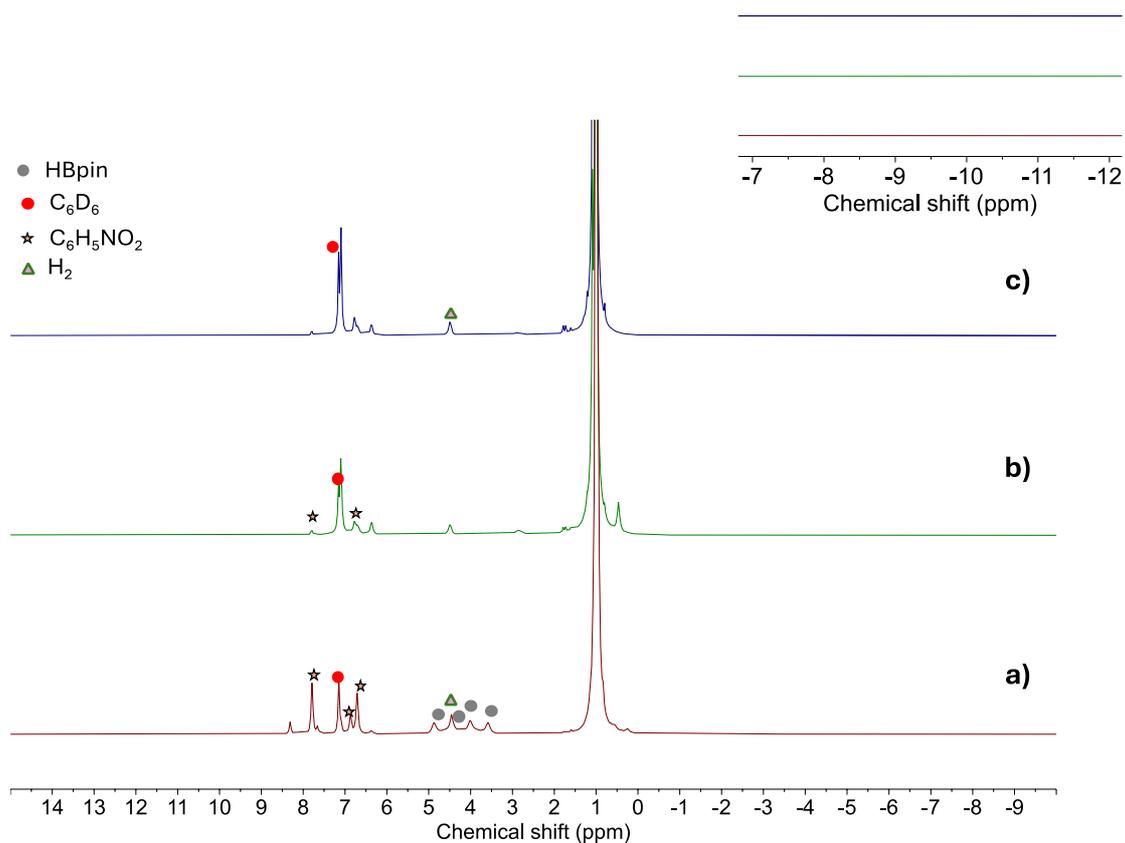


Figure S61: ^1H NMR spectrum (300 MHz, C_6D_6 , 298 K) monitoring of the reaction mixture obtained by reacting **2** with 100 equiv. of HBpin and 20 equiv. of nitrobenzene in C_6D_6 suspension at 50°C a) 15 min after, b) 2 h after, and c) 5 h after.

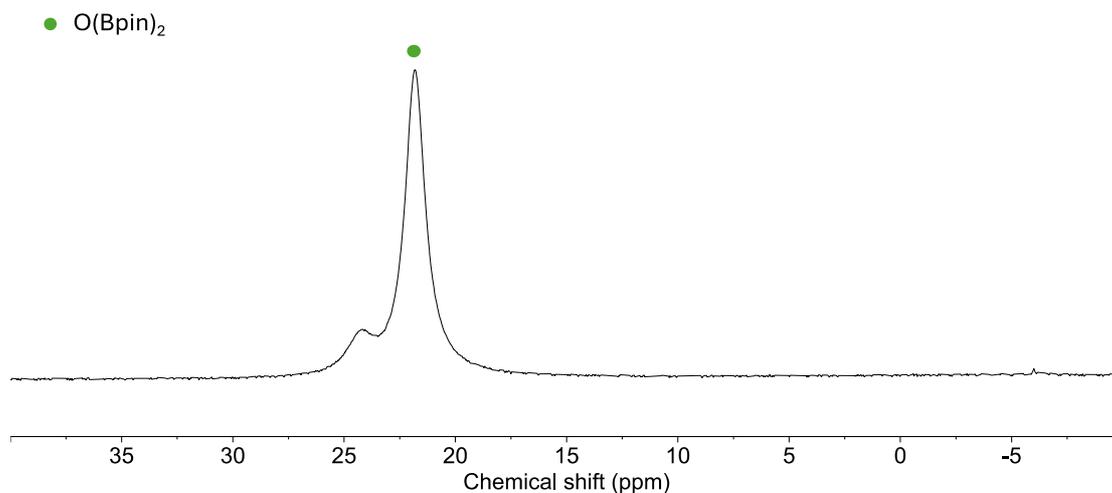


Figure S62: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (96.29 MHz, C_6D_6 , 298 K) of the reaction mixture obtained by reacting **2** with 100 equiv. of HBpin and 20 equiv. of nitrobenzene in C_6D_6 suspension at 80°C for 30 min.

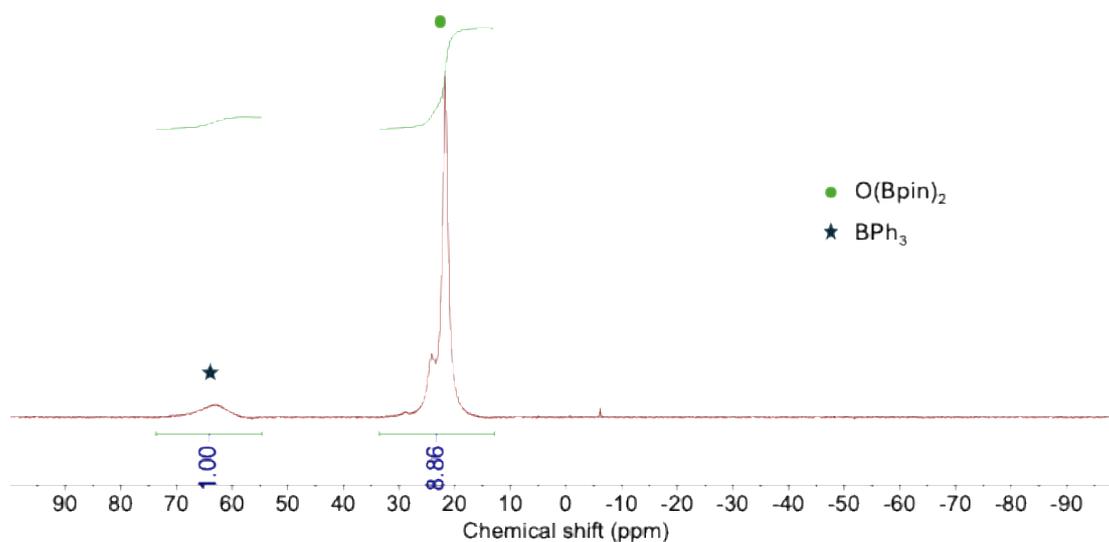


Figure S63: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (96.29 MHz, C_6D_6 , 298 K) of the reaction mixture obtained by reacting **2** with 100 equiv. of HBpin and 20 equiv. of nitrobenzene in C_6D_6 suspension at 80°C for 30 min, using BPh_3 (20 mg, 0.083 mmol, 35 equiv.) as internal standard.

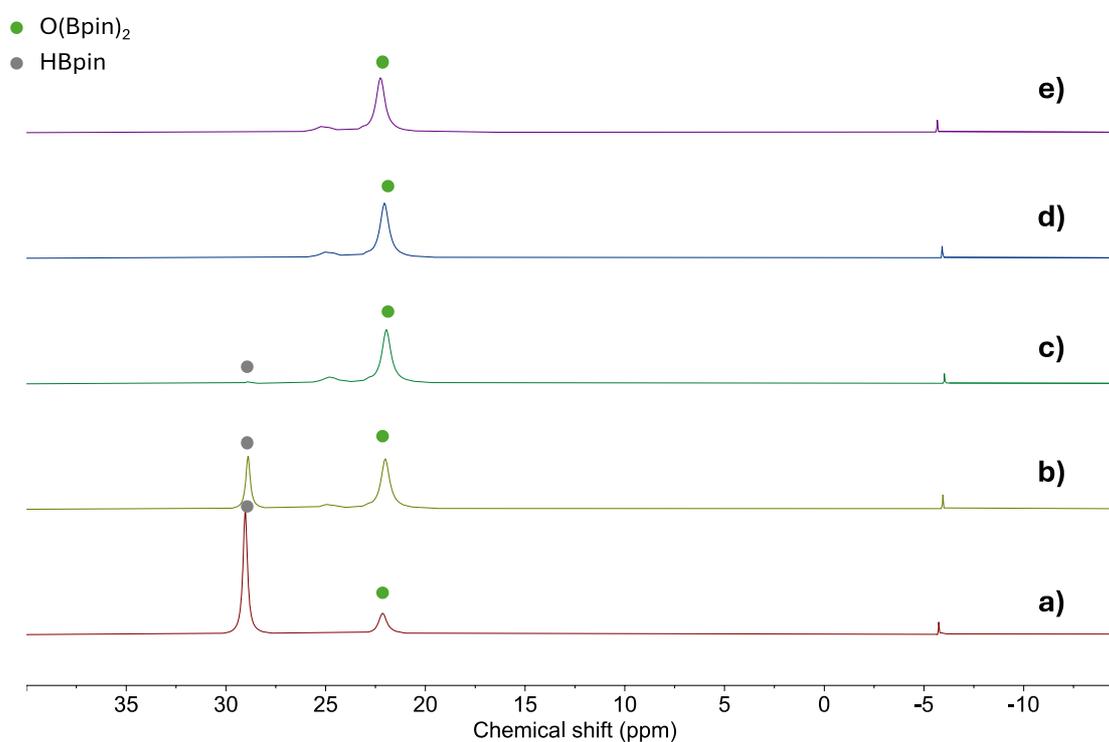


Figure S64: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (96.29 MHz, Et_2O , 298 K) monitoring of the reaction mixture obtained by reacting **2** with 100 equiv. of HBpin and 20 equiv. of nitrobenzene in Et_2O solution at 25°C a) 15 min after, b) 1 h after, and c) 6 h after, d) 21 h after, and e) 24 h after.

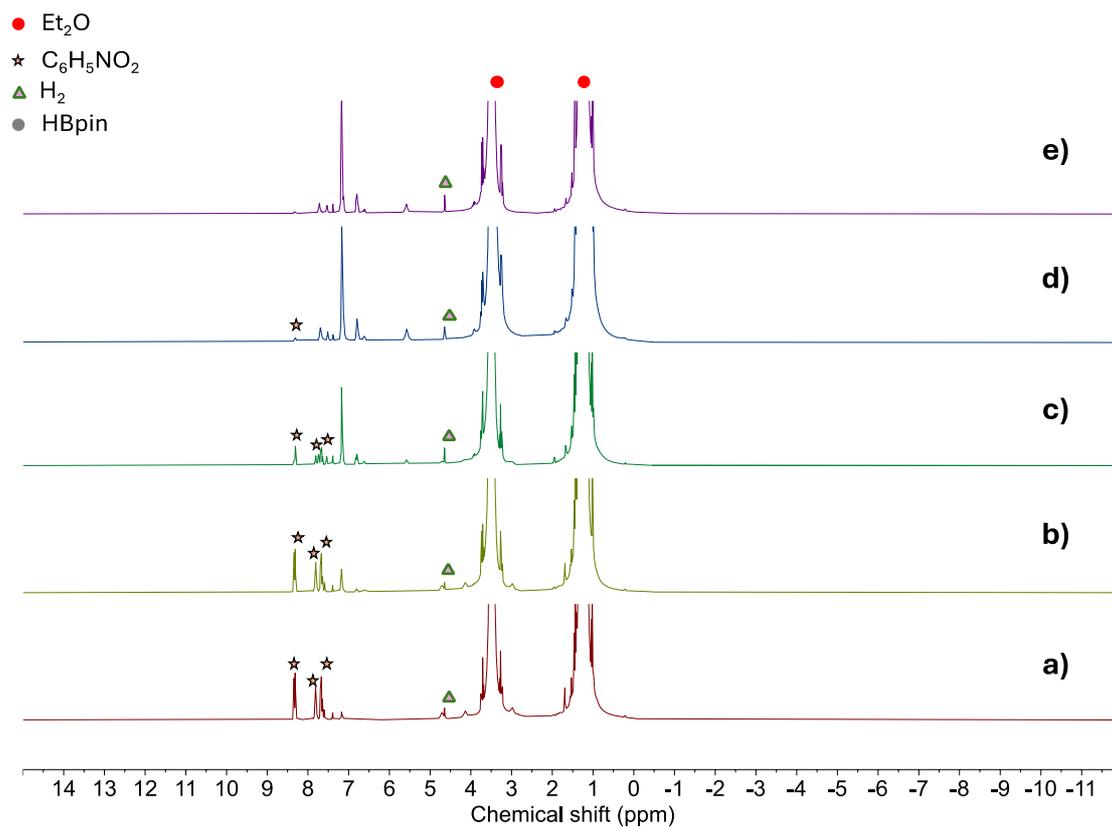


Figure S65: ¹H NMR spectrum (300 MHz, Et₂O, 298 K) monitoring of the reaction mixture obtained by reacting **2** with 100 equiv. of HBpin and 20 equiv. of nitrobenzene in Et₂O solution at 25°C a) 15 min after, b) 1 h after, and c) 6 h after, d) 21 h after, and e) 24 h after.

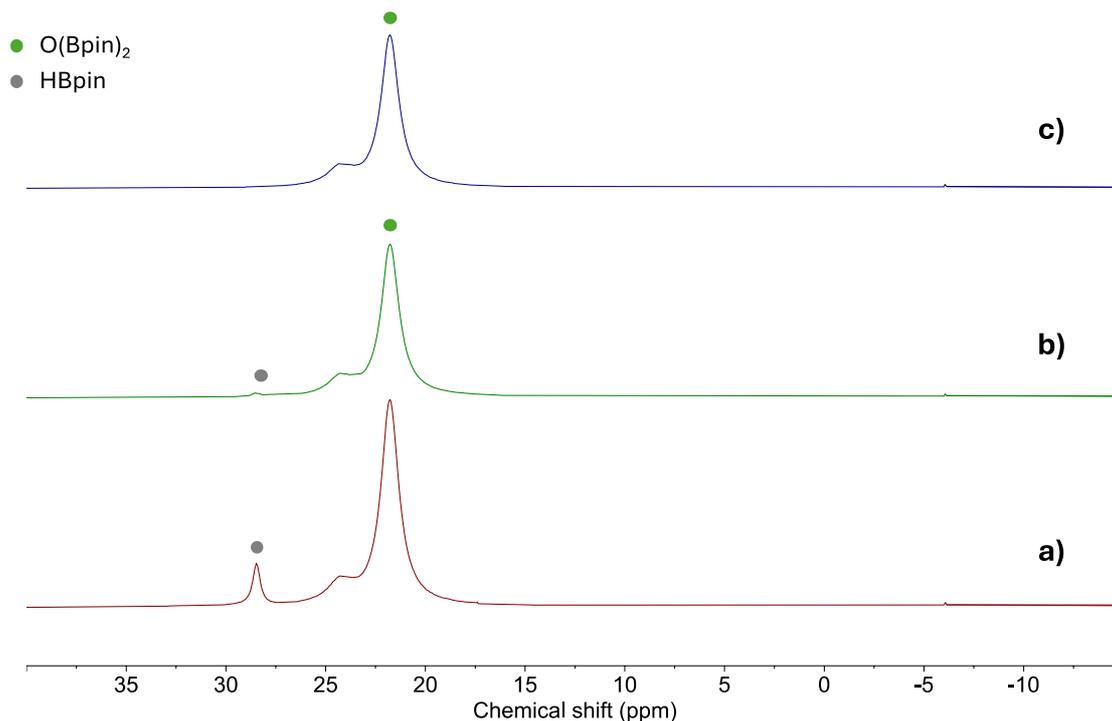


Figure S66: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (96.29 MHz, C_6D_6 , 298 K) monitoring of the reaction mixture obtained by reacting **2** with 500 equiv. of HBpin and 100 equiv. of nitrobenzene in C_6D_6 suspension at 80°C a) 10 min after, b) 20 min after, and c) 30 min after.

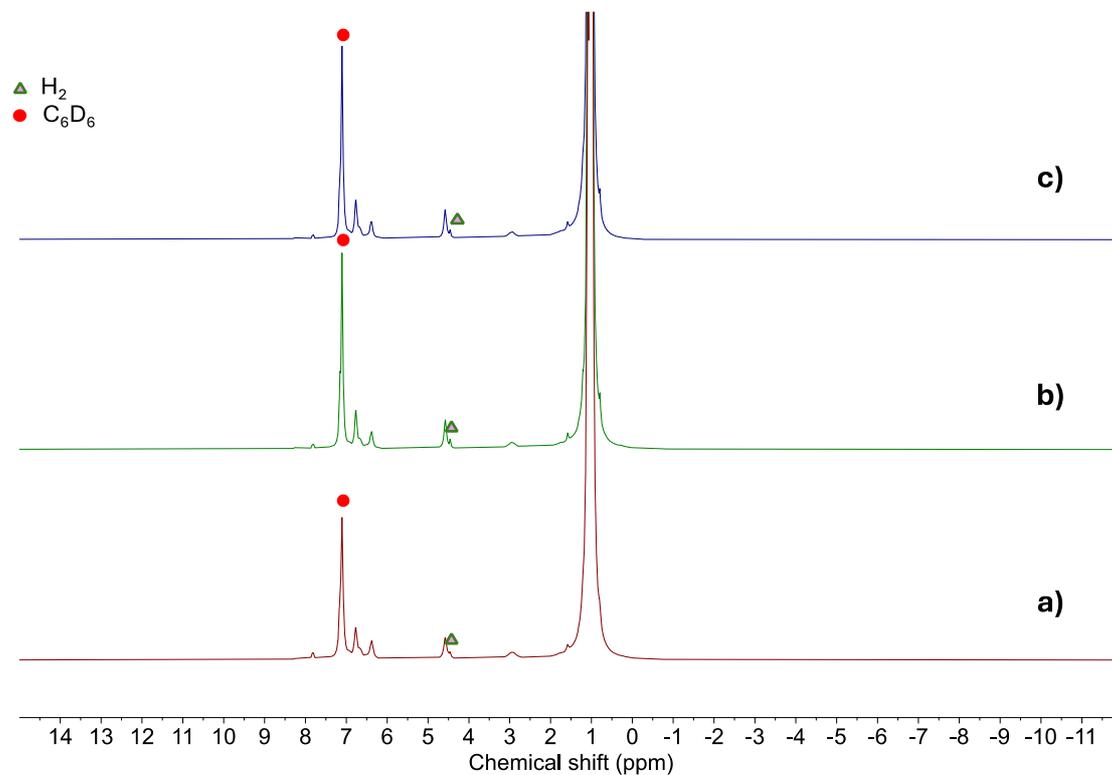


Figure S67: ^1H NMR spectrum (300 MHz, C_6D_6 , 298 K) monitoring of the reaction mixture obtained by reacting **2** with 500 equiv. of HBpin and 100 equiv. of nitrobenzene in C_6D_6 suspension at 80°C a) 10 min after, b) 20 min after, and c) 30 min after.

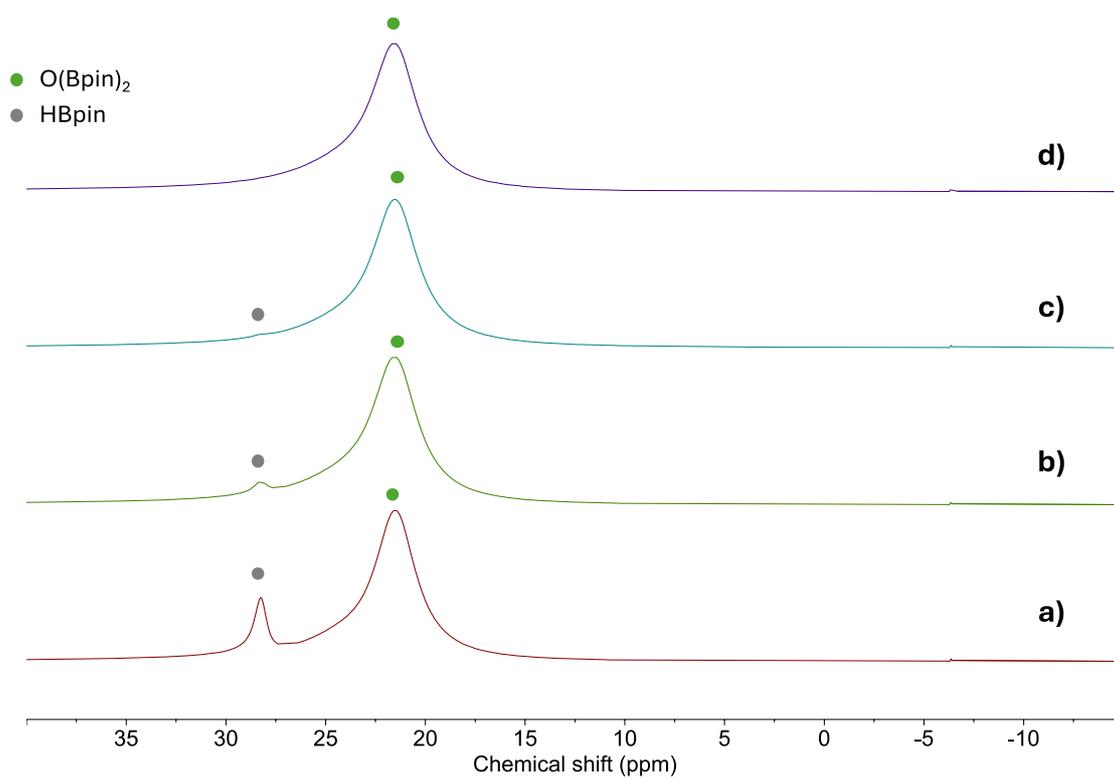


Figure S68: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (96.29 MHz, C_6D_6 , 298 K) monitoring of the reaction mixture obtained by reacting **2** with 5000 equiv. of HBpin and 1000 equiv. of nitrobenzene in C_6D_6 suspension at 80°C a) 30 min after, b) 1h 30 min after, c) 3 h after, and d) 4 h after.

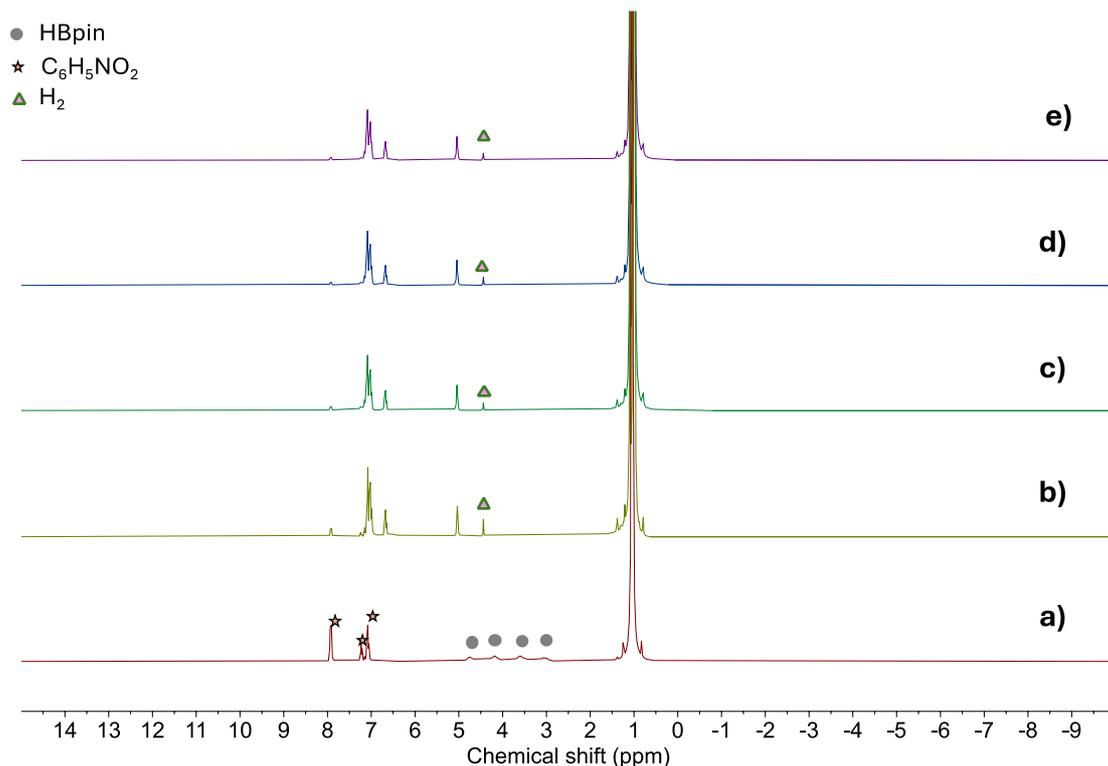


Figure S69: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (96.29 MHz, C_6D_6 , 298 K) monitoring of the reaction mixture obtained by reacting **2** with 5000 equiv. of HBpin and 1000 equiv. of nitrobenzene in C_6D_6 suspension at 80°C a) before warming, b) 30 min after, c) 1 h 30 min after, d) 3 h after, and e) 4 h after.

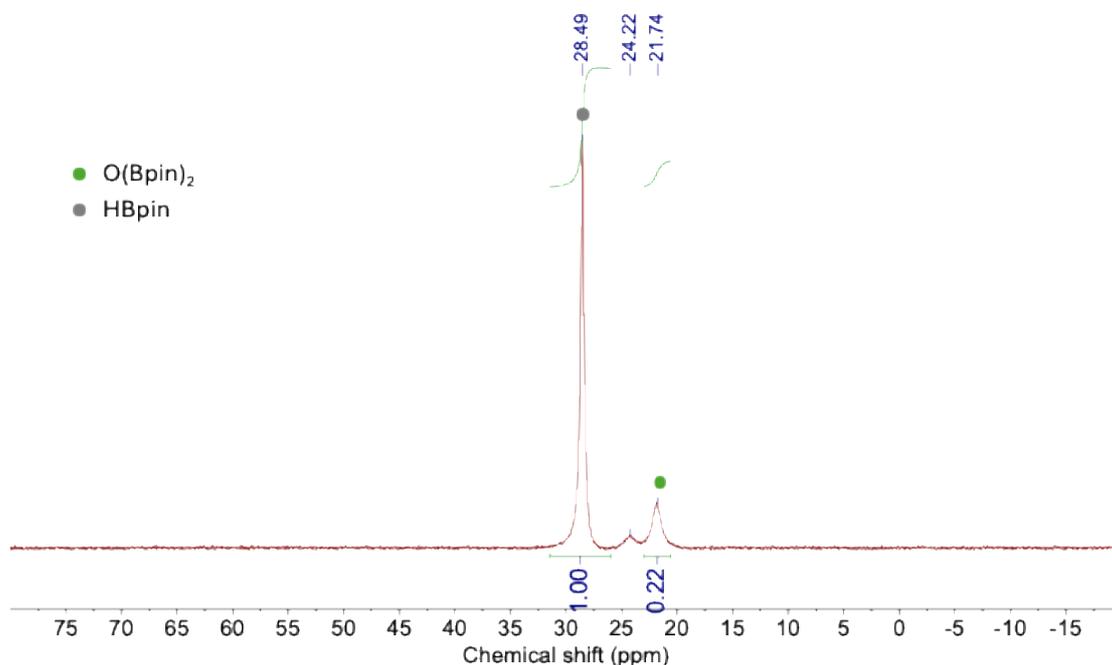


Figure S70: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (96.29 MHz, C_6D_6 , 298 K) of the reaction mixture obtained by reacting $[\text{Fe}(\text{depe})_2\text{Cl}_2]$ with 100 equiv. of HBpin and 20 equiv. of nitrobenzene in C_6D_6 suspension at 80°C for 16 h (**no conversion observed after 30 min**).

C. X-ray Crystal Structure Determination Details

Bragg-intensities of **1**, **2**, **3**, **4**, **5**, **6-O**, **6-N** and **7** were collected at 150K or 193 K. Data collection was performed on a Bruker D8 Quest APEX-III CCD area detector PhotonIII using monochromatic radiation λ (Mo K α 1) = 0.71073 Å by a I μ S 3.0 microfocus X-ray source. Data collections were processed with APEX-W2D-NT (Bruker, 2004), cell refinement and data reduction with SAINT-Plus (Bruker, 2004) and the absorption was corrected by multiscan method applied by SADABS. The space-group assignment was based upon systematic absences, E statistics, and successful refinement of the structure

The structures were solved by direct methods and expanded through successive difference Fourier maps, F2 (SHELXTL).¹¹ In the last cycles of refinement, ordered non-hydrogen atoms were refined anisotropically. Hydrogen atoms connected to carbon atoms were included in idealized positions and a riding model was used for their refinement.

Complexes **2**, **3**, **4**, **5**, **6-O** and **7** required of split and disorder modelling of the CF₃ groups at the BAr^F counteranion. In the case of **3**, **5** and **7** also RIGU, DELU, SIMU and fix position of the fluor atoms were used in one of the CF₃ groups to improve the ellipsoids ADPs. In complex **2** the refinement of the N–N fragment bonded to the iron center and the depe ligand required RIGU restrains. The crystals of complex **3** were very small and therefore the pattern of limited quality, though enough to build a good model that fully agrees with other experimental and computational data. In complex **4** the two hydrogen atoms bonded to the nitrogen atom were located in the Fourier electron density map and refined using a DFIX 1.0Å.

A summary of the fundamental crystal and refinement data are given in Tables **S3-5**. Atomic coordinates, anisotropic displacement parameters and bond lengths and angles can be found in the cif files, which have been deposited in the Cambridge Crystallographic Data Centre with no. CCDC 2475085-2475092. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S3: Crystallographic parameters for complexes **1**, **2**, and **3**.

	[Fe(depe)Cp*Cl], 1	[Fe(depe)Cp*N ₂][BAr ^F], 2	[Fe(depe)Cp*OH][BAr ^F], 3
CCDC number	2475085	2475091	2475087
Empirical formula	C ₄₀ H ₇₈ Cl ₂ Fe ₂ P ₄	C ₅₂ H ₅₁ BF ₂₄ FeN ₂ P ₂	C ₅₂ H ₅₀ BF ₂₄ FeOP ₂
Formula weight	865.50	1288.54	1225.12
Temperature/K	193.0	193.0	193.0
Crystal system	monoclinic	triclinic	triclinic
Space group	P21/n	P-1	P-1
a/Å	8.5732(6)	12.3633(7)	12.3363(14)
b/Å	14.6314(8)	12.7575(7)	12.7312(15)
c/Å	17.7652(12)	18.6259(11)	18.623(2)
α/°	90	96.758(2)	96.854(5)
β/°	94.176(3)	90.524(2)	90.903(5)
γ/°	90	96.518(2)	96.757(4)
Volume/Å ³	2222.5(2)	2897.7(3)	2882.4(6)
Z	2	2	2
ρ _{calc} /cm ³	1.293	1.477	1.470
μ/mm ⁻¹	0.943	0.429	0.431
F(000)	928.0	1308.0	1295.0
Crystal size/mm ³	0.2 × 0.2 × 0.2	0.1 × 0.1 × 0.1	0.1 × 0.1 × 0.05
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2θ range for data collection/°	3.61 to 56.66	4.024 to 54.35	4.046 to 50.772
Index ranges	-11 ≤ h ≤ 11, -19 ≤ k ≤ 19, -23 ≤ l ≤ 23	-15 ≤ h ≤ 15, -16 ≤ k ≤ 16, -23 ≤ l ≤ 23	-14 ≤ h ≤ 14, -15 ≤ k ≤ 15, -22 ≤ l ≤ 22
Reflections collected	63557	122997	70732
Independent reflections	5538 [R _{int} = 0.0855, R _{sigma} = 0.0359]	12852 [R _{int} = 0.0976, R _{sigma} = 0.0448]	10524 [R _{int} = 0.1307, R _{sigma} = 0.0790]
Data/restraints/parameters	5538/0/226	12852/243/845	10525/999/895
Goodness-of-fit on F ²	1.045	1.024	1.137
Final R indexes [I >= 2σ (I)]	R ₁ = 0.0361, wR ₂ = 0.0707	R ₁ = 0.0940, wR ₂ = 0.2508	R ₁ = 0.1689, wR ₂ = 0.3717
Final R indexes [all data]	R ₁ = 0.0569, wR ₂ = 0.0809	R ₁ = 0.1312, wR ₂ = 0.2862	R ₁ = 0.2406, wR ₂ = 0.4259
Largest diff. peak/hole /eÅ ⁻³	0.47/-0.41	2.38/-1.14	2.67/-0.61

Table S4: Crystallographic parameters for complexes **4**, **5**, and **6-O**

	[Fe(depe)Cp*(ONN H ₂)] [BAR ^F], 4	[Fe(depe')Cp*] [BAR ^F], 5	[Fe(depe)Cp*(κ ¹ O-C ₆ H ₅ NO)] [BAR ^F], 6-O
CCDC number	2475090	2475092	2475088
Empirical formula	C ₅₂ H ₅₂ BF ₂₄ FeN ₂ OP ₂	C ₅₂ H ₄₉ BF ₂₄ FeP ₂	C ₅₈ H ₅₆ BF ₂₄ FeNOP ₂
Formula weight	1305.55	1258.51	1367.63
Temperature/K	150.0	110.0	150.00
Crystal system	triclinic	triclinic	monoclinic
Space group	P-1	P-1	P2 ₁ /c
a/Å	12.4178(15)	12.801(2)	13.1363(7)
b/Å	12.6184(15)	13.0443(18)	18.0228(10)
c/Å	18.884(2)	17.892(3)	25.0443(11)
α/°	102.952(4)	78.220(6)	90
β/°	92.919(4)	69.724(6)	96.049(3)
γ/°	95.205(4)	78.417(6)	90
Volume/Å ³	2864.0(6)	2715.9(7)	5896.3(5)
Z	2	2	4
ρ _{calc} /cm ³	1.514	1.539	1.541
μ/mm ⁻¹	0.437	0.455	0.428
F(000)	1326.0	1276.0	2784.0
Crystal size/mm ³	0.36 × 0.22 × 0.12	0.2 × 0.2 × 0.1	0.26 × 0.04 × 0.04
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2θ range for data collection/°	3.842 to 52.846	4.164 to 52.744	3.85 to 50.762
Index ranges	-15 ≤ h ≤ 15, -15 ≤ k ≤ 15, -23 ≤ l ≤ 23	-15 ≤ h ≤ 15, -16 ≤ k ≤ 16, -22 ≤ l ≤ 22	-15 ≤ h ≤ 15, -21 ≤ k ≤ 21, -30 ≤ l ≤ 30
Reflections collected	137121	122496	92148
Independent reflections	11723 [R _{int} = 0.0473, R _{sigma} = 0.0212]	11101 [R _{int} = 0.1221, R _{sigma} = 0.0507]	10810 [R _{int} = 0.1039, R _{sigma} = 0.0544]
Data/restraints/parameters	11726/53/820	11101/272/813	10810/42/828
Goodness-of-fit on F ²	1.098	1.054	1.083
Final R indexes [I > 2σ (I)]	R ₁ = 0.0665, wR ₂ = 0.1712	R ₁ = 0.0668, wR ₂ = 0.1557	R ₁ = 0.0665, wR ₂ = 0.1298
Final R indexes [all data]	R ₁ = 0.0678, wR ₂ = 0.1720	R ₁ = 0.0911, wR ₂ = 0.1694	R ₁ = 0.0890, wR ₂ = 0.1862
Largest diff. peak/hole /eÅ ⁻³	1.58/-0.73	1.25/-0.61	0.93/-0.53

Table S5: Crystallographic parameters for complexes **6-N** and **7**

	[Fe(depe)Cp*(κ ¹ N-C ₆ H ₅ NO)][BAR ^F], 6-N	[Fe(depe)Cp*(H) ₂][BAR ^F], 7
CCDC number	2475089	2475086
Empirical formula	C ₆₂ H ₆₆ BF ₂₄ FeNO ₂ P ₂	C ₅₂ H ₅₁ BF ₂₄ FeP ₂
Formula weight	1441.75	1260.52
Temperature/K	150.0	193.0
Crystal system	monoclinic	triclinic
Space group	C2/c	P-1
a/Å	42.284(5)	12.801(2)
b/Å	14.2783(15)	13.0443(18)
c/Å	25.921(3)	17.892(3)
α/°	90	78.220(6)
β/°	123.837(4)	69.724(6)
γ/°	90	78.417(6)
Volume/Å ³	2864.0(6)	2715.9(7)
Z	8	4
ρ _{calc} /cm ³	1.473	1.469
μ/mm ⁻¹	0.393	0.434
F(000)	5904.0	2560.0
Crystal size/mm ³	0.2 × 0.2 × 0.1	0.2 × 0.2 × 0.1
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2θ range for data collection/°	3.936 to 50.242	3.836 to 53.002
Index ranges	-50 ≤ h ≤ 50, -16 ≤ k ≤ 16, -30 ≤ l ≤ 30	-15 ≤ h ≤ 15, -16 ≤ k ≤ 16, -45 ≤ l ≤ 45
Reflections collected	108796	66992
Independent reflections	11544 [R _{int} = 0.1681, R _{sigma} = 0.0718]	23426 [R _{int} = 0.0441, R _{sigma} = 0.0544]
Data/restraints/parameters	11544/285/953	23426/798/1668
Goodness-of-fit on F ²	1.016	1.011
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0928, wR ₂ = 0.2136	R ₁ = 0.0667, wR ₂ = 0.2948
Final R indexes [all data]	R ₁ = 0.1436, wR ₂ = 0.2445	R ₁ = 0.1395, wR ₂ = 0.2948
Largest diff. peak/hole /eÅ ⁻³	0.68/-0.72	2.15/-1.26

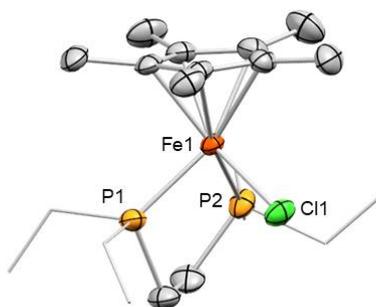


Figure S71: ORTEP diagram for complex **1**. Hydrogen atoms have been excluded, and ethyl groups of depe ligand are represented in wire-frame format for clarity. Thermal ellipsoids are set at 50 % probability.

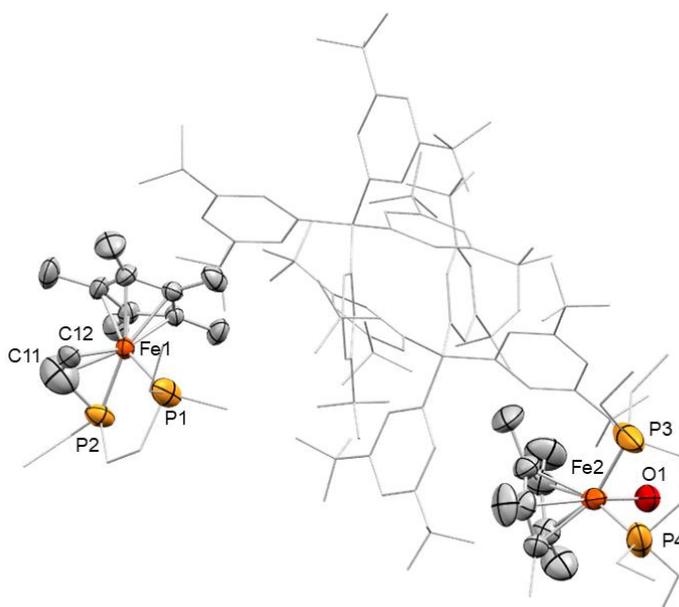


Figure S72: ORTEP diagram for co-crystallized **3** and **5**. Hydrogen atoms have been excluded, and ethyl groups of depe ligand and BAr^F counter anion are represented in wire-frame format for clarity. Thermal ellipsoids are set at 50 % probability.

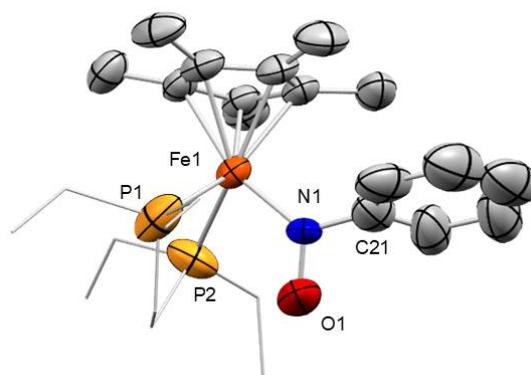


Figure S73: ORTEP diagram for complex **6-N**. Hydrogen atoms have been excluded, and ethyl groups of depe ligand are represented in wire-frame format for clarity. Thermal ellipsoids are set at 50 % probability.

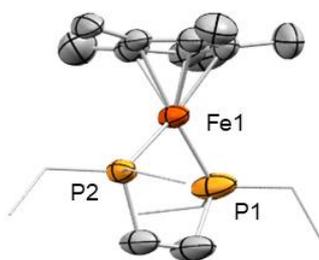


Figure S74: ORTEP diagram for complex **7**. Hydrogen atoms have been excluded, and ethyl groups of depe ligand are represented in wire-frame format for clarity. The iron-hydride ligands could not be located in the Fourier difference electron density map. Thermal ellipsoids are set at 50 % probability.

D. IR spectroscopy

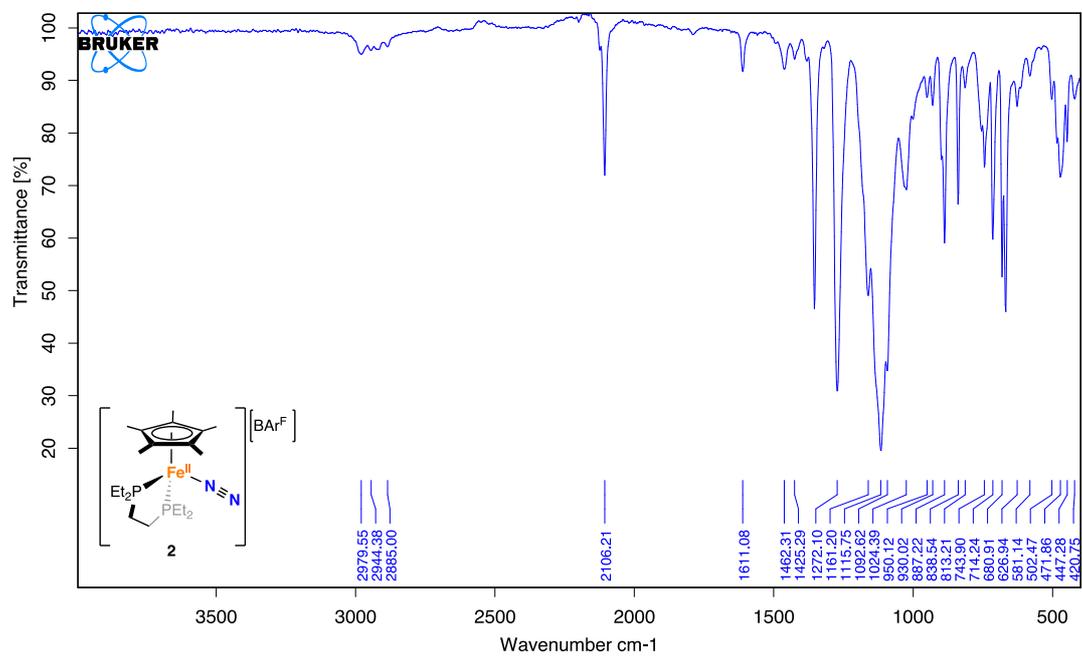


Figure S75: IR spectrum of isolated complex 2.

E. EPR data

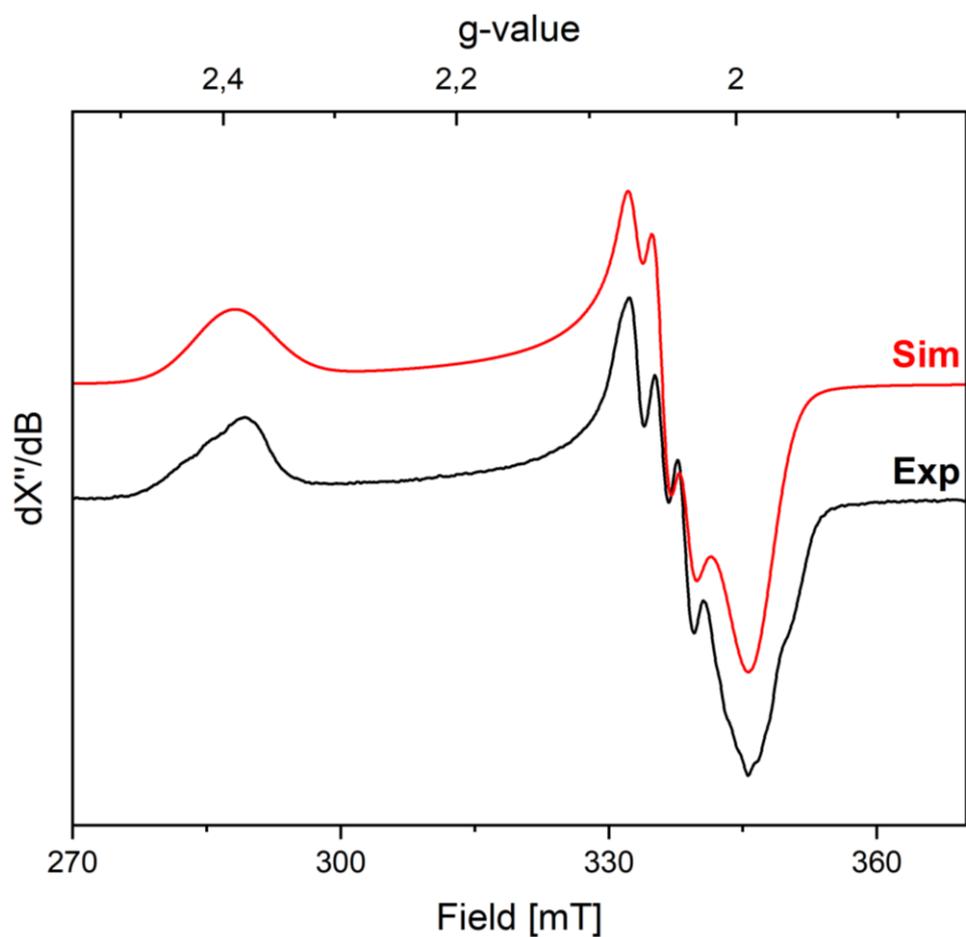


Figure S76: Experimental (black) and simulated (red) X-band EPR spectra of the reaction mixture obtained 24 h after addition of 1 bar of H₂ to a d₈-THF solution of **2** at 25°C to yield compound **7** (diamagnetic, EPR silent) and **8** (proposed as the main component of this EPR spectrum). Et₂O added to form a 1:1 mixture as a way of obtaining a good glass (modulation amplitude: 4 G, 9.6361 GHz, 77 K, 8 scans, g_x = 2.392, g_y = 2.049 and g_z = 1.990; A(³¹P_α)=[31 80 4] MHz and A(³¹P_β)=[-51 80 9] MHz)

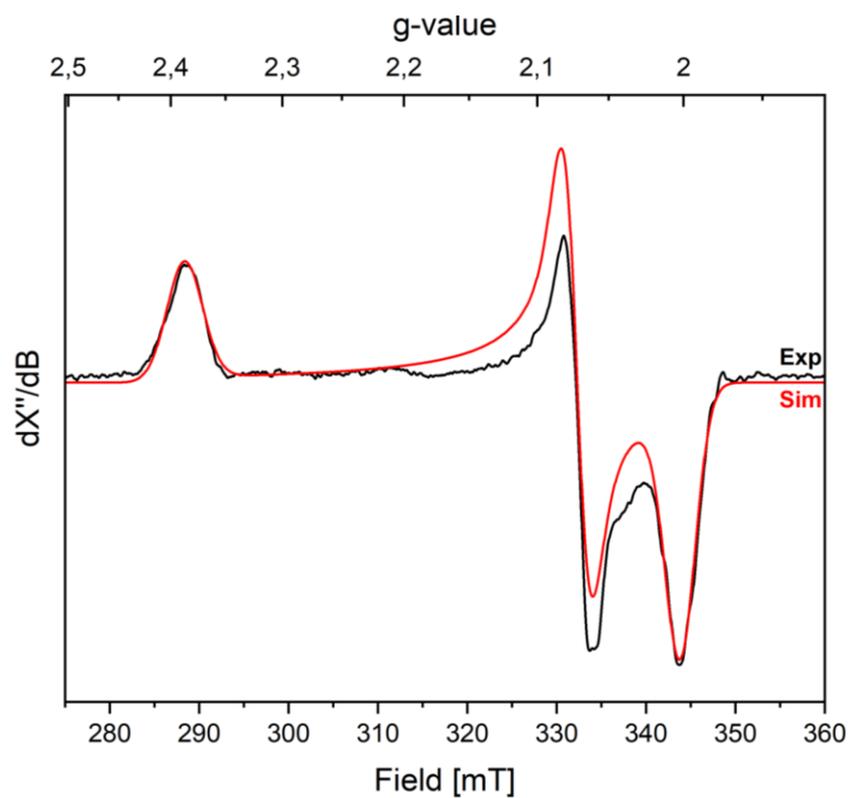


Figure S77: Experimental (black) and simulated (red) X-band EPR spectra of a frozen 1:1 THF:Et₂O solution of the reaction mixture of **2** with 7 equiv. of C₆H₅NO₂ (1.5 mM, modulation amplitude: 4 G, 9.6353 GHz, 77 K, 8 scans, $g = 2.387, 2.072$ and 2.002)

F. Computational details

All the geometry optimizations and frequency calculations reported in this paper were obtained with the ORCA 6.0.1 program.¹² Electron correlation was partially taken into account using the BP86^{13,14} functional in conjunction with the D3(BJ) dispersion correction suggested by Grimme et al.^{15,16}, the resolution-of-identity approach,¹⁷ RI, and the triple- ζ quality plus polarization functions def2-TZVP¹⁸ basis set for all atoms. All species were characterized by frequency calculations: reactants and adducts exhibited positive definite Hessian matrices, while transition states showed a single negative eigenvalue in their diagonalized force constant matrices. This level is denoted (RI)-BP86-D3(BJ)/def2-TZVP.

For the calculations of the reaction profiles shown in Figure 4, a smaller basis-sets (def2-SVP) were used. Therefore, for these calculations the level is denoted (RI)-BP86-D3(BJ)/def2-SVP.

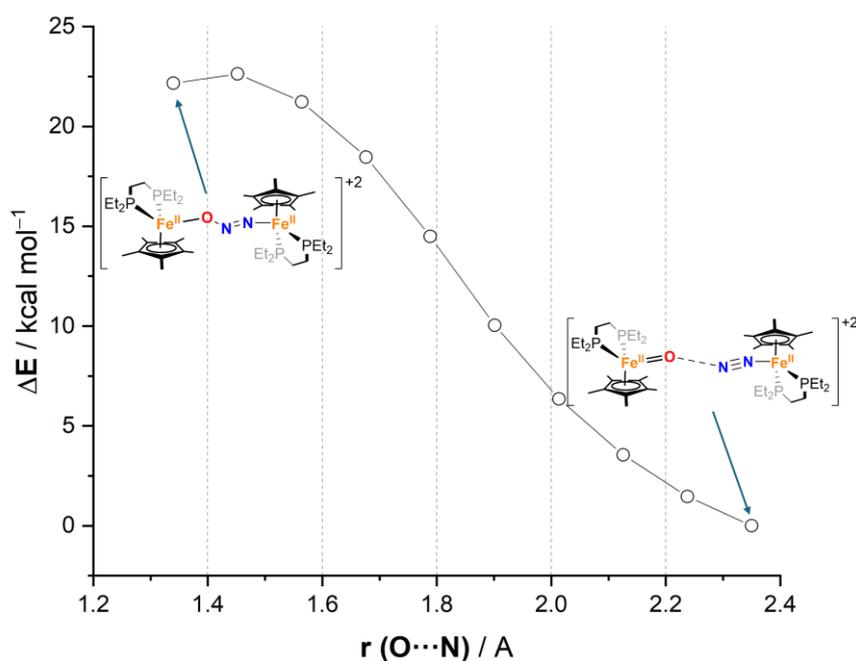


Figure S78. Relaxed scan calculations for the transformation of INT2 into Fe(IV)=O complex (3') and Fe(II)-N₂ complex 2. All data were computed at the RI-BP86-D3(BJ)/def2-SVP level.

Cartesian coordinates (in Å) and free energies (in a.u., at 298 K) of all the stationary points discussed in the text. All calculations have been performed at the (RI)-BP86-D3(BJ)/def2-SVP level.

2: G= -2840.44541974

Fe	0.171908000	0.542662000	-0.140938000
P	1.090759000	-1.484968000	-0.238731000
P	-1.768966000	-0.516976000	-0.209605000
N	0.156895000	0.656168000	-1.908918000
C	1.703015000	1.444590000	1.038892000
C	-0.570429000	1.943969000	1.266071000
C	0.518340000	1.178919000	1.834736000
C	-0.087268000	2.614354000	0.091584000
C	1.327482000	2.310787000	-0.038875000
C	3.113468000	1.092741000	1.404299000
H	3.159206000	0.316093000	2.188786000
H	3.620537000	1.992507000	1.812773000
H	3.705908000	0.749845000	0.536235000
C	0.486161000	0.477341000	3.158526000
H	-0.475989000	-0.041238000	3.334339000
H	0.618385000	1.205696000	3.987369000
H	1.294319000	-0.271492000	3.251302000
C	-1.895188000	2.189667000	1.921624000
H	-2.726145000	2.293820000	1.197802000
H	-1.843148000	3.146389000	2.483885000
H	-2.156704000	1.401854000	2.650243000
C	2.248286000	2.902820000	-1.060048000
H	3.206802000	2.354683000	-1.118786000
H	2.484371000	3.954377000	-0.791097000
H	1.799902000	2.919114000	-2.072362000
C	-0.858755000	3.558483000	-0.777152000
H	-0.545169000	3.496295000	-1.837110000
H	-0.696579000	4.607471000	-0.448984000
H	-1.947071000	3.364479000	-0.734086000
C	-2.552992000	-1.099858000	1.380703000
H	-1.728642000	-1.160903000	2.119837000
H	-3.203285000	-0.267394000	1.717157000
C	2.502009000	-3.650169000	1.022019000
H	1.661451000	-4.348136000	0.837664000
H	3.014297000	-3.990444000	1.944091000
H	3.224347000	-3.758668000	0.189228000
C	-3.339104000	-2.415082000	1.342617000
H	-3.794778000	-2.607733000	2.334543000
H	-2.690510000	-3.282648000	1.110328000
H	-4.158573000	-2.396694000	0.599680000
C	2.030215000	-2.202159000	1.188952000
H	2.889270000	-1.529749000	1.378261000
H	1.356097000	-2.098440000	2.064858000
C	-3.090970000	0.379862000	-1.145716000
H	-3.248049000	1.335255000	-0.602521000
H	-2.616895000	0.658391000	-2.110602000
C	-4.421330000	-0.344539000	-1.371757000
H	-4.952027000	-0.547452000	-0.420935000
H	-4.286717000	-1.306796000	-1.904558000
H	-5.092645000	0.281632000	-1.992897000
N	0.155297000	0.808608000	-3.037208000
C	-1.464047000	-2.079514000	-1.168811000
H	-2.355795000	-2.736169000	-1.184665000

H	-1.256270000	-1.780356000	-2.217111000
C	2.181966000	-1.764862000	-1.716201000
H	2.463044000	-2.838624000	-1.726070000
H	1.533751000	-1.601851000	-2.602180000
C	-0.251977000	-2.763425000	-0.532848000
H	0.133941000	-3.597619000	-1.152411000
H	-0.520491000	-3.187893000	0.457553000
C	3.414334000	-0.863430000	-1.781470000
H	3.982375000	-1.046382000	-2.714780000
H	3.127570000	0.206160000	-1.769276000
H	4.106126000	-1.047355000	-0.934757000

2' : G = -2730.93726291

Fe	0.149525000	0.567109000	-0.144609000
P	1.203106000	-1.379295000	-0.151467000
P	-1.723658000	-0.612554000	-0.271420000
C	1.634067000	1.765330000	0.686964000
C	-0.681055000	2.110446000	0.941136000
C	0.503608000	1.554794000	1.578756000
C	-0.310908000	2.559964000	-0.370669000
C	1.120580000	2.346208000	-0.517290000
C	3.078688000	1.564552000	1.030088000
H	3.210528000	0.852062000	1.865575000
H	3.525501000	2.527678000	1.357571000
H	3.674910000	1.202244000	0.171020000
C	0.577007000	1.028969000	2.976103000
H	-0.371553000	0.550102000	3.288339000
H	0.779050000	1.852144000	3.696705000
H	1.388980000	0.285431000	3.093641000
C	-2.003993000	2.333002000	1.605157000
H	-2.854466000	2.268205000	0.898632000
H	-2.024977000	3.355762000	2.039786000
H	-2.181379000	1.627254000	2.436713000
C	1.895217000	2.691997000	-1.751018000
H	2.958390000	2.399292000	-1.674076000
H	1.863065000	3.787836000	-1.930988000
H	1.468924000	2.213552000	-2.658524000
C	-1.189695000	3.233309000	-1.379599000
H	-0.959021000	2.908898000	-2.414127000
H	-1.050892000	4.336066000	-1.348593000
H	-2.261997000	3.034888000	-1.193595000
C	-2.552757000	-0.973348000	1.367898000
H	-1.754475000	-0.865332000	2.129817000
H	-3.251454000	-0.129122000	1.535610000
C	3.049532000	-3.318536000	0.889779000
H	2.265931000	-4.096746000	0.976375000
H	3.810332000	-3.530950000	1.667237000
H	3.544484000	-3.440973000	-0.094210000
C	-3.272278000	-2.314891000	1.528778000
H	-3.746884000	-2.364819000	2.529519000
H	-2.577066000	-3.174572000	1.458794000
H	-4.070514000	-2.463092000	0.777113000
C	2.484730000	-1.907356000	1.076620000
H	3.287878000	-1.145262000	1.036406000
H	2.003528000	-1.793145000	2.071274000
C	-3.058112000	0.002517000	-1.406494000
H	-3.344743000	1.000421000	-1.013246000
H	-2.542441000	0.201588000	-2.370753000
C	-4.292034000	-0.880969000	-1.611681000
H	-4.876651000	-0.997279000	-0.678389000

H	-4.026488000	-1.891660000	-1.980204000
H	-4.965929000	-0.423676000	-2.363728000
C	-1.287784000	-2.314764000	-0.911411000
H	-2.131395000	-3.025202000	-0.808441000
H	-1.080625000	-2.215008000	-1.998300000
C	2.001531000	-1.629060000	-1.825457000
H	2.170735000	-2.719773000	-1.951422000
H	1.239038000	-1.344515000	-2.582189000
C	-0.041634000	-2.783410000	-0.153037000
H	0.395321000	-3.702172000	-0.594245000
H	-0.286563000	-3.011097000	0.906431000
C	3.291785000	-0.836232000	-2.034065000
H	3.688061000	-0.998852000	-3.055888000
H	3.118915000	0.249089000	-1.909019000
H	4.083675000	-1.140698000	-1.321111000

3: G = -2808.08700941 (def2-TZVP)

Fe	0.033033000	0.524566000	-0.239594000
P	1.561987000	-1.076971000	-0.261382000
P	-1.434392000	-1.140352000	-0.297906000
O	0.116053000	0.636824000	-2.092119000
C	-1.147525000	1.959168000	0.835913000
C	-0.145280000	1.389371000	1.705111000
C	-0.472152000	2.618317000	-0.240724000
C	0.939344000	2.470686000	-0.042917000
C	1.142585000	1.738049000	1.169310000
C	-2.600798000	2.091253000	1.158240000
H	-3.235131000	2.078192000	0.265423000
H	-2.770330000	3.053925000	1.666975000
H	-2.945578000	1.308323000	1.842875000
C	2.294535000	-1.812581000	1.263486000
H	3.036398000	-2.556225000	0.934797000
H	2.861037000	-1.006238000	1.747514000
C	0.826318000	-2.527866000	-1.144732000
H	0.794054000	-2.276227000	-2.216465000
H	1.466667000	-3.415364000	-1.043390000
C	3.037613000	-0.604404000	-1.258527000
H	2.631934000	-0.089093000	-2.141390000
H	3.567172000	0.165370000	-0.676224000
C	-2.568700000	-1.060031000	-1.755205000
H	-1.926493000	-1.122136000	-2.646652000
H	-3.178438000	-1.976602000	-1.744214000
C	-0.580368000	-2.769824000	-0.595393000
H	-0.531195000	-3.291768000	0.368784000
H	-1.182268000	-3.391971000	-1.271947000
C	-2.539701000	-1.510825000	1.129836000
H	-1.875879000	-1.630323000	1.999232000
H	-3.137701000	-0.608910000	1.316656000
C	-3.442821000	0.188329000	-1.822976000
H	-4.074541000	0.164484000	-2.720910000
H	-2.822302000	1.091562000	-1.870896000
H	-4.110089000	0.263189000	-0.953429000
C	3.989393000	-1.735918000	-1.655543000
H	4.816814000	-1.333267000	-2.255648000
H	3.485628000	-2.498491000	-2.264355000
H	4.432233000	-2.233359000	-0.782730000
C	-0.397294000	0.815377000	3.061992000
H	-1.344851000	0.265307000	3.108507000
H	-0.454691000	1.622314000	3.810635000
H	0.404839000	0.137831000	3.377584000

C	1.305157000	-2.444414000	2.245089000
H	0.919578000	-3.401541000	1.871769000
H	0.449241000	-1.784600000	2.437572000
H	1.796527000	-2.647929000	3.205790000
C	-3.450431000	-2.731746000	0.971838000
H	-4.174373000	-2.600524000	0.157293000
H	-4.023272000	-2.891144000	1.895532000
H	-2.881341000	-3.650345000	0.776332000
C	1.988430000	3.010706000	-0.954142000
H	2.982931000	2.619032000	-0.709132000
H	2.035622000	4.108455000	-0.879739000
H	1.760210000	2.757312000	-1.998438000
C	2.449186000	1.581049000	1.877266000
H	2.408783000	0.803250000	2.647885000
H	2.694564000	2.526222000	2.387019000
H	3.281952000	1.362033000	1.196588000
C	-1.091786000	3.335823000	-1.390088000
H	-0.777724000	2.874988000	-2.338743000
H	-2.186562000	3.320596000	-1.338465000
H	-0.769709000	4.387825000	-1.405072000
H	0.103335000	-0.194660000	-2.597563000

3: G = -2806.73817911

Fe	0.033094000	0.523941000	-0.221406000
P	1.575213000	-1.071719000	-0.252577000
P	-1.444180000	-1.135878000	-0.287030000
O	0.126354000	0.608898000	-2.068340000
C	-1.148250000	1.946910000	0.842077000
C	-0.137671000	1.382102000	1.716560000
C	-0.473027000	2.608717000	-0.242814000
C	0.944873000	2.463613000	-0.047758000
C	1.153979000	1.730907000	1.172033000
C	-2.603165000	2.082232000	1.172896000
H	-3.247254000	2.093180000	0.275594000
H	-2.765648000	3.043422000	1.706376000
H	-2.958212000	1.282912000	1.848788000
C	2.306962000	-1.829629000	1.273851000
H	3.037463000	-2.594675000	0.937016000
H	2.900674000	-1.027092000	1.753570000
C	0.824562000	-2.519153000	-1.156879000
H	0.786162000	-2.243148000	-2.232582000
H	1.474892000	-3.413718000	-1.077972000
C	3.048654000	-0.587157000	-1.264914000
H	2.614189000	-0.081873000	-2.151864000
H	3.565402000	0.208632000	-0.688310000
C	-2.570335000	-1.037866000	-1.763846000
H	-1.904201000	-1.077856000	-2.650440000
H	-3.171784000	-1.971256000	-1.779134000
C	-0.578974000	-2.771947000	-0.600126000
H	-0.524040000	-3.301451000	0.370773000
H	-1.188536000	-3.401126000	-1.279391000
C	-2.562592000	-1.525052000	1.139364000
H	-1.890041000	-1.667762000	2.011015000
H	-3.145749000	-0.606110000	1.346513000
C	-3.457225000	0.203251000	-1.822028000
H	-4.073241000	0.197314000	-2.742837000
H	-2.840317000	1.121356000	-1.833918000
H	-4.152966000	0.253773000	-0.960589000
C	4.019409000	-1.705053000	-1.655588000
H	4.844327000	-1.292098000	-2.269998000

H	3.526372000	-2.492409000	-2.259840000
H	4.482554000	-2.190139000	-0.773538000
C	-0.389866000	0.816195000	3.081038000
H	-1.314512000	0.210526000	3.120126000
H	-0.508956000	1.637970000	3.820182000
H	0.446175000	0.183118000	3.431896000
C	1.302441000	-2.429076000	2.262313000
H	0.878711000	-3.383599000	1.893980000
H	0.462314000	-1.734441000	2.456695000
H	1.792561000	-2.647424000	3.231494000
C	-3.492237000	-2.729238000	0.958441000
H	-4.218868000	-2.575709000	0.136467000
H	-4.078343000	-2.897184000	1.884051000
H	-2.934607000	-3.664092000	0.750589000
C	1.986659000	2.999040000	-0.975815000
H	2.998657000	2.631941000	-0.723303000
H	2.012490000	4.108409000	-0.934638000
H	1.757480000	2.708389000	-2.020344000
C	2.467376000	1.573483000	1.875003000
H	2.437657000	0.782386000	2.646123000
H	2.712758000	2.522875000	2.396985000
H	3.306822000	1.364728000	1.183932000
C	-1.092395000	3.310867000	-1.406913000
H	-0.816279000	2.788996000	-2.347211000
H	-2.194758000	3.346192000	-1.332749000
H	-0.722012000	4.353956000	-1.477862000
H	0.112438000	-0.231222000	-2.566996000

3`: G = -2807.44387651 (def2-TZVP)

Fe	0.027787000	0.512920000	-0.258821000
P	1.530799000	-1.101502000	-0.331065000
P	-1.443735000	-1.145327000	-0.297383000
O	0.100730000	0.409139000	-1.949381000
C	-1.108932000	1.935808000	0.880532000
C	-0.065779000	1.411961000	1.718719000
C	-0.495552000	2.628746000	-0.231545000
C	0.907944000	2.503703000	-0.101896000
C	1.180257000	1.744679000	1.099951000
C	-2.553576000	2.030118000	1.250572000
H	-3.221247000	1.860287000	0.398708000
H	-2.761379000	3.043429000	1.630005000
H	-2.816370000	1.328598000	2.049995000
C	2.274398000	-1.817457000	1.194944000
H	3.008312000	-2.568700000	0.865079000
H	2.850621000	-1.009135000	1.664282000
C	0.775258000	-2.527573000	-1.215624000
H	0.707681000	-2.220700000	-2.268127000
H	1.416204000	-3.417184000	-1.145203000
C	2.966634000	-0.600286000	-1.362110000
H	2.506837000	-0.228304000	-2.289814000
H	3.424838000	0.272020000	-0.873144000
C	-2.574337000	-1.004474000	-1.744861000
H	-1.892797000	-0.977056000	-2.608019000
H	-3.150688000	-1.941248000	-1.796896000
C	-0.613740000	-2.772525000	-0.629527000
H	-0.547200000	-3.307437000	0.326492000
H	-1.241111000	-3.375368000	-1.300071000
C	-2.523684000	-1.489497000	1.151848000
H	-1.854946000	-1.601322000	2.018365000

H	-3.119430000	-0.584688000	1.329962000
C	-3.497769000	0.209003000	-1.754805000
H	-4.111125000	0.208068000	-2.665615000
H	-2.918347000	1.139912000	-1.746418000
H	-4.185366000	0.210831000	-0.897339000
C	4.011958000	-1.683311000	-1.639198000
H	4.783065000	-1.288550000	-2.314670000
H	3.570655000	-2.562833000	-2.126931000
H	4.519328000	-2.015547000	-0.724170000
C	-0.244391000	0.833893000	3.085880000
H	-1.171565000	0.253554000	3.170356000
H	-0.294882000	1.637070000	3.838623000
H	0.589143000	0.178918000	3.365582000
C	1.292034000	-2.434333000	2.193411000
H	0.893402000	-3.390153000	1.831245000
H	0.445766000	-1.764761000	2.393302000
H	1.794745000	-2.635861000	3.148596000
C	-3.438204000	-2.710108000	1.006441000
H	-4.153164000	-2.589571000	0.182306000
H	-4.020011000	-2.850070000	1.927589000
H	-2.871058000	-3.634042000	0.832767000
C	1.908603000	3.052753000	-1.061011000
H	2.923649000	2.700945000	-0.842369000
H	1.921319000	4.152745000	-1.014960000
H	1.652026000	2.765915000	-2.090366000
C	2.529183000	1.604563000	1.727244000
H	2.536185000	0.853246000	2.524481000
H	2.809925000	2.565626000	2.186828000
H	3.316562000	1.358922000	1.003317000
C	-1.185298000	3.327645000	-1.352958000
H	-0.916877000	2.857723000	-2.311707000
H	-2.275656000	3.305828000	-1.242955000
H	-0.874213000	4.381791000	-1.400510000

3\': G = -2806.09530567

Fe	0.027622000	0.511416000	-0.246150000
P	1.544163000	-1.098491000	-0.322248000
P	-1.453005000	-1.145037000	-0.285176000
O	0.098510000	0.406334000	-1.932765000
C	-1.109881000	1.920615000	0.883231000
C	-0.057971000	1.401457000	1.725713000
C	-0.498701000	2.618280000	-0.235295000
C	0.912397000	2.495386000	-0.109986000
C	1.191167000	1.734340000	1.096224000
C	-2.556669000	2.018649000	1.260799000
H	-3.235207000	1.838249000	0.407954000
H	-2.764511000	3.044858000	1.632431000
H	-2.821727000	1.322540000	2.077214000
C	2.284406000	-1.834556000	1.207768000
H	3.012718000	-2.601463000	0.869871000
H	2.881018000	-1.027713000	1.676713000
C	0.775034000	-2.519500000	-1.229277000
H	0.698449000	-2.179778000	-2.281139000
H	1.425634000	-3.416032000	-1.187471000
C	2.982318000	-0.583184000	-1.361121000
H	2.505723000	-0.224744000	-2.297312000
H	3.419357000	0.314617000	-0.877569000
C	-2.581824000	-0.990607000	-1.746298000
H	-1.878434000	-0.954177000	-2.603838000

H	-3.155331000	-1.939145000	-1.814744000
C	-0.610632000	-2.777296000	-0.636292000
H	-0.539569000	-3.323942000	0.324063000
H	-1.245063000	-3.384029000	-1.312871000
C	-2.531794000	-1.511552000	1.172918000
H	-1.840358000	-1.681669000	2.024695000
H	-3.087439000	-0.582186000	1.403916000
C	-3.508917000	0.221384000	-1.755715000
H	-4.109174000	0.235556000	-2.686755000
H	-2.927792000	1.161607000	-1.721221000
H	-4.221436000	0.210715000	-0.906027000
C	4.049969000	-1.648134000	-1.625281000
H	4.820798000	-1.244858000	-2.312000000
H	3.625894000	-2.551799000	-2.106811000
H	4.570989000	-1.962537000	-0.699455000
C	-0.235879000	0.831977000	3.100547000
H	-1.141640000	0.201346000	3.178338000
H	-0.342860000	1.649275000	3.846254000
H	0.630345000	0.219475000	3.412138000
C	1.289317000	-2.429889000	2.208540000
H	0.859764000	-3.384040000	1.846640000
H	0.454155000	-1.732363000	2.412430000
H	1.790873000	-2.647172000	3.172055000
C	-3.494078000	-2.691359000	0.995345000
H	-4.232441000	-2.507187000	0.190358000
H	-4.064446000	-2.857958000	1.930912000
H	-2.963761000	-3.636065000	0.762444000
C	1.904136000	3.039783000	-1.086789000
H	2.939396000	2.731613000	-0.850721000
H	1.878162000	4.149579000	-1.089913000
H	1.658781000	2.697134000	-2.112294000
C	2.546910000	1.594151000	1.718009000
H	2.563895000	0.832882000	2.518871000
H	2.830213000	2.561543000	2.185036000
H	3.339481000	1.353731000	0.983532000
C	-1.189498000	3.307655000	-1.366847000
H	-0.943433000	2.795529000	-2.321066000
H	-2.287856000	3.319220000	-1.243085000
H	-0.846849000	4.359000000	-1.453473000

4: G = -2916.09460639

Fe	-0.067394000	0.379370000	0.202429000
P	1.535741000	-0.969952000	-0.550932000
P	-1.486277000	-1.188400000	-0.491114000
O	-0.202813000	1.115615000	-1.481195000
C	0.452083000	0.585355000	2.307390000
C	1.042883000	1.618021000	1.476813000
C	-0.049031000	2.298624000	0.818244000
C	-0.974872000	0.675252000	2.192405000
C	-2.206823000	-2.440052000	0.670466000
H	-2.890234000	-1.874251000	1.334187000
H	-2.848299000	-3.118162000	0.069756000
C	-2.963300000	-0.488074000	-1.357384000
H	-3.584800000	-0.019328000	-0.567017000
H	-2.554737000	0.345279000	-1.964418000
C	-1.300666000	1.727708000	1.265462000
C	0.067310000	3.205278000	-0.374702000
H	1.140067000	3.412971000	-0.604902000
H	-0.439486000	4.179571000	-0.227943000
C	2.417589000	-0.269189000	-2.028053000

H	3.046704000	-1.079416000	-2.452247000
H	1.607729000	-0.057703000	-2.755460000
C	2.477085000	2.048094000	1.509997000
H	3.178295000	1.192913000	1.542542000
H	2.662282000	2.654484000	2.422220000
H	2.745629000	2.673018000	0.639228000
C	-0.613267000	-2.209726000	-1.781443000
H	-1.188915000	-3.127574000	-2.017782000
H	-0.584028000	-1.587068000	-2.699986000
C	3.237133000	0.991066000	-1.766182000
H	4.042079000	0.824884000	-1.022291000
H	2.589926000	1.807205000	-1.392554000
H	3.721105000	1.341927000	-2.699525000
C	2.872439000	-1.615777000	0.558643000
H	3.364866000	-0.732476000	1.014009000
H	2.345305000	-2.132325000	1.387574000
C	0.801957000	-2.522728000	-1.290524000
H	1.449419000	-2.903805000	-2.105775000
H	0.788316000	-3.291887000	-0.493082000
C	-3.786799000	-1.463776000	-2.203829000
H	-3.191323000	-1.899609000	-3.030123000
H	-4.646425000	-0.935746000	-2.663042000
H	-4.200982000	-2.298407000	-1.603712000
N	-0.589708000	2.525849000	-1.504346000
C	-1.184795000	-3.233067000	1.490157000
H	-1.683602000	-3.788065000	2.309164000
H	-0.423834000	-2.565738000	1.943666000
H	-0.651154000	-3.982167000	0.872866000
C	1.178760000	-0.267348000	3.302443000
H	0.756363000	-1.289245000	3.366730000
H	1.098297000	0.180036000	4.316798000
H	2.255228000	-0.354755000	3.070800000
N	-0.285882000	3.102507000	-2.707925000
C	3.905125000	-2.534878000	-0.100640000
H	4.633273000	-2.893796000	0.653950000
H	4.481370000	-2.012680000	-0.889653000
H	3.436707000	-3.429789000	-0.556379000
C	-2.662604000	2.231026000	0.903341000
H	-2.707010000	2.506023000	-0.168301000
H	-2.900923000	3.141951000	1.493376000
H	-3.453028000	1.487529000	1.119893000
C	-1.952429000	-0.067247000	3.047601000
H	-2.963379000	-0.100496000	2.599986000
H	-2.049977000	0.457208000	4.022607000
H	-1.626170000	-1.099853000	3.268476000
H	-0.932881000	2.781459000	-3.436395000
H	0.693795000	2.930288000	-3.001091000

5: G = -2731.02183330 (def2-TZVP)

Fe	5.554032000	9.887301000	2.831914000
P	3.931074000	8.455991000	3.210911000
P	4.397623000	11.174313000	4.127044000
C	7.276050000	8.997545000	3.635435000
C	6.946173000	8.334400000	2.398587000
C	7.523124000	10.382029000	3.332506000
C	6.948456000	9.307305000	1.347561000
C	7.326834000	10.570356000	1.922714000
C	4.608264000	11.678380000	2.456513000
C	2.692779000	10.603250000	4.536038000
C	4.130999000	7.263332000	4.609323000

C	2.369261000	9.360476000	3.696348000
C	3.379675000	7.388132000	1.808384000
C	4.848252000	12.509907000	5.289995000
C	6.750529000	9.028981000	-0.106116000
H	7.701826000	8.721412000	-0.569650000
H	6.025492000	8.222840000	-0.274795000
H	6.400477000	9.916971000	-0.646699000
C	6.874940000	6.856897000	2.191154000
H	7.896636000	6.471908000	2.041891000
H	6.458704000	6.318874000	3.050761000
H	6.299705000	6.589671000	1.296942000
C	7.567631000	11.826540000	1.152539000
H	8.543254000	11.773681000	0.644581000
H	6.811047000	11.988561000	0.372245000
H	7.587781000	12.710783000	1.801473000
C	7.557394000	8.333358000	4.943900000
H	6.973855000	7.415207000	5.075755000
H	8.621805000	8.053742000	5.005538000
H	7.345076000	8.995099000	5.792769000
C	8.060566000	11.395266000	4.289999000
H	7.697628000	11.224120000	5.311078000
H	9.160486000	11.340617000	4.319347000
H	7.800420000	12.420614000	3.997275000
C	2.077736000	6.605157000	2.000368000
H	1.859678000	6.016896000	1.098517000
H	2.137218000	5.900248000	2.840265000
H	1.220049000	7.268450000	2.172978000
C	3.809419000	13.634423000	5.380792000
H	3.614859000	14.078542000	4.395498000
H	2.855681000	13.276298000	5.789437000
H	4.175690000	14.428195000	6.045707000
C	4.204477000	7.915730000	5.991194000
H	3.233273000	8.331060000	6.290270000
H	4.487711000	7.176097000	6.751695000
H	4.946936000	8.724864000	6.014465000
C	4.241508000	10.758027000	1.438881000
H	4.646681000	10.935747000	0.440380000
H	3.247787000	10.313452000	1.410518000
H	5.272993000	12.518900000	2.246144000
H	5.821577000	12.890777000	4.951140000
H	5.019618000	12.042373000	6.272091000
H	2.693859000	10.373635000	5.611069000
H	1.972413000	11.414930000	4.369539000
H	1.856119000	9.651271000	2.770616000
H	1.696420000	8.677230000	4.232008000
H	3.292285000	6.552394000	4.565677000
H	5.041430000	6.683466000	4.407379000
H	4.214052000	6.702608000	1.602794000
H	3.310743000	8.054299000	0.935773000

5: G = -2729.76546187

Fe	5.558082000	9.891452000	2.830551000
P	3.935580000	8.445489000	3.199738000
P	4.406436000	11.175749000	4.151894000
C	7.267413000	9.003120000	3.642624000
C	6.936824000	8.331512000	2.404442000
C	7.510352000	10.393518000	3.330082000
C	6.933976000	9.302869000	1.342646000
C	7.316419000	10.573729000	1.911927000
C	4.622050000	11.684517000	2.469393000

C	2.685875000	10.596316000	4.541818000
C	4.137602000	7.251030000	4.610507000
C	2.365087000	9.360719000	3.688310000
C	3.381017000	7.375245000	1.786610000
C	4.852505000	12.517563000	5.324342000
C	6.734629000	9.012520000	-0.112497000
H	7.689460000	8.681751000	-0.575149000
H	5.990573000	8.210124000	-0.278747000
H	6.397240000	9.906725000	-0.669729000
C	6.866780000	6.848826000	2.203817000
H	7.898453000	6.459782000	2.065920000
H	6.440050000	6.307747000	3.068810000
H	6.296798000	6.571133000	1.297735000
C	7.565407000	11.826263000	1.130449000
H	8.548542000	11.761636000	0.617795000
H	6.804825000	11.989849000	0.341345000
H	7.593567000	12.724880000	1.775326000
C	7.560693000	8.347223000	4.957057000
H	6.987903000	7.412827000	5.101306000
H	8.638128000	8.080267000	5.018385000
H	7.341193000	9.014788000	5.811957000
C	8.056580000	11.413105000	4.281950000
H	7.698890000	11.248025000	5.315986000
H	9.166038000	11.356532000	4.305741000
H	7.796709000	12.447572000	3.984588000
C	2.078159000	6.591615000	1.973589000
H	1.866838000	5.985675000	1.069869000
H	2.127388000	5.888773000	2.829281000
H	1.207347000	7.258437000	2.129445000
C	3.827037000	13.655778000	5.401251000
H	3.653185000	14.112710000	4.406809000
H	2.851222000	13.309337000	5.794742000
H	4.192735000	14.450348000	6.081737000
C	4.200846000	7.907238000	5.992246000
H	3.215232000	8.309379000	6.298741000
H	4.501343000	7.169457000	6.762159000
H	4.934433000	8.737777000	6.016312000
C	4.254610000	10.757339000	1.448196000
H	4.656802000	10.948991000	0.439251000
H	3.245593000	10.318896000	1.409779000
H	5.277638000	12.546339000	2.259911000
H	5.845265000	12.881929000	4.993486000
H	5.010350000	12.038710000	6.314247000
H	2.679951000	10.359591000	5.625175000
H	1.964447000	11.420644000	4.375312000
H	1.856575000	9.658696000	2.750477000
H	1.680539000	8.666233000	4.214594000
H	3.299537000	6.525225000	4.558143000
H	5.061783000	6.675200000	4.405803000
H	4.228183000	6.690546000	1.580384000
H	3.319347000	8.053664000	0.910584000

5 \: G = -2730.34201948

Fe	5.602682000	9.821873000	2.854850000
P	3.940959000	8.441410000	3.213966000
P	4.444884000	11.257023000	4.070656000
C	7.366816000	8.905790000	3.649059000
C	7.039823000	8.252288000	2.410159000
C	7.563749000	10.312128000	3.364498000
C	7.029098000	9.243166000	1.362629000

C	7.372836000	10.516324000	1.945285000
C	4.161042000	11.937865000	2.352803000
C	2.790137000	10.605574000	4.606152000
C	4.127009000	7.218274000	4.601462000
C	2.413665000	9.412955000	3.714467000
C	3.369349000	7.386509000	1.797303000
C	4.891308000	12.621673000	5.226534000
C	6.811411000	8.967129000	-0.091798000
H	7.767736000	8.668470000	-0.572483000
H	6.088948000	8.144595000	-0.255162000
H	6.440041000	9.857954000	-0.632750000
C	6.934149000	6.774124000	2.195328000
H	7.944311000	6.357161000	1.994680000
H	6.540214000	6.240012000	3.080524000
H	6.302720000	6.521004000	1.323117000
C	7.574807000	11.799195000	1.201484000
H	8.585223000	11.828258000	0.740721000
H	6.843775000	11.924366000	0.378074000
H	7.494533000	12.679185000	1.867948000
C	7.643611000	8.236502000	4.960442000
H	7.073605000	7.296491000	5.080883000
H	8.721363000	7.974641000	5.038314000
H	7.406819000	8.891387000	5.820595000
C	8.093131000	11.320342000	4.339611000
H	7.685579000	11.169057000	5.357369000
H	9.198465000	11.234474000	4.412875000
H	7.871556000	12.359084000	4.028493000
C	1.999645000	6.715368000	1.941141000
H	1.792349000	6.079507000	1.057253000
H	1.940901000	6.059208000	2.832648000
H	1.179353000	7.456771000	2.009265000
C	3.839903000	13.731929000	5.342477000
H	3.617322000	14.191984000	4.358929000
H	2.888639000	13.360107000	5.771239000
H	4.208532000	14.536578000	6.009553000
C	4.258217000	7.846476000	5.991438000
H	3.295951000	8.271121000	6.339263000
H	4.564995000	7.087861000	6.738274000
H	5.015262000	8.655912000	6.002141000
C	4.392990000	10.692733000	1.476486000
H	4.930740000	10.921454000	0.537790000
H	3.437513000	10.204262000	1.203734000
H	4.913799000	12.731220000	2.172777000
H	3.150311000	12.395642000	2.255436000
H	5.860630000	13.017700000	4.861334000
H	5.100250000	12.151977000	6.211524000
H	2.887542000	10.307309000	5.669346000
H	2.028773000	11.410832000	4.557542000
H	1.938987000	9.766454000	2.776850000
H	1.683386000	8.743461000	4.211566000
H	3.263807000	6.521099000	4.561586000
H	5.025564000	6.617719000	4.352890000
H	4.169093000	6.630180000	1.657147000
H	3.403645000	8.037897000	0.900219000

Fe-ON2: G = -2915.50326874

Fe	-0.071387000	-0.437710000	0.143276000
P	-1.372518000	1.335694000	-0.067973000
P	1.560062000	0.852517000	-0.656091000
O	-0.512745000	-0.856026000	-1.860477000

C	1.137169000	-1.817456000	1.202535000
C	0.509203000	-0.853157000	2.088282000
C	0.096496000	-2.504991000	0.502279000
C	-1.189207000	-1.998364000	0.951588000
C	-0.924874000	-1.002480000	1.954799000
C	2.584433000	-2.203103000	1.218533000
H	2.904797000	-2.687322000	0.278599000
H	2.763087000	-2.928983000	2.041228000
H	3.252332000	-1.341794000	1.406357000
C	-1.642329000	2.570246000	1.295453000
H	-2.272740000	3.380239000	0.873804000
H	-2.263165000	2.058628000	2.056569000
C	-0.654281000	2.379075000	-1.444489000
H	-0.886712000	1.855754000	-2.395906000
H	-1.147615000	3.371176000	-1.488549000
C	-3.117171000	0.987011000	-0.623811000
H	-3.049674000	0.188163000	-1.391184000
H	-3.615068000	0.515549000	0.250230000
C	2.330868000	0.252280000	-2.246261000
H	1.499356000	0.222707000	-2.980657000
H	3.027021000	1.043159000	-2.595896000
C	0.301641000	-3.624295000	-0.472470000
H	0.447562000	-4.579761000	0.075873000
H	1.200333000	-3.475210000	-1.102183000
C	0.859963000	2.499053000	-1.243551000
H	1.094569000	3.252832000	-0.466703000
H	1.373526000	2.822631000	-2.171058000
C	3.001104000	1.375200000	0.390369000
H	2.548933000	1.867027000	1.276662000
H	3.481035000	0.448891000	0.764897000
C	3.027056000	-1.103471000	-2.162268000
H	3.424188000	-1.404019000	-3.152289000
H	2.322508000	-1.889442000	-1.827315000
H	3.880725000	-1.090084000	-1.455568000
C	-3.937730000	2.168872000	-1.150090000
H	-4.955482000	1.833114000	-1.433341000
H	-3.479931000	2.622882000	-2.051214000
H	-4.058328000	2.966576000	-0.390687000
C	1.208347000	-0.083863000	3.165222000
H	2.204921000	0.275285000	2.849215000
H	1.363647000	-0.734079000	4.054058000
H	0.620235000	0.789364000	3.503634000
C	-0.370608000	3.143547000	1.925411000
H	0.136773000	3.860365000	1.251451000
H	0.352471000	2.343008000	2.175180000
H	-0.608953000	3.691101000	2.858628000
C	4.031589000	2.289658000	-0.277589000
H	4.554896000	1.786807000	-1.114581000
H	4.805556000	2.590848000	0.456479000
H	3.574150000	3.219416000	-0.670949000
C	-2.538617000	-2.543837000	0.591619000
H	-3.329581000	-1.772318000	0.656442000
H	-2.825541000	-3.364174000	1.285013000
H	-2.570205000	-2.972157000	-0.428940000
N	-1.298547000	-1.558381000	-2.440013000
N	-2.022533000	-2.214237000	-3.039365000
C	-1.947575000	-0.405717000	2.871463000
H	-1.595469000	0.532353000	3.337942000
H	-2.153887000	-1.120331000	3.697044000
H	-2.914573000	-0.210403000	2.368695000
H	-0.569491000	-3.778919000	-1.137164000

Fe-ON2H: G = -2916.10134059

Fe	0.128817000	0.468814000	0.101491000
P	1.355982000	-1.396627000	-0.015516000
P	-1.556448000	-0.831581000	-0.641093000
O	0.603001000	0.583380000	-1.724699000
C	-1.061861000	1.684165000	1.408349000
C	-0.197472000	0.791941000	2.154000000
C	-0.235612000	2.552498000	0.613177000
C	1.139353000	2.207893000	0.859209000
C	1.168927000	1.148693000	1.833329000
C	-2.529535000	1.877555000	1.641906000
H	-3.099979000	2.028583000	0.706634000
H	-2.677730000	2.787160000	2.262257000
H	-2.977024000	1.034803000	2.198693000
C	1.571009000	-2.569546000	1.404590000
H	2.381964000	-3.271070000	1.116809000
H	1.969668000	-1.969182000	2.245929000
C	0.625636000	-2.430567000	-1.378452000
H	0.903843000	-1.912023000	-2.317209000
H	1.082898000	-3.440610000	-1.392633000
C	3.083058000	-1.030925000	-0.576781000
H	2.961292000	-0.251201000	-1.355400000
H	3.591393000	-0.543149000	0.280346000
C	-2.294441000	-0.144976000	-2.197494000
H	-1.450448000	-0.123898000	-2.915486000
H	-3.026439000	-0.891464000	-2.571622000
C	-0.701784000	3.697300000	-0.227242000
H	-0.381480000	4.653909000	0.237819000
H	-1.802491000	3.724787000	-0.320870000
C	-0.895514000	-2.487279000	-1.218334000
H	-1.186970000	-3.235972000	-0.456776000
H	-1.397984000	-2.774116000	-2.163771000
C	-2.997238000	-1.300817000	0.424031000
H	-2.559061000	-1.760410000	1.335291000
H	-3.472293000	-0.356942000	0.752446000
C	-2.921325000	1.240363000	-2.062494000
H	-3.293091000	1.593077000	-3.044659000
H	-2.178667000	1.977472000	-1.703905000
H	-3.784676000	1.243796000	-1.366409000
C	3.898682000	-2.218480000	-1.096809000
H	4.911808000	-1.879320000	-1.391646000
H	3.435981000	-2.679999000	-1.991351000
H	4.031237000	-3.010835000	-0.332935000
C	-0.625804000	-0.122621000	3.260740000
H	-1.599788000	-0.604390000	3.052307000
H	-0.739270000	0.446254000	4.208887000
H	0.115406000	-0.921031000	3.446716000
C	0.319398000	-3.344076000	1.826597000
H	0.034287000	-4.102944000	1.072335000
H	-0.548082000	-2.674223000	1.985810000
H	0.502078000	-3.884580000	2.776169000
C	-4.028816000	-2.232111000	-0.221032000
H	-4.524364000	-1.761053000	-1.092623000
H	-4.823078000	-2.481140000	0.510692000
H	-3.581985000	-3.188494000	-0.557845000
C	2.332792000	2.897432000	0.281059000
H	3.210743000	2.225621000	0.225751000
H	2.617934000	3.761737000	0.919316000
H	2.122531000	3.276225000	-0.735630000

N	0.840947000	1.831985000	-2.283832000
N	1.154196000	1.798259000	-3.482394000
C	2.393596000	0.714076000	2.578672000
H	2.257809000	-0.248121000	3.105285000
H	2.624227000	1.472544000	3.357012000
H	3.288783000	0.641147000	1.932494000
H	-0.253650000	3.652721000	-1.238966000
H	1.179670000	0.794922000	-3.814612000

TS1: G = -2916.06761173 (i = -1214 cm-1)

Fe	-0.100543000	-0	
474065000	0.060759000		
P	-1.329523000	1.394813000	-0.182412000
P	1.651132000	0.854466000	-0.550175000
O	-0.261832000	-0.632433000	-1.912320000
C	1.014486000	-1.865849000	1.211484000
C	0.333028000	-0.910228000	2.063465000
C	0.026003000	-2.562055000	0.440172000
C	-1.296702000	-2.123440000	0.875334000
C	-1.086302000	-1.037567000	1.820818000
C	2.455937000	-2.261076000	1
328255000			
H	2.817704000	-2.804080000	0.436665000
H	2.571700000	-2.940317000	2.201549000
H	3.126409000	-1.398686000	1.504348000
C	-1.638333000	2.599251000	1.199592000
H	-2.178854000	3.461670000	0.755427000
H	-2.355087000	2.105651000	1.885266000
C	-0.496760000	2.415999000	-1.499382000
H	-0.669157000	1.872739000	-2.450963000
H	-0.966719000	3.417983000	-1.582838000
C	-3.024255000	1.040080000	-0.861259000
H	-2.837551000	0.526104000	-1.826888000
H	-3.467600000	0.270810000	-0.193791000
C	2.578620000	0.241270000	-2.042663000
H	1.811555000	0.184921000	-2.841165000
H	3.295761000	1.040264000	-2.327583000
C	0.319051000	-3.681866000	-0.516443000
H	0.643869000	-4.587955000	0.039524000
H	1.133940000	-3.414608000	-1.217909000
C	1.004030000	2.505283000	-1.189629000
H	1.202418000	3.261531000	-0.403703000
H	1.586388000	2.811883000	-2.082963000
C	2.964301000	1.376168000	0.655436000
H	2.415252000	1.870457000	1.484666000
H	3.396196000	0.447231000	1.081061000
C	3.280404000	-1.105534000	-1.870300000
H	3.807162000	-1.390264000	-2.803767000
H	2.547379000	-1.904738000	-1.642965000
H	4.034566000	-1.086886000	-1.056734000
C	-3.964936000	2.238053000	-1.049413000
H	-4.903802000	1.910457000	-1.541283000
H	-3.515438000	3.023843000	-1.690985000
H	-4.247501000	2.702843000	-0.083563000
C	0.967924000	-0.179453000	3.208564000
H	1.975387000	0.202031000	2.959854000
H	1.085549000	-0.874112000	4.069625000
H	0.354235000	0.671284000	3.559973000
C	-0.387324000	3.067776000	1.952161000
H	0.213014000	3.780088000	1.352065000

H	0.266152000	2.213275000	2.215530000
H	-0.665751000	3.587990000	2.890796000
C	4.075407000	2.283883000	0.108906000
H	4.700790000	1.765241000	-0.645282000
H	4.749196000	2.598116000	0.932249000
H	3.674792000	3.207215000	-0.357779000
C	-2.547285000	-2.538240000	0.317218000
H	-3.469402000	-2.126247000	0.759752000
H	-2.629781000	-3.598428000	0.014339000
H	-2.269499000	-2.148362000	-1.084491000
N	-1.100224000	-1.150447000	-2.734319000
N	-1.925341000	-2.024414000	-2.270443000
C	-2.177701000	-0.440379000	2.659898000
H	-1.844161000	0.466366000	3.197981000
H	-2.491911000	-1.182063000	3.425942000
H	-3.082059000	-0.186767000	2.071779000
H	-0.561881000	-3.950139000	-1.126711000
H	-2.587259000	-2.308801000	-3.009354000

INT1: G = -2916.07097328

Fe	-0.102134000	0.445011000	0
180632000			
P	1.604390000	-0.771644000	-0.628712000
P	-1.329606000	-1.361554000	-0.172603000
O	-0.423606000	1.108812000	-1.653197000
C	1.043668000	1.574974000	1.577247000
C	0.271998000	2.458177000	0.762627000
C	-1.150784000	2.195613000	0.992755000
C	0.139492000	0.665307000	2.249816000
C	-1.578475000	-2.650148000	1.142015000
H	-2.038928000	-2.111753000	1.994263000
H	-2.350207000	-3.355386000	0.768008000
C	-3.067294000	-1.020577000	-0.733641000
H	-3.623176000	-0.740314000	0.184922000
H	-3.009057000	-0.095748000	-1.344054000
C	-1.205932000	1.012665000	1.860716000
C	-2.215131000	2.836373000	0.373662000
H	-2.054959000	3.725301000	-0.250583000
H	-3.252212000	2.517758000	0.545372000
C	2.435632000	-0.014283000	-2.115479000
H	3.087363000	-0.789622000	-2.570280000
H	1.612589000	0.179348000	-2.833209000
C	0.780636000	3.603940000	-0.054140000
H	1.884192000	3.616301000	-0.116701000
H	0.461866000	4.566020000	0.401058000
H	0.378903000	3.586992000	-1.087058000
C	-0.553596000	-2.281166000	-1.597884000
H	-1.018489000	-3.278769000	-1.735840000
H	-0.781697000	-1.682908000	-2.505014000
C	3.214987000	1.267495000	-1.829540000
H	4.056677000	1.092810000	-1.128763000
H	2.558159000	2.041628000	-1.390273000
H	3.649295000	1.681559000	-2.761550000
C	3.020611000	-1.364168000	0.419131000
H	3.518934000	-0.462142000	0.823333000
H	2.551896000	-1.869137000	1.290429000
C	0.957871000	-2.374461000	-1.373165000
H	1.500341000	-2.604449000	-2.312265000
H	1.196777000	-3.184390000	-0.657375000
C	-3.780083000	-2.148866000	-1.485734000

H	-3.287414000	-2.378979000	-2.451033000
H	-4.824910000	-1.856015000	-1.713157000
H	-3.827906000	-3.088209000	-0.898431000
N	-1.554928000	1.536896000	-2.028309000
C	-0.325159000	-3.404986000	1.591056000
H	-0.530392000	-3.988848000	2.510055000
H	0.509423000	-2.711544000	1.812627000
H	0.019668000	-4.123193000	0.821830000
C	2.506687000	1.719486000	1.866921000
H	2.924911000	0.821528000	2.356585000
H	2.656567000	2.568907000	2.567185000
H	3.102579000	1.934914000	0.960564000
N	-1.502281000	2.135964000	-3.202993000
C	4.037515000	-2.279661000	-0.268427000
H	4.816084000	-2.597082000	0.454023000
H	4.557159000	-1.769105000	-1.103466000
H	3.570467000	-3.200137000	-0.671517000
C	-2.464740000	0.539673000	2.519945000
H	-3.314974000	0.465557000	1.814927000
H	-2.763348000	1.269361000	3.303216000
H	-2.341289000	-0.437491000	3.022814000
C	0.522649000	-0.299514000	3.329079000
H	-0.220920000	-1.109816000	3.444694000
H	0.593830000	0.221334000	4.308829000
H	1.506818000	-0.768721000	3.137368000
H	-2.385927000	2.494614000	-3.571070000
H	-0.599854000	2.305410000	-3.672889000

TS2: G = -2916.06644147 (i = -188 cm-1)

Fe	-0.090088000	0.430083000	0.172919000
P	1.602744000	-0.763403000	-0.657732000
P	-1.304888000	-1.397421000	-0.151397000
O	-0.527429000	1.075490000	-1.605839000
C	1.036853000	1.541955000	1.615702000
C	0.346286000	2.443405000	0.745070000
C	-1.084057000	2.205327000	0.869187000
C	0.063718000	0.686623000	2.256771000
C	-1.499721000	-2.683786000	1.173997000
H	-1.966323000	-2.151613000	2.028273000
H	-2.257801000	-3.410852000	0.813525000
C	-3.059888000	-1.083726000	-0.663135000
H	-3.609678000	-0.872339000	0.276567000
H	-3.038267000	-0.129634000	-1.231938000
C	-1.247603000	1.074301000	1.782304000
C	-2.062851000	2.787879000	0.036376000
H	-1.843201000	3.735298000	-0.474703000
H	-3.124486000	2.541200000	0.170558000
C	2.409777000	0.028071000	-2.137587000
H	3.009552000	-0.753592000	-2.649442000
H	1.571115000	0.292262000	-2.813913000
C	0.935468000	3.554031000	-0.067481000
H	2.037625000	3.586975000	0.007046000
H	0.549796000	4.532415000	0.290283000
H	0.668028000	3.468150000	-1.139753000
C	-0.548534000	-2.291868000	-1.598075000
H	-1.004804000	-3.292983000	-1.737890000
H	-0.801408000	-1.680699000	-2.489634000
C	3.260763000	1.255613000	-1.818577000
H	4.123583000	1.006906000	-1.167647000
H	2.661490000	2.033399000	-1.311226000

H	3.671203000	1.700882000	-2.746851000
C	3.032040000	-1.346321000	0.376056000
H	3.519926000	-0.443974000	0.791005000
H	2.577932000	-1.873278000	1.241852000
C	0.966791000	-2.367705000	-1.403032000
H	1.494218000	-2.579894000	-2.354572000
H	1.231453000	-3.179817000	-0.698751000
C	-3.746701000	-2.198559000	-1.458888000
H	-3.267399000	-2.360864000	-2.444137000
H	-4.805390000	-1.931443000	-1.650850000
H	-3.749778000	-3.167508000	-0.919252000
N	-1.703272000	1.582243000	-1.792888000
C	-0.222769000	-3.399756000	1.617858000
H	-0.405401000	-3.986739000	2.539579000
H	0.590966000	-2.680102000	1.833394000
H	0.139833000	-4.109184000	0.848784000
C	2.489708000	1.628337000	1.970225000
H	2.853416000	0.711998000	2.469183000
H	2.642466000	2.467553000	2.682086000
H	3.128635000	1.826269000	1.089084000
N	-1.768986000	2.203944000	-2.977478000
C	4.057265000	-2.233447000	-0.336441000
H	4.846746000	-2.551214000	0.373878000
H	4.561353000	-1.700005000	-1.166680000
H	3.601465000	-3.153879000	-0.752200000
C	-2.560020000	0.656982000	2.370433000
H	-3.393508000	0.765812000	1.651451000
H	-2.796478000	1.303283000	3.242925000
H	-2.552851000	-0.386013000	2.739244000
C	0.352907000	-0.267676000	3.374142000
H	-0.425117000	-1.047620000	3.471309000
H	0.396980000	0.271248000	4.345630000
H	1.326093000	-0.777473000	3.238890000
H	-2.664262000	2.661992000	-3.162125000
H	-0.911612000	2.621805000	-3.368509000

INT2: G = -5646.43478620

Fe	-0.285196000	0.593823000	-0.135864000
P	1.570659000	-0.607392000	-0.370250000
P	-1.357166000	-1.274634000	-0.765688000
N	-0.151037000	1.155130000	-1.805565000
C	-1.775083000	1.225235000	1.276299000
C	-0.587375000	0.745426000	1.955134000
C	-1.396497000	2.328824000	0.442287000
C	0.022779000	2.553776000	0.611050000
C	0.512421000	1.605438000	1.570343000
C	-3.186078000	0.832997000	1.593103000
H	-3.814807000	0.719531000	0.691030000
H	-3.647415000	1.629540000	2.214751000
H	-3.238585000	-0.099321000	2.182341000
C	2.332598000	-1.555038000	1.028070000
H	3.337159000	-1.874204000	0.680361000
H	2.508000000	-0.827768000	1.843671000
C	1.228750000	-1.895491000	-1.665044000
H	1.239981000	-1.357117000	-2.632577000
H	2.045889000	-2.644281000	-1.691637000
C	2.964648000	0.378066000	-1.094683000
H	2.494089000	0.966860000	-1.909395000
H	3.272036000	1.113107000	-0.322246000
C	-2.438475000	-1.016485000	-2.248519000

H	-1.748815000	-0.694864000	-3.054889000
H	-2.831047000	-2.010852000	-2.546917000
C	-2.318129000	3.163527000	-0.390386000
H	-2.240637000	4.231535000	-0.100491000
H	-3.372365000	2.857501000	-0.266202000
C	-0.133076000	-2.541009000	-1.408767000
H	-0.053027000	-3.331633000	-0.638496000
H	-0.540264000	-3.021361000	-2.320998000
C	-2.393087000	-2.262249000	0.412211000
H	-1.743781000	-2.457561000	1.291405000
H	-3.203107000	-1.598097000	0.768113000
C	-3.564021000	-0.002094000	-2.066357000
H	-4.137465000	0.116767000	-3.006707000
H	-3.163903000	0.990574000	-1.786235000
H	-4.285541000	-0.320659000	-1.287448000
C	4.165722000	-0.423611000	-1.603717000
H	4.942946000	0.261542000	-1.994503000
H	3.886248000	-1.107297000	-2.429243000
H	4.644506000	-1.027220000	-0.807737000
C	-0.573210000	-0.249001000	3.074258000
H	-1.279904000	-1.081961000	2.902485000
H	-0.876620000	0.244205000	4.022590000
H	0.429889000	-0.681450000	3.239979000
C	1.532865000	-2.761570000	1.526911000
H	1.534521000	-3.589630000	0.791912000
H	0.480810000	-2.498919000	1.749763000
H	1.980952000	-3.158570000	2.458868000
C	-2.971868000	-3.565780000	-0.148840000
H	-3.673801000	-3.382690000	-0.985815000
H	-3.540457000	-4.093387000	0.642303000
H	-2.186532000	-4.261289000	-0.504548000
C	0.817946000	3.664181000	0.001265000
H	1.876427000	3.378855000	-0.148819000
H	0.806345000	4.553296000	0.667496000
H	0.405552000	3.970960000	-0.975343000
N	-0.248658000	1.680104000	-2.877135000
C	1.850203000	1.692685000	2.237727000
H	2.093899000	0.791599000	2.828272000
H	1.834164000	2.544518000	2.950471000
H	2.677555000	1.887638000	1.529027000
H	-2.069775000	3.098603000	-1.468772000
O	0.703734000	2.183147000	-3.677891000
C	0.670662000	2.272284000	-7.618051000
C	-0.708612000	2.208630000	-7.210468000
C	1.402802000	1.266711000	-6.870240000
C	-0.836843000	1.208213000	-6.183965000
C	0.475064000	0.635174000	-5.981319000
Fe	0.525115000	2.678690000	-5.541620000
P	-0.597430000	4.539803000	-5.047175000
P	2.294874000	4.050105000	-5.389163000
C	0.808646000	-0.500987000	-5.068397000
H	1.784903000	-0.344510000	-4.568324000
H	0.036687000	-0.637687000	-4.287981000
H	0.875804000	-1.451427000	-5.639664000
C	-2.090682000	0.745991000	-5.509366000
H	-2.062992000	0.955315000	-4.419110000
H	-2.986026000	1.240918000	-5.928321000
H	-2.229833000	-0.347898000	-5.635018000
C	2.795303000	0.771160000	-7.122671000
H	2.752486000	-0.231447000	-7.599402000
H	3.355795000	1.426202000	-7.813591000

H	3.387062000	0.663458000	-6.192484000
C	-1.823465000	2.894538000	-7.935049000
H	-1.567850000	3.930708000	-8.229135000
H	-2.031792000	2.341577000	-8.876457000
H	-2.763539000	2.912106000	-7.354672000
C	1.152709000	3.048587000	-8.806641000
H	2.251002000	3.011039000	-8.916002000
H	0.719044000	2.623632000	-9.737170000
H	0.847819000	4.113164000	-8.768474000
C	3.616628000	4.112125000	-6.696825000
H	3.104470000	4.470846000	-7.611462000
H	3.928176000	3.071624000	-6.904018000
C	1.762664000	5.859698000	-5.334148000
H	1.864915000	6.223303000	-4.291533000
H	2.450802000	6.469906000	-5.951038000
C	0.313913000	5.968865000	-5.810059000
H	-0.149094000	6.941235000	-5.545153000
H	0.238367000	5.853657000	-6.911566000
C	-2.379613000	4.941031000	-5.378798000
H	-2.499064000	6.020550000	-5.149301000
H	-2.552836000	4.843415000	-6.466235000
C	3.270583000	3.841958000	-3.820653000
H	2.529068000	3.866259000	-2.996569000
H	3.937846000	4.720031000	-3.697289000
C	-0.469270000	4.916251000	-3.228552000
H	-1.033405000	4.105977000	-2.726845000
H	0.589338000	4.738938000	-2.956947000
C	4.055357000	2.531030000	-3.794531000
H	4.588191000	2.411939000	-2.830376000
H	3.375011000	1.665936000	-3.925281000
H	4.820455000	2.488984000	-4.595081000
C	4.832103000	4.987737000	-6.375797000
H	5.430250000	4.583377000	-5.536268000
H	5.501427000	5.040242000	-7.257550000
H	4.552092000	6.029579000	-6.120664000
C	-0.944029000	6.291058000	-2.759846000
H	-0.362568000	7.114545000	-3.220826000
H	-2.013741000	6.468730000	-2.986062000
H	-0.822998000	6.387506000	-1.661469000
C	-3.374692000	4.099974000	-4.576372000
H	-4.415064000	4.335871000	-4.874926000
H	-3.215798000	3.016450000	-4.731883000
H	-3.294973000	4.295862000	-3.488209000

INT3: G = -5898.26297618

Fe	-2.827462000	-0.410854000	0.734253000
P	-2.983644000	-1.678478000	-1.075752000
P	-3.996080000	1.079800000	-0.447374000
O	-0.972774000	0.112101000	0.325296000
C	-3.902139000	-0.027867000	2.550836000
C	-4.201271000	-1.340899000	2.018965000
C	-2.494695000	0.039019000	2.800085000
C	-1.926872000	-1.255621000	2.503613000
C	-2.965302000	-2.107989000	2.022443000
C	-4.898836000	0.966850000	3.064316000
H	-4.651227000	2.010339000	2.794885000
H	-4.907778000	0.912411000	4.173825000
H	-5.927138000	0.747156000	2.728357000
C	-4.349077000	-2.908766000	-1.360383000

H	-4.007568000	-3.571301000	-2.182700000
H	-4.405953000	-3.547184000	-0.457905000
C	-3.107548000	-0.568641000	-2.561622000
H	-2.072182000	-0.230344000	-2.742211000
H	-3.424167000	-1.140712000	-3.456894000
C	-1.445830000	-2.658087000	-1.439463000
H	-0.607878000	-1.975447000	-1.193510000
H	-1.406363000	-3.469909000	-0.684593000
C	-3.400888000	2.836895000	-0.514492000
H	-2.445522000	2.803116000	-1.063932000
H	-4.110314000	3.395329000	-1.159898000
C	-1.758124000	1.182635000	3.419598000
H	-1.407475000	0.909257000	4.438040000
H	-2.396971000	2.078353000	3.521648000
C	-4.023990000	0.618303000	-2.274850000
H	-5.071803000	0.365999000	-2.526629000
H	-3.753202000	1.504049000	-2.883623000
C	-5.815750000	1.283652000	-0.103712000
H	-6.239764000	0.258784000	-0.125028000
H	-5.911407000	1.633972000	0.939186000
C	-3.218118000	3.520765000	0.835716000
H	-2.814541000	4.543927000	0.700446000
H	-2.506588000	2.957679000	1.469768000
H	-4.173211000	3.620535000	1.390163000
C	-1.312525000	-3.210531000	-2.861838000
H	-0.379563000	-3.798505000	-2.963645000
H	-1.274443000	-2.402337000	-3.618598000
H	-2.147046000	-3.886211000	-3.135048000
C	-5.578276000	-1.904911000	1.854713000
H	-6.302206000	-1.149780000	1.496134000
H	-5.951999000	-2.271185000	2.835526000
H	-5.607820000	-2.763553000	1.160542000
C	-5.717984000	-2.314791000	-1.698962000
H	-5.717271000	-1.810693000	-2.685143000
H	-6.053934000	-1.583046000	-0.940131000
H	-6.481483000	-3.115906000	-1.746260000
C	-6.588533000	2.213471000	-1.043610000
H	-6.244653000	3.263735000	-0.968494000
H	-7.664044000	2.206441000	-0.776228000
H	-6.517112000	1.906636000	-2.106046000
C	-0.498780000	-1.619840000	2.727968000
H	-0.329585000	-2.708047000	2.639507000
H	-0.169391000	-1.306549000	3.739850000
H	0.141316000	-1.102712000	1.984865000
N	-0.010498000	0.461808000	-0.476986000
C	-2.830969000	-3.588853000	1.833283000
H	-3.634957000	-4.019712000	1.210200000
H	-2.895122000	-4.092113000	2.821557000
H	-1.858469000	-3.871067000	1.386431000
H	-0.866436000	1.458047000	2.825864000
O	1.171431000	-0.001481000	-0.181513000
C	5.001281000	-0.022314000	-1.422704000
C	4.614964000	1.365434000	-1.375724000
C	4.021305000	-0.714011000	-2.236249000
C	3.378417000	1.533339000	-2.081212000
C	3.015155000	0.239257000	-2.612426000
Fe	3.115370000	0.095679000	-0.497864000
P	3.404149000	0.992147000	1.557957000
P	3.209696000	-1.879475000	0.601566000
C	1.884443000	-0.082492000	-3.540662000
H	1.105474000	-0.709381000	-3.057740000

H	1.403654000	0.835135000	-3.920914000
H	2.259285000	-0.650759000	-4.415791000
C	2.794003000	2.864597000	-2.429531000
H	2.740789000	3.537806000	-1.553497000
H	3.432308000	3.365670000	-3.189048000
H	1.780448000	2.782945000	-2.853943000
C	4.183956000	-2.051724000	-2.892814000
H	4.571018000	-1.892776000	-3.922876000
H	4.919648000	-2.698448000	-2.383029000
H	3.236837000	-2.612200000	-2.985430000
C	5.543944000	2.474974000	-0.997724000
H	6.294262000	2.169794000	-0.246550000
H	6.111882000	2.756786000	-1.911735000
H	5.029479000	3.386603000	-0.649639000
C	6.352325000	-0.520896000	-1.005357000
H	6.447908000	-1.616415000	-1.095311000
H	7.133907000	-0.074257000	-1.656849000
H	6.604599000	-0.239135000	0.036385000
C	4.685789000	-3.008851000	0.458031000
H	5.547258000	-2.418324000	0.829003000
H	4.874253000	-3.179689000	-0.617086000
C	3.250125000	-1.567381000	2.445920000
H	2.212407000	-1.406952000	2.799327000
H	3.641580000	-2.457123000	2.977167000
C	4.103617000	-0.323016000	2.672593000
H	4.108982000	0.009805000	3.729407000
H	5.160952000	-0.492641000	2.378353000
C	4.426081000	2.480268000	1.993314000
H	4.615077000	2.427267000	3.085751000
H	5.413211000	2.358774000	1.512135000
C	1.771259000	-3.033292000	0.400051000
H	0.869430000	-2.407924000	0.533991000
H	1.804912000	-3.753043000	1.244471000
C	1.807724000	1.409924000	2.430059000
H	1.474811000	2.358741000	1.965088000
H	1.070206000	0.644964000	2.124251000
C	1.730513000	-3.757296000	-0.943560000
H	0.882787000	-4.469447000	-0.976383000
H	1.600945000	-3.038993000	-1.776037000
H	2.650806000	-4.341539000	-1.139731000
C	4.592042000	-4.348097000	1.196219000
H	3.804720000	-5.005204000	0.778644000
H	5.552967000	-4.892251000	1.102999000
H	4.395198000	-4.229150000	2.280327000
C	1.887606000	1.560820000	3.949813000
H	2.090005000	0.595512000	4.454399000
H	2.672651000	2.276533000	4.264563000
H	0.928017000	1.941386000	4.351581000
C	3.773213000	3.816527000	1.622683000
H	4.512563000	4.640354000	1.661880000
H	3.341377000	3.799085000	0.601015000
H	2.956549000	4.080506000	2.323176000
C	-0.160558000	1.717867000	-1.185047000
C	0.053253000	2.903161000	-0.459643000
C	-0.572139000	1.767723000	-2.523615000
C	-0.148243000	4.142271000	-1.081717000
C	-0.787529000	3.012629000	-3.137411000
C	-0.576121000	4.201434000	-2.419392000
H	0.356453000	2.843746000	0.591775000
H	-0.713001000	0.841676000	-3.089730000
H	0.018290000	5.069007000	-0.513231000

H	-1.114747000	3.050655000	-4.186792000
H	-0.743644000	5.174569000	-2.903185000

TS3: G = -5898.24389805 (i = -265 cm-1)

Fe	-2.815490000	-0.465665000	0.550099000
P	-2.688110000	-1.255861000	-1.517657000
P	-3.992189000	1.205417000	-0.395330000
O	-1.113966000	0.364284000	0.468317000
C	-4.069932000	-0.573152000	2.296297000
C	-4.217149000	-1.756130000	1.476155000
C	-2.696187000	-0.475611000	2.702349000
C	-1.998088000	-1.616187000	2.177121000
C	-2.921206000	-2.404708000	1.411279000
C	-5.186772000	0.223622000	2.898897000
H	-4.982102000	1.309998000	2.917246000
H	-5.319311000	-0.099223000	3.953641000
H	-6.151558000	0.051563000	2.390659000
C	-3.960067000	-2.428159000	-2.199769000
H	-3.522731000	-2.868166000	-3.119985000
H	-4.040035000	-3.260145000	-1.472525000
C	-2.718603000	0.185879000	-2.690866000
H	-1.705051000	0.622510000	-2.606800000
H	-2.858463000	-0.156523000	-3.735865000
C	-1.093584000	-2.107435000	-1.936144000
H	-0.300963000	-1.510071000	-1.441445000
H	-1.134012000	-3.088667000	-1.422690000
C	-3.498523000	2.947779000	0.018112000
H	-2.465964000	3.062891000	-0.356449000
H	-4.135108000	3.605587000	-0.610219000
C	-2.090994000	0.554900000	3.600527000
H	-1.782327000	0.098677000	4.565394000
H	-2.798965000	1.370639000	3.831833000
C	-3.783767000	1.192625000	-2.263494000
H	-4.768673000	0.931075000	-2.695216000
H	-3.544269000	2.217698000	-2.610486000
C	-5.841622000	1.249316000	-0.199804000
H	-6.199457000	0.226562000	-0.435834000
H	-6.039257000	1.403160000	0.876457000
C	-3.588020000	3.333109000	1.490454000
H	-3.223496000	4.368824000	1.638781000
H	-2.963380000	2.666314000	2.114022000
H	-4.628211000	3.296851000	1.872640000
C	-0.812245000	-2.279565000	-3.432459000
H	0.129089000	-2.844349000	-3.583757000
H	-0.696230000	-1.306251000	-3.946450000
H	-1.606719000	-2.846000000	-3.957605000
C	-5.520770000	-2.355823000	1.048355000
H	-6.270509000	-1.586454000	0.784869000
H	-5.951847000	-2.957748000	1.877435000
H	-5.409666000	-3.032989000	0.182435000
C	-5.337057000	-1.836686000	-2.504206000
H	-5.295325000	-1.105471000	-3.334761000
H	-5.775926000	-1.331255000	-1.623400000
H	-6.039560000	-2.636211000	-2.811217000
C	-6.589110000	2.298325000	-1.028337000
H	-6.302181000	3.331997000	-0.752156000
H	-7.679294000	2.207089000	-0.851374000
H	-6.426270000	2.178649000	-2.117675000
C	-0.553886000	-1.905914000	2.410989000
H	-0.331510000	-2.983355000	2.304490000

H	-0.253088000	-1.597342000	3.431869000
H	0.066691000	-1.338145000	1.683885000
N	-0.357649000	0.741425000	-0.536846000
C	-2.634846000	-3.786136000	0.905342000
H	-3.334953000	-4.110338000	0.114211000
H	-2.741963000	-4.512613000	1.739128000
H	-1.603437000	-3.883997000	0.516122000
H	-1.185438000	0.997848000	3.140370000
O	1.183037000	-0.132099000	-0.108806000
C	4.820049000	-0.043958000	-1.522619000
C	4.603473000	1.316171000	-1.149407000
C	3.685260000	-0.464999000	-2.319165000
C	3.337351000	1.757500000	-1.682347000
C	2.783169000	0.658017000	-2.432240000
Fe	2.918083000	0.037286000	-0.414822000
P	3.338537000	0.642326000	1.748131000
P	3.065847000	-2.091919000	0.399816000
C	1.571263000	0.666683000	-3.309197000
H	0.667170000	0.345595000	-2.755062000
H	1.389673000	1.679900000	-3.712868000
H	1.709565000	-0.014066000	-4.170115000
C	2.869240000	3.180173000	-1.662342000
H	2.288510000	3.436214000	-0.755891000
H	3.732532000	3.872178000	-1.715961000
H	2.216036000	3.390626000	-2.527596000
C	3.625480000	-1.687574000	-3.181880000
H	4.187385000	-1.495684000	-4.121640000
H	4.081941000	-2.578120000	-2.714114000
H	2.589641000	-1.945043000	-3.466184000
C	5.678514000	2.203854000	-0.608258000
H	6.379213000	1.668099000	0.058119000
H	6.281510000	2.566971000	-1.469800000
H	5.291394000	3.095814000	-0.088287000
C	6.145006000	-0.735056000	-1.398752000
H	6.114273000	-1.780487000	-1.748342000
H	6.889840000	-0.205478000	-2.030875000
H	6.543080000	-0.724888000	-0.365028000
C	4.572982000	-3.138442000	0.085480000
H	5.441381000	-2.542300000	0.427370000
H	4.683766000	-3.230641000	-1.012060000
C	3.103815000	-2.003562000	2.259979000
H	2.068989000	-1.830885000	2.614127000
H	3.441227000	-2.969613000	2.683227000
C	4.011576000	-0.838279000	2.640910000
H	4.041475000	-0.655817000	3.733586000
H	5.057354000	-1.002708000	2.306063000
C	4.429277000	2.018685000	2.339880000
H	4.581411000	1.834167000	3.424421000
H	5.421611000	1.889242000	1.870806000
C	1.656332000	-3.243686000	0.059416000
H	0.750820000	-2.619544000	0.165132000
H	1.650805000	-3.985522000	0.885553000
C	1.765308000	0.994259000	2.666129000
H	1.534530000	2.040232000	2.392219000
H	0.984736000	0.378471000	2.182099000
C	1.685596000	-3.934699000	-1.301250000
H	0.808864000	-4.602811000	-1.413551000
H	1.650451000	-3.197265000	-2.121612000
H	2.588745000	-4.559498000	-1.444363000
C	4.583296000	-4.524599000	0.739317000
H	3.748181000	-5.164238000	0.394192000

H	5.524694000	-5.049056000	0.480437000
H	4.539794000	-4.474206000	1.844864000
C	1.805340000	0.828112000	4.185101000
H	1.929978000	-0.229778000	4.490714000
H	2.616479000	1.415442000	4.660481000
H	0.853166000	1.180950000	4.629508000
C	3.865291000	3.423353000	2.105029000
H	4.637960000	4.190491000	2.309065000
H	3.511935000	3.565528000	1.064922000
H	3.010920000	3.638441000	2.776024000
C			
	0.201646000	2.162643000	-0.537138000
C	-0.141554000	2.908445000	0.660478000
C	-0.318157000	2.842308000	-1.766255000
C	-0.114819000	4.305954000	0.620027000
C	-0.332037000	4.245084000	-1.799450000
C	-0.205544000	4.982933000	-0.612139000
H	-0.172160000	2.371688000	1.612867000
H	-0.444931000	2.268860000	-2.690657000
H	-0.057383000	4.878478000	1.558052000
H	-0.444762000	4.764839000	-2.762492000
H	-0.205877000	6.082296000	-0.640579000

6-O: G = -3092.24545702

Fe	-0.158028000	-0.208607000	0.326324000
P	1.362986000	-1.542469000	-0.567507000
P	0.691567000	1.318310000	-1.028799000
N	-1.283193000	-1.152184000	-2.085764000
C	-0.167623000	-1.143598000	2.221935000
O	-1.443743000	-0.682495000	-0.894529000
C	-1.519129000	-0.845538000	1.826349000
C	0.563603000	0.107360000	2.288916000
C	-1.635851000	0.577728000	1.638515000
C	-0.354268000	1.164542000	1.935803000
C	0.294950000	-2.484248000	2.708066000
C	1.931702000	0.307626000	2.867218000
C	-0.097237000	2.631441000	2.101333000
C	-2.620527000	-1.841987000	1.646296000
C	2.947211000	-1.895197000	0.337190000
C	2.178387000	2.288625000	-0.460880000
C	-3.766253000	-1.018013000	-2.283128000
C	-2.478964000	-1.376411000	-2.766660000
C	-2.350836000	-1.993152000	-4.038670000
C	-3.489500000	-2.266361000	-4.802352000
C	-4.763481000	-1.919700000	-4.315476000
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C	-2.883590000	1.315424000	1.267553000
C	0.672205000	-3.239537000	-0.938924000
C	2.038664000	-0.801607000	-2.162359000
C	1.230985000	0.431896000	-2.566401000
C	-0.554531000	2.551996000	-1.627666000
H	-0.426095000	-3.142855000	-0.836374000
H	0.978768000	2.879763000	2.061020000
H	1.396320000	-2.560521000	2.761228000
H	-3.267222000	-1.872264000	2.548859000
H	1.859366000	0.564059000	3.946291000
H	-2.228395000	-2.863185000	1.481224000
H	2.478464000	1.135970000	2.376101000
H	-0.087552000	-2.660275000	3.736058000
H	-0.628665000	3.248283000	1.351251000

H	-0.466792000	2.954603000	3.098113000
H	-2.662635000	2.260309000	0.735736000
H	-0.079273000	-3.312121000	2.075657000
H	2.555931000	-0.600366000	2.789436000
H	1.776477000	3.190206000	0.044725000
H	-3.262468000	-1.582856000	0.783639000
H	-3.473501000	1.573241000	2.173166000
H	-3.536186000	0.704560000	0.615249000
H	2.670997000	-2.297663000	1.331074000
H	-1.344233000	-2.252163000	-4.398211000
H	-3.851921000	-0.516296000	-1.310618000
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H	-5.658984000	-2.130976000	-4.918437000
H	-5.892311000	-1.013817000	-2.688329000
H	3.410007000	-0.903156000	0.523921000
H	2.648140000	1.676163000	0.335356000
H	1.015839000	-3.878952000	-0.098002000
C	3.212830000	2.673393000	-1.523221000
H	4.015967000	3.285319000	-1.065648000
H	3.697048000	1.783186000	-1.971351000
H	2.771776000	3.267344000	-2.346486000
C	1.014245000	-3.868529000	-2.289813000
H	0.598887000	-3.263862000	-3.119633000
H	2.105092000	-3.976147000	-2.449600000
H	0.566555000	-4.880238000	-2.362297000
C	-0.103121000	3.550773000	-2.697179000
H	0.691088000	4.227415000	-2.324524000
H	0.275233000	3.043703000	-3.606832000
H	-0.955399000	4.188108000	-3.007703000
H	-0.923415000	3.078601000	-0.723143000
H	-1.404534000	1.932559000	-1.984630000
H	3.092564000	-0.527024000	-1.949460000
H	2.058012000	-1.559306000	-2.968305000
H	1.789931000	1.100927000	-3.249087000
H	0.294049000	0.116646000	-3.065488000
C	3.925645000	-2.840331000	-0.367006000
H	4.214159000	-2.475640000	-1.372999000
H	4.856921000	-2.938294000	0.226234000
H	3.502702000	-3.857503000	-0.482589000

INT4: G = -3092.23745358

Fe	0.037878000	-0.112629000	0.456905000
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P	1.038267000	1.503035000	-0.710037000
N	-1.262616000	0.126425000	-1.134395000
C	0.178535000	-1.209094000	2.245255000
O	-0.818316000	-1.131125000	-0.968492000
C	-1.218837000	-1.017090000	1.967472000
C	0.792980000	0.099574000	2.373702000
C	-1.489939000	0.393915000	1.961025000
C	-0.247064000	1.086321000	2.171668000
C	0.781394000	-2.525145000	2.631684000
C	2.146300000	0.388292000	2.947298000
C	-0.111879000	2.558436000	2.414837000
C	-2.222627000	-2.118588000	1.843470000
C	3.350004000	-1.516810000	0.233854000
C	2.681808000	2.135788000	-0.082967000
C	-3.508823000	-0.904452000	-1.050084000
C	-2.669703000	0.235339000	-1.047020000
C	-3.253155000	1.522849000	-1.114463000

C	-4.644556000	1.667191000	-1.140462000
C	-5.477259000	0.533792000	-1.113294000
C	-4.900122000	-0.749190000	-1.078837000
C	-2.836098000	1.035355000	1.943132000
C	1.112885000	-3.140147000	-0.714246000
C	2.032061000	-0.641941000	-2.184495000
C	1.376397000	0.730811000	-2.361836000
C	0.068761000	3.022750000	-1.133214000
H	0.054980000	-3.173200000	-0.392819000
H	0.891771000	2.940706000	2.149621000
H	1.879386000	-2.553634000	2.509531000
H	-2.425646000	-2.560293000	2.842638000
H	2.090562000	0.341236000	4.056555000
H	-1.855626000	-2.932356000	1.188869000
H	2.500977000	1.402212000	2.687517000
H	0.574069000	-2.716825000	3.706660000
H	-0.867182000	3.143713000	1.857140000
H	-0.266870000	2.775777000	3.493561000
H	-2.829597000	2.016563000	1.434849000
H	0.344776000	-3.366753000	2.063179000
H	2.915312000	-0.338799000	2.631865000
H	2.458215000	3.057190000	0.495736000
H	-3.179375000	-1.757097000	1.427862000
H	-3.158073000	1.208833000	2.993308000
H	-3.603327000	0.407277000	1.456746000
H	3.228293000	-1.877786000	1.274208000
H	-2.606084000	2.409359000	-1.133771000
H	-3.044388000	-1.898129000	-1.060657000
H	-5.085879000	2.674105000	-1.185210000
H	-6.570679000	0.648977000	-1.140654000
H	-5.545485000	-1.640854000	-1.089623000
H	3.754124000	-0.486579000	0.309971000
H	3.034513000	1.396074000	0.660195000
H	1.702150000	-3.723575000	0.022188000
C	3.774710000	2.399895000	-1.123884000
H	4.683450000	2.797622000	-0.628865000
H	4.071093000	1.471269000	-1.651207000
H	3.464373000	3.137410000	-1.887719000
C	1.248835000	-3.734022000	-2.117909000
H	0.589860000	-3.211442000	-2.838578000
H	2.287974000	-3.696940000	-2.501041000
H	0.939914000	-4.798662000	-2.103210000
C	0.828078000	4.161525000	-1.818893000
H	1.627788000	4.581282000	-1.177528000
H	1.285025000	3.842663000	-2.776698000
H	0.129334000	4.990206000	-2.050990000
H	-0.406098000	3.371046000	-0.194127000
H	-0.745057000	2.637972000	-1.776903000
H	3.135828000	-0.574963000	-2.259861000
H	1.701376000	-1.344589000	-2.970426000
H	1.975721000	1.399739000	-3.009154000
H	0.366467000	0.627829000	-2.802998000
C	4.316884000	-2.427965000	-0.530151000
H	4.478018000	-2.091901000	-1.573957000
H	5.307569000	-2.434316000	-0.032968000
H	3.960358000	-3.476170000	-0.563273000

6-N: G = -3092.25060148

Fe	-0.013048000	-0.012022000	0.469881000
P	1.592538000	-1.285804000	-0.447618000

P	0.887525000	1.567961000	-0.795054000
N	-1.067045000	-0.591070000	-0.904977000
C	-0.002775000	-1.044669000	2.291236000
O	-0.628012000	-1.224042000	-1.914619000
C	-1.354276000	-0.607699000	2.023083000
C	0.822792000	0.137263000	2.445061000
C	-1.364793000	0.827508000	1.977401000
C	-0.015735000	1.277380000	2.210994000
C	0.374296000	-2.454970000	2.632215000
C	2.200444000	0.200163000	3.035636000
C	0.357392000	2.705127000	2.475347000
C	-2.547761000	-1.510312000	1.982353000
C	3.228669000	-1.482031000	0.420281000
C	2.444674000	2.373813000	-0.151830000
C	-3.260512000	-1.624315000	-1.288927000
C	-2.509314000	-0.474776000	-0.973469000
C	-3.132745000	0.769089000	-0.813804000
C	-4.526746000	0.864254000	-0.942993000
C	-5.289813000	-0.284237000	-1.209201000
C	-4.653222000	-1.528065000	-1.381514000
C	-2.560233000	1.728964000	2.034666000
C	1.095252000	-3.067349000	-0.727713000
C	2.163623000	-0.523797000	-2.072295000
C	1.380031000	0.754797000	-2.386717000
C	-0.216812000	2.965663000	-1.312131000
H	0.010032000	-3.116156000	-0.516306000
H	1.450442000	2.863779000	2.477364000
H	1.455428000	-2.650966000	2.504477000
H	-2.812052000	-1.821889000	3.015665000
H	2.138036000	0.586111000	4.075498000
H	-2.352161000	-2.431637000	1.401356000
H	2.882524000	0.877345000	2.485225000
H	0.130566000	-2.665855000	3.695817000
H	-0.099810000	3.411416000	1.755056000
H	-0.015300000	2.997559000	3.480818000
H	-2.429107000	2.651166000	1.435676000
H	-0.179179000	-3.189978000	2.018177000
H	2.678764000	-0.792888000	3.089243000
H	2.114936000	3.284772000	0.387040000
H	-3.433481000	-1.017392000	1.543384000
H	-2.718761000	2.050908000	3.087268000
H	-3.485014000	1.229722000	1.697579000
H	3.014702000	-1.913584000	1.416964000
H	-2.518578000	1.653331000	-0.615410000
H	-2.738681000	-2.578089000	-1.445589000
H	-5.018479000	1.843049000	-0.840151000
H	-6.383692000	-0.209630000	-1.297451000
H	-5.249146000	-2.426702000	-1.599395000
H	3.618843000	-0.459957000	0.604881000
H	2.839808000	1.688964000	0.624309000
H	1.603686000	-3.642809000	0.074012000
C	3.536748000	2.712890000	-1.170576000
H	4.384901000	3.211842000	-0.660183000
H	3.940996000	1.806388000	-1.662398000
H	3.179549000	3.397472000	-1.963138000
C	1.389607000	-3.663874000	-2.104266000
H	0.821987000	-3.133198000	-2.892710000
H	2.466898000	-3.629076000	-2.360632000
H	1.079085000	-4.728048000	-2.128919000
C	0.418885000	4.105358000	-2.113560000
H	1.195142000	4.640450000	-1.532017000

H	0.880027000	3.744024000	-3.053993000
H	-0.352978000	4.850581000	-2.392050000
H	-0.688589000	3.346552000	-0.381614000
H	-1.030071000	2.480653000	-1.891436000
H	3.243792000	-0.300173000	-1.959806000
H	2.068405000	-1.264255000	-2.887662000
H	1.957895000	1.451129000	-3.025150000
H	0.438446000	0.512887000	-2.915934000
C	4.269036000	-2.338483000	-0.309892000
H	4.505986000	-1.946727000	-1.319119000
H	5.217181000	-2.359590000	0.264019000
H	3.933469000	-3.387684000	-0.425568000

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