Supporting Information

to the manuscript

Aminophosphine PN^H complexes of Mn(I), Fe(II), and Co(II) and evaluation of their activities in the transfer hydrogenation of nitriles

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1. General information

All manipulations were carried out using conventional inert atmosphere glovebox (LC Technology Solutions Inc.) and Schlenk techniques. All solvents, including deuterated solvents for NMR analysis, were purchased from VWR and/or Sigma-Aldrich (Merk) and additionally dried by distillation from appropriate drying agents. All reagents, including ammonia borane (AB), nitriles, and reagents and precursors for the synthesis of Mn, Fe, and Co complexes were purchased from VWR and/or Sigma-Aldrich (Merk) and used without further purification. (2-diphenylphosphinobenzylidene)-2,6-dimethylphenylenamine (PN^{DMP} ligand, **2**) was synthesized according to the literature procedure.[1] *cis*-$FeBr_2(CO)_4$ was prepared by the treatment of $Fe(CO)_5$ with Br_2 by the literature procedure.[2] NMR spectra were obtained with JEOL ECA-500 MHz spectrometer (^{1}H: 500 MHz, ^{13}C: 126 MHz, ^{31}P: 202.5 MHz, ^{11}B: 160 MHz, and ^{19}F: 471 MHz). IR spectra were measured using a Nicolet iS10 FT-IR spectrometer. Elemental analyses were performed in the "Nazarbayev University Core Facilities" laboratories using Elementar Unicube CNHS/O elemental analyzer. UV-vis analysis was performed in CH_2Cl_2 using a Thermo Scientific Evolution 60S UV-Vis Spectrophotometer. X-ray crystallographic analysis was performed using Bruker D8 Quest and Bruker Apex II CCD diffractometers at Nazarbayev University Core Facilities (Kazakhstan), University of Windsor (Canada), and Lomonosov Moscow State University (Russia) by Dr. Aishabibi Kassymbek, Dr. Anton Dmitrienko and Dr. Konstantin A. Lyssenko, respectively. Full details can be found in the independently deposited crystallography information files (CIFs). All catalytic transfer hydrogenation reactions were performed under an inert atmosphere (unless noted otherwise) using 10 mL pressure vials (Supelco headspace vials) equipped with magnetic screw caps having PTFE-faced butyl septa. Mechanistic studies were performed using NMR tubes equipped with Teflon valves (J. Young NMR tubes). For details of computational studies, see Section 6 below.

2. Experimental details

Synthesis of ligands and metal complexes

*Preparation of N-(2-(diphenylphosphanyl)benzyl)aniline (PN^H, **1**)*

2-(diphenylphosphino)benzaldehyde (1 g, 3.44 mmol), aniline (336 mg, 3.61 mmol), and (2.18 g, 10.32 mmol) $NaBH(OAc)_3$ were mixed in dichloroethane (DCE) (80 mL) under inert atmosphere and the resulting mixture was stirred at room temperature for 24 h. After the reaction completion, 40 ml saturated $NaHCO_3$ solution were added to the mixture portion-wise. The solvent was evaporated, 25 ml of degassed water were added, and the product was extracted with CH_2Cl_2 (7 mL x 3 times). The organic fraction was collected and dried with Na_2SO_4. The solvent was pumped off resulting in a white solid product, which was dried in a vacuum for 4 h. Yield: 677.4 mg, 64 %. ^{1}H-NMR (500 MHz; $CDCl_3$; δ, ppm): 7.51–7.48 (m, 1 H, aromatic), 7.39–7.27 (m, 11 H, aromatic), 7.19 (t, J = 7.4 Hz, 1 H, aromatic), 7.10 (t, J = 7.8 Hz, 2 H, aromatic), 6.95–6.91 (m, 1 H, aromatic), 6.67 (t, J = 7.3 Hz, 1 H, aromatic), 6.41 (d, J = 8.1 Hz, 2 H, aromatic), 4.50 (s, 2 H, –CH_2N(H)Ph), 3.94 (br s, 1 H, N*H*). ^{13}C{1H}-NMR (126 MHz; $CDCl_3$; δ, ppm): 147.8 (s), 143.4 (d, J = 23.1 Hz), 136.4 (d, J = 9.7 Hz), 135.9 (d, J = 14.9 Hz), 134.1 (d, J = 19.8 Hz), 133.7 (s), 129.21 (s), 129.18 (s), 129.0 (s), 128.8 (d, J = 7.1 Hz), 128.3 (d, J = 5.3 Hz), 127.6 (s), 117.5 (s), 113.0 (s), 47.0 (d, J = 23.4 Hz). ^{31}P{^{1}H}-NMR (202.5 MHz;

$CDCl_3$; δ, ppm): -15.3 (s, 1 P, PPh_2). NMR data are consistent with those previously reported in the literature.[3]

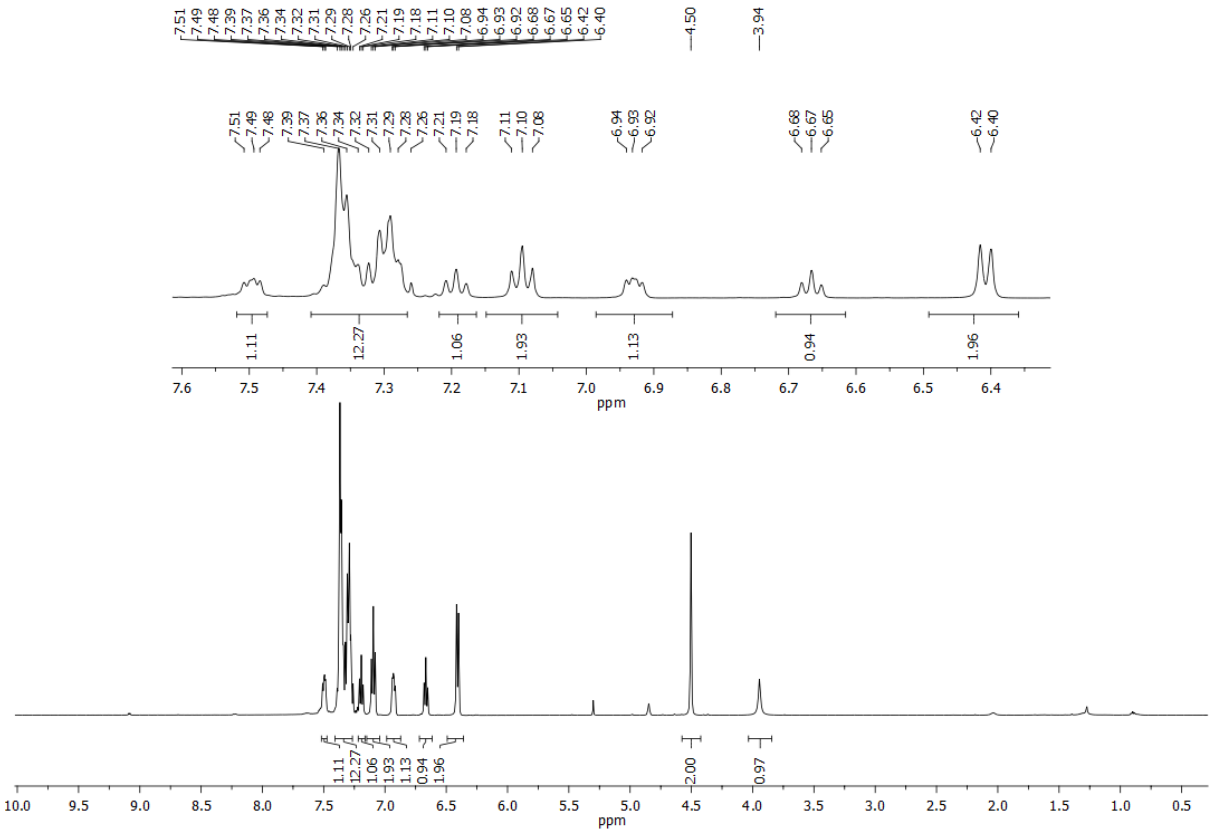


Figure S1. The ^{1}H-NMR spectrum of *N*-(2-(diphenylphosphanyl)benzyl)aniline (PN^H, **1**) in $CDCl_3$.

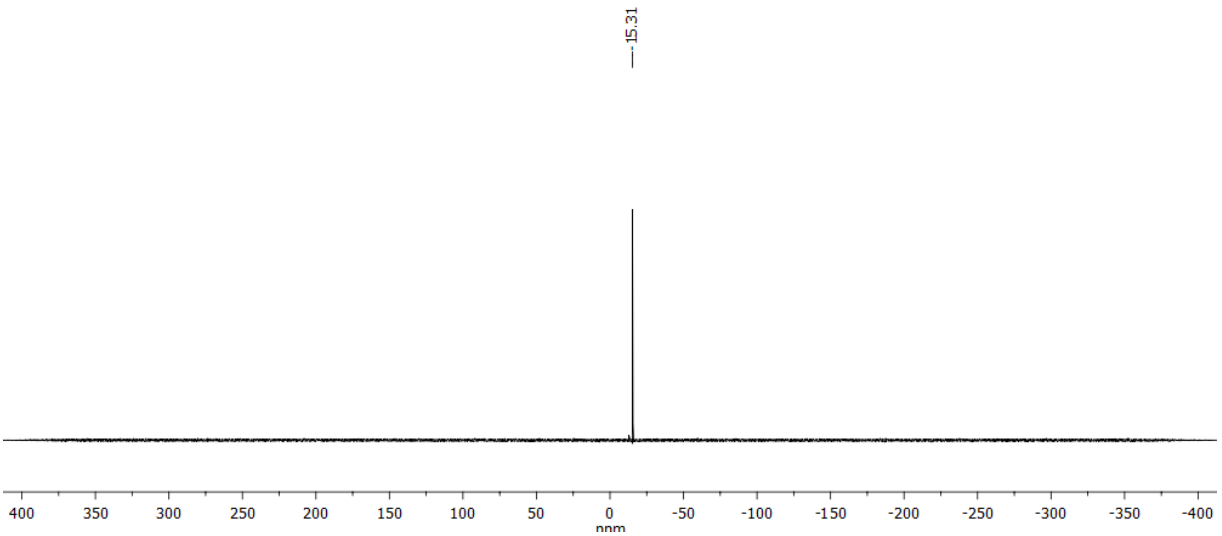


Figure S2. The $^{31}P\{^1H\}$-NMR spectrum of N-(2-(diphenylphosphanyl)benzyl) aniline (PN^H, **1**) in $CDCl_3$.

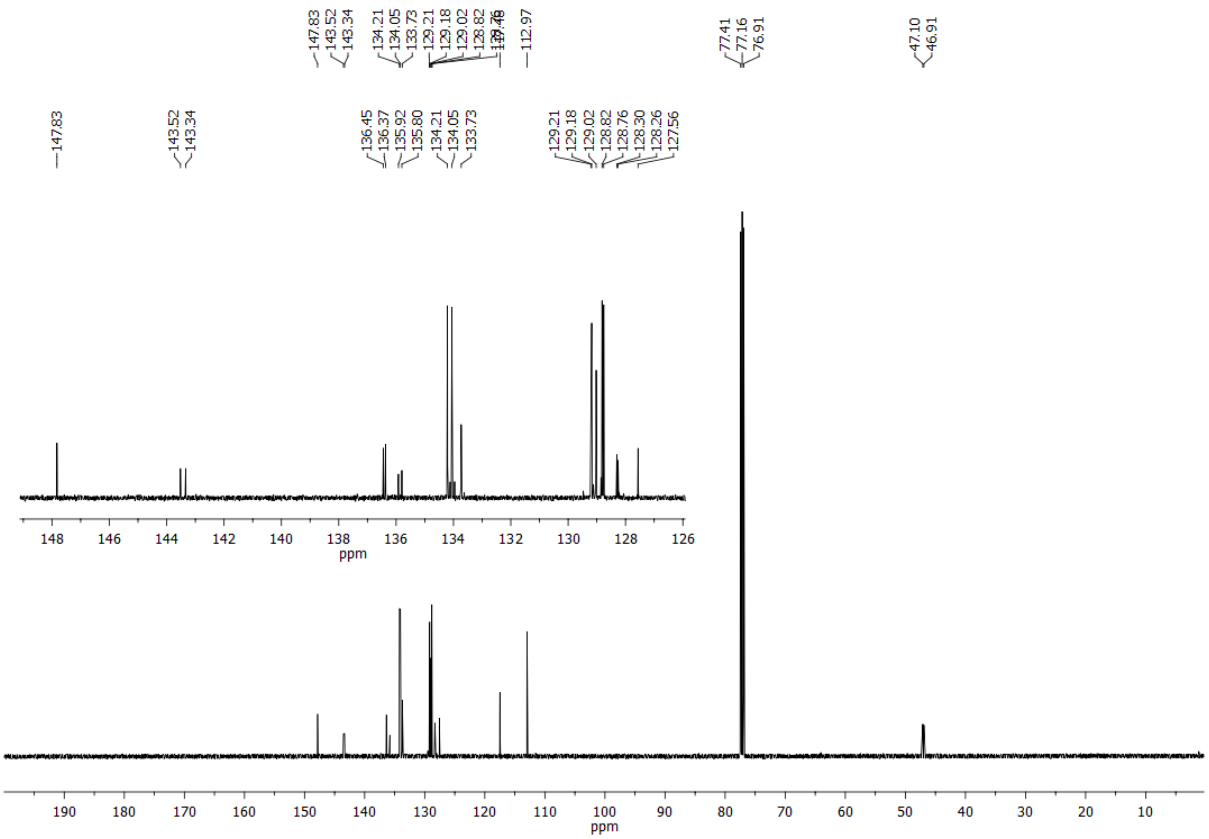


Figure S3. The $^{13}C\{^{1}H\}$-NMR spectrum of N-(2-(diphenylphosphanyl)benzyl) aniline (PN^{H}, **1**) in $CDCl_3$.

*Preparation of 1-(2-(diphenylphosphanyl)phenyl)-N,N-dimethylmethanamine (PN^{Me2}, **3**)*

$[Me_2NH_2]Cl$ (252.8 mg, 3.10 mmol) and NEt_3 (432 µL, 3.10 mmol) were added one by one at room temperature to a solution of 2-(diphenylphosphino)benzaldehyde (300 mg, 1.03 mmol) in 5 mL of MeOH. The reaction mixture was stirred overnight at room temperature forming a yellow suspension. The mixture was cooled to -5 °C, and $NaBH_4$ (101.6 mg, 2.69 mmol) was added portionwise during 1 h. When the addition of $NaBH_4$ was complete, the reaction was stirred at room temperature overnight. After that, the solvent was pumped off, and the residue was redissolved in 25 mL of benzene and filtered through a short column of silica gel. Removal of benzene in a vacuum yielded a yellowish oil of the ligand **3** in 46% yield (151.3 mg). ^{1}H-NMR (500 MHz; $CDCl_3$; δ, ppm): 7.44–7.46 (m, 1 H, aromatic), 7.28–7.33 (m, 7 H, aromatic), 7.22–7.27 (m, 4 H, aromatic) 7.14 (t, J = 7.5 Hz, 1 H, aromatic), 6.86–6.92 (m, 1 H, aromatic), 3.60 (s, 2 H, $-CH_2NMe_2$), 2.06 (s, 6 H, NMe_2). $^{31}P\{^{1}H\}$-NMR (202.5 MHz; $CDCl_3$; δ, ppm): -14.77 (s, 1 P, PPh_2). $^{13}C\{^{1}H\}$-NMR (126 MHz; $CDCl_3$; δ, ppm): 144.2 (d, J = 22.2 Hz), 137.9 (d, J = 10.2 Hz), 136.8 (d, J = 15.2 Hz), 134.0 (s), 133.8 (s), 129.1 (d, J = 5.4 Hz), 128.7 (s), 128.5 (d, J = 6.9 Hz), 128.4 (s), 127.2 (s), 62.3 (d, J = 17.9 Hz), 44.8 (s). NMR data are consistent with those previously reported in the literature.[4]

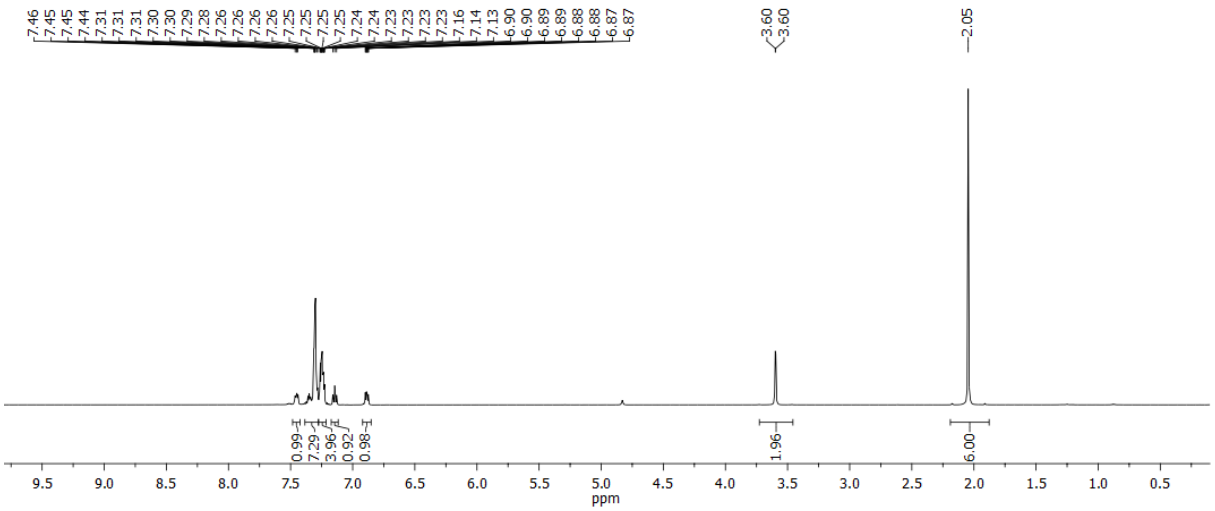


Figure S4. The ^{1}H-NMR spectrum of 1-(2-(diphenylphosphanyl)phenyl)-*N*,*N*-dimethylmethanamine (PN^{Me2}, **3**) in $CDCl_3$.

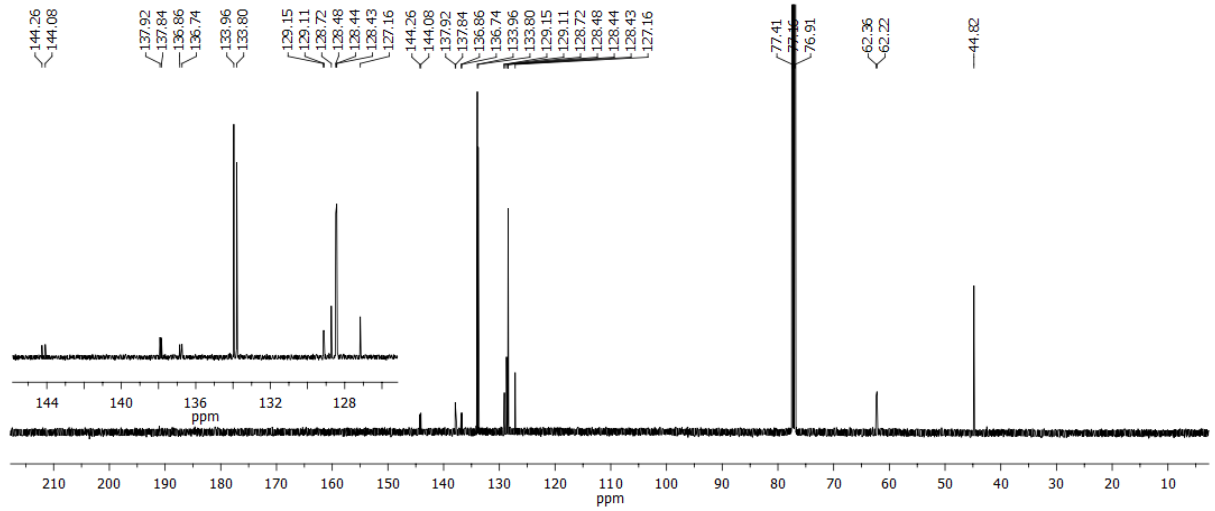


Figure S5. The ^{13}C{^{1}H}-NMR spectrum of 1-(2-(diphenylphosphanyl)phenyl)-*N*,*N*-dimethylmethanamine (PN^{Me2}, **3**) in $CDCl_3$.

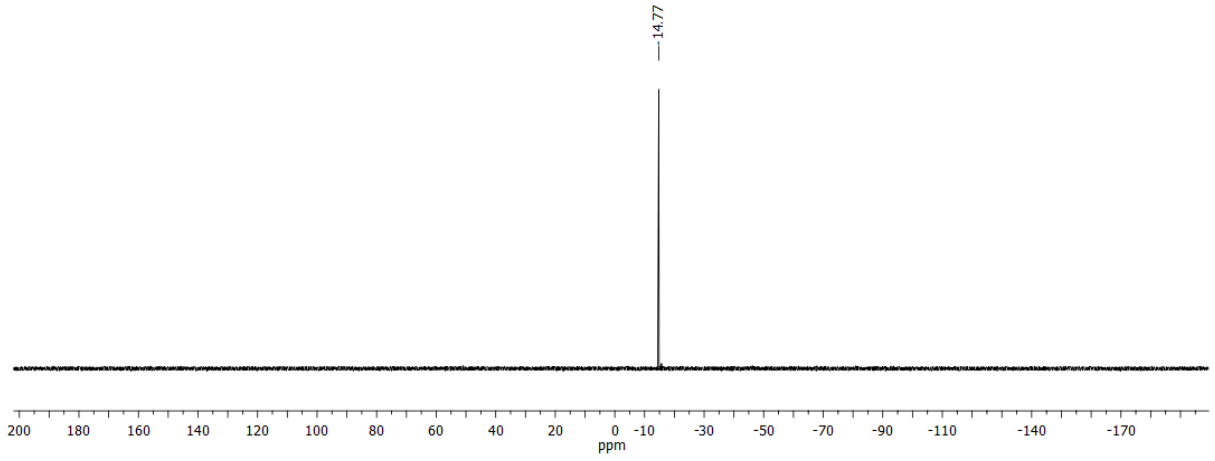


Figure S6. The ^{31P}C{^{1}H}-NMR spectrum of 1-(2-(diphenylphosphanyl)phenyl)-*N*,*N*-dimethylmethanamine (PN^{Me2}, **3**) in $CDCl_3$.

*Preparation of (PN^{H})MnBr(CO)$_3$ (**1-Mn**)*

A solution of *N*-(2-(diphenylphosphanyl)benzyl)aniline ligand **1** (93.6 mg, 0.255 mmol) in 10 mL of toluene was added at room temperature to $Mn(CO)_5Br$ (70.0 mg, 0.255 mmol) in 10 mL of toluene. The resulting mixture was stirred at 80 ºC for 24 h to give an orange suspension. The solvent was pumped off, and the residue was dried in vacuum and recrystallized from CH_2Cl_2/hexanes to give an orange solid. Yield: 106.3 mg, 71%. Single crystals of **1-Mn** suitable for X-ray diffraction analysis were grown at room temperature by layering a dichloroethane (DCE) solution of **1-Mn** with hexanes. ^{1}H-NMR (500 MHz; C_6D_6; δ, ppm): 8.30 (br s, 2 H, aromatic), 7.30–7.36 (m, 2 H, aromatic), 6.86–7.10 (m, 13 H, aromatic), 6.78–6.82 (m, 1 H, aromatic), 6.56–6.61 (m, 1 H, aromatic), 5.02 (d, *J* = 10.1 Hz, 1 H), 4.23–4.33 (m, 1 H), 3.60 (dd, *J* = 12.0, 3.9 Hz, 1 H). ^{31}P{^{1}H}-NMR (202.5 MHz; C_6D_6; δ, ppm): 38.3 (s, 1 P, *P*Ph$_2$). ^{31}P{^{1}H}-NMR (202.5 MHz; $CDCl_3$; δ, ppm): 37.9 (s, 1 P, *P*Ph$_2$). ^{13}C{^{1}H}-NMR (126 MHz; $CDCl_3$; δ, ppm): 223.3 (br s, CO), 222.7 (br d, *J* = 21.9 Hz, CO), 212.6 (br d, *J* = 36.2 Hz, CO), 153.5 (s), 138.7 (d, *J* = 16.1 Hz, s), 136.1 (d, *J* = 9.7 Hz), 133.5 (s), 132.8 (d, *J* = 10.3 Hz), 131.7 (s), 131.41 (s), 131.37 (d, *J* = 6.3 Hz), 130.7 (s), 130.4 (d, *J* = 6.0 Hz), 129.8 (s), 129.1 (d, *J* = 9.3 Hz), 128.9 (d, *J* = 9.7 Hz), 121.5 (s), 118.6 (s), 59.8 (d, *J* = 10.7 Hz). IR (nujol; selected stretches): 1897 cm^{-1} (CO), 1941 cm^{-1} (CO), 2023 cm^{-1} (CO). Elem. analysis (%): calcd. for $C_{28}H_{22}BrMnNO_3P$: C 57.36, H 3.78, N 2.39; found: C: 57.26, H 3.48, N 2.77.

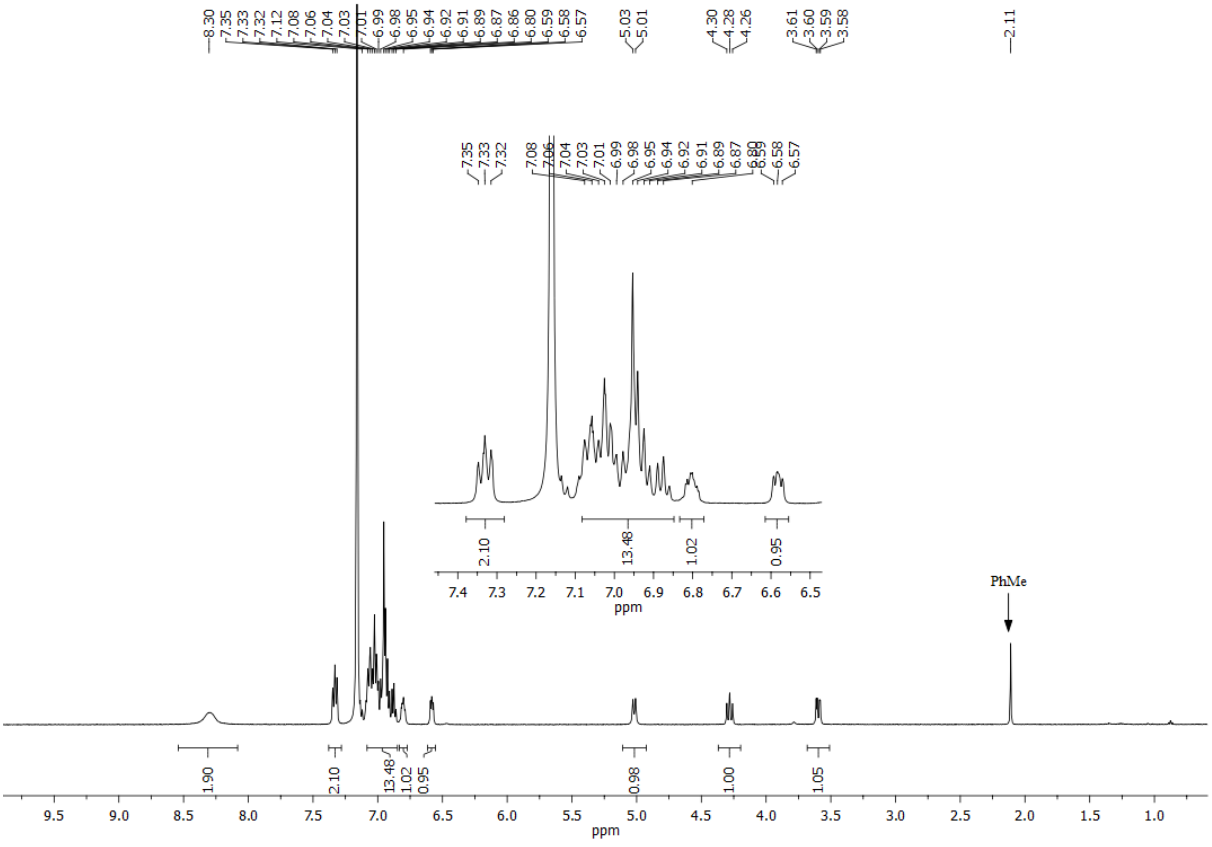


Figure S7. The ^{1}H-NMR spectrum of (PN^{H})MnBr(CO)$_3$ (**1-Mn**) in C_6D_6.

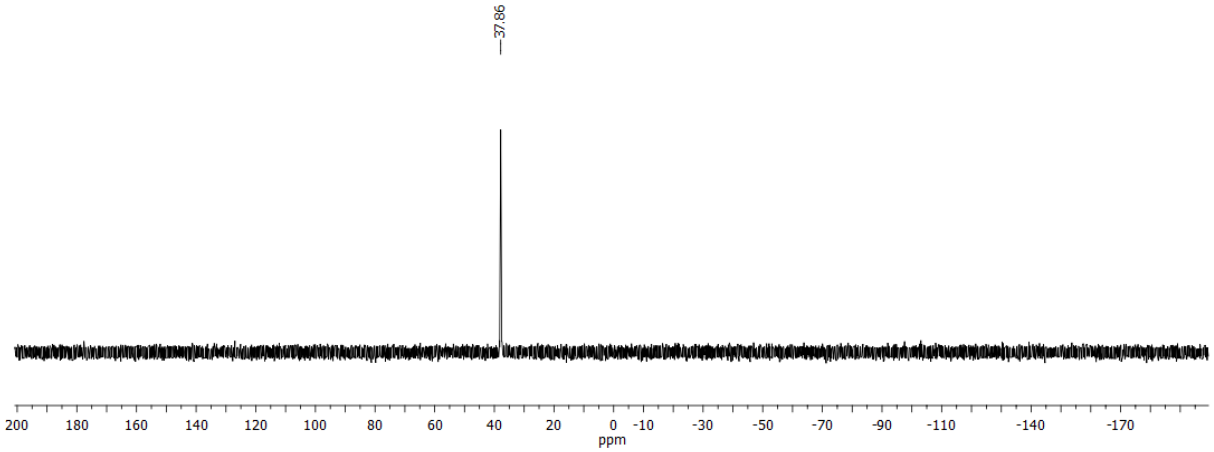


Figure S8. The $^{31}P\{^{1}H\}$-NMR spectrum of $(PN^{H})MnBr(CO)_3$ (**1-Mn**) in $CDCl_3$.

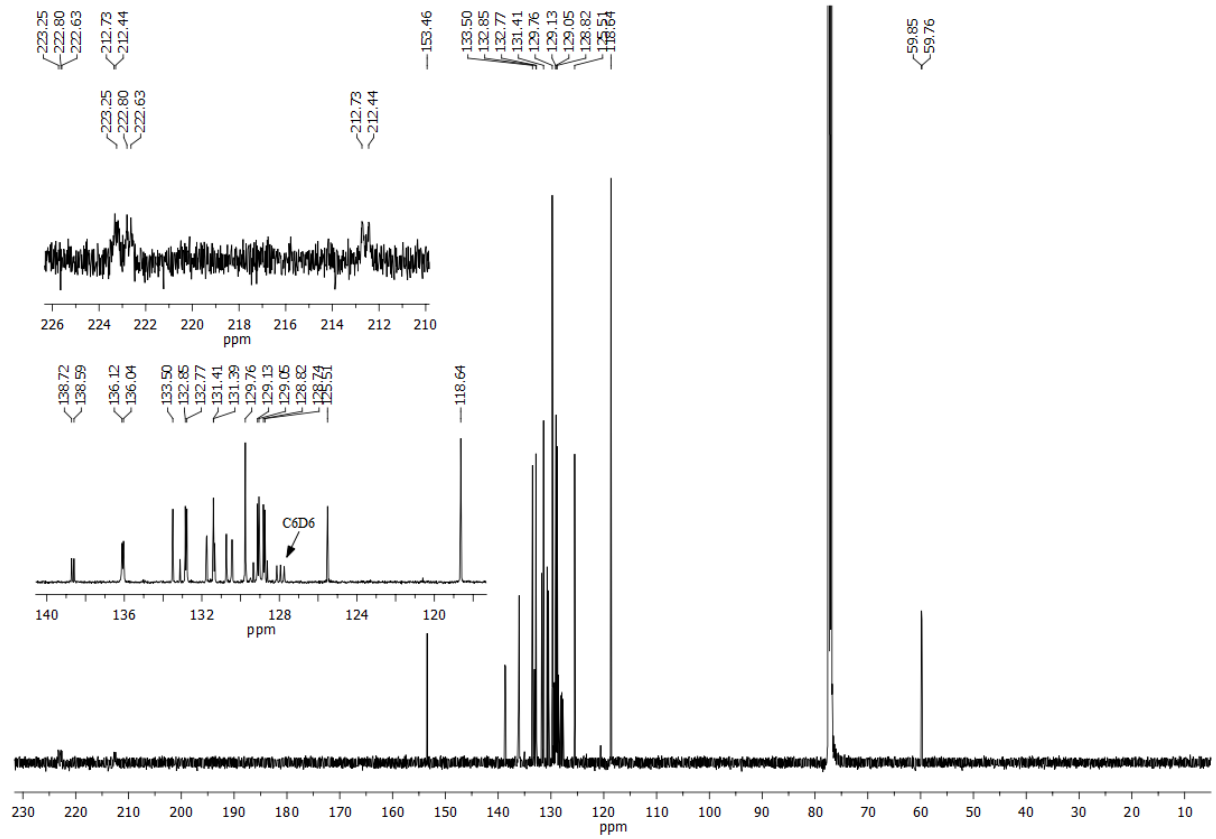


Figure S9. The $^{13}C\{^{1}H\}$-NMR spectrum of $(PN^{H})MnBr(CO)_3$ (**1-Mn**) in $CDCl_3$.

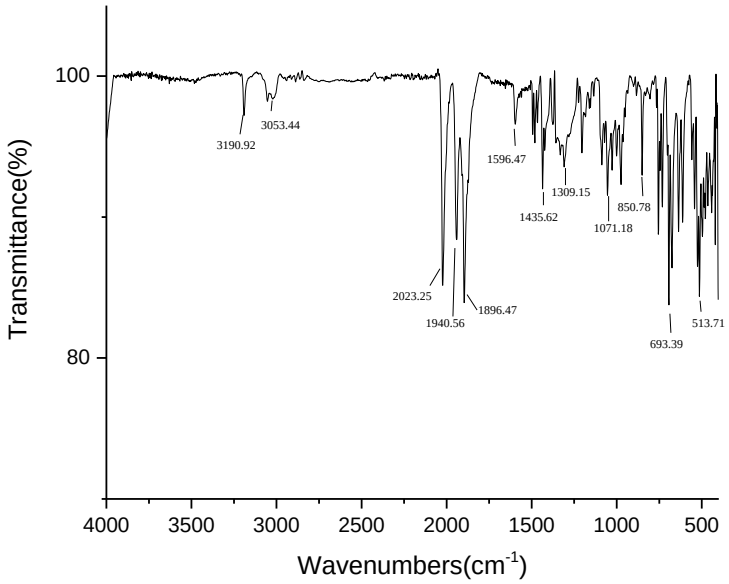


Figure S10. The IR spectrum of $(PN^{H})MnBr(CO)_3$ (**1-Mn**) in nujol.

*Preparation of $(PN^{H})CoCl_2$ (**1-Co**)*

A solution of *N*-(2-(diphenylphosphanyl)benzyl)aniline ligand **1** (100 mg, 0.27 mmol) in 20 mL of THF was added at room temperature to anhydrous $CoCl_2$ (35.3 mg, 0.27 mmol). The resulting mixture was stirred at room temperature for 24 h. The solvent was pumped off, and the blue residue was dried in vacuum and recrystallized from CH_2Cl_2/hexanes to give bright blue crystals of **1-Co**. Yield: 57.1 mg, 42%. The produced compound is paramagnetic, μ_{eff}.= 4.19 μB (determined in $CHCl_3$ with a $CDCl_3$ insert by Evans method[5]), which corresponds to S = 3/2 and 3 unpaired electrons. Elem. analysis (%): calcd. for $C_{25}H_{22}Cl_2CoNP$: C 60.39, H 4.46, N 2.82; found: C: 60.02, H 4.77, N 3.01. Single crystals of **1-Co** suitable for X-ray diffraction analysis were grown from CH_2Cl_2 solution at -28 °C.

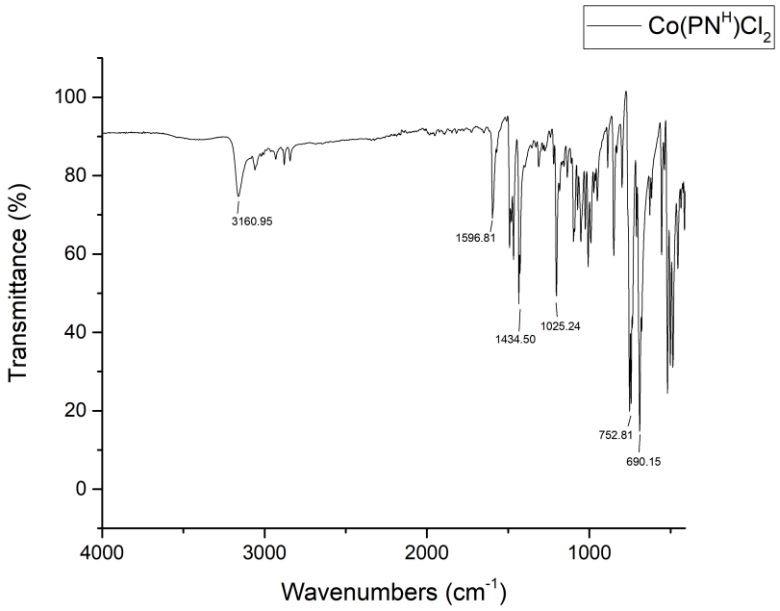


Figure S11. The IR spectrum of $(PN^{H})CoCl_2$ (**1-Co**) in nujol.

*Preparation of (PN^H)$FeBr_2$ (**1-Fe**)*

A solution of *N*-(2-(diphenylphosphanyl)benzyl)aniline ligand **1** (136 mg, 0.37 mmol) in 20 mL of toluene was added at room temperature to $FeBr_2$ (79.8 mg, 0.37 mmol) in 10 mL of toluene. The resulting mixture was stirred at room temperature for 24 h, the solvent was pumped off to give a brown residue which was dried in vacuum and recrystallized from CH_2Cl_2/hexanes. Yield: 168.3 mg, 78%. The produced compound is paramagnetic, $\mu_{eff.}$= 5.3 μB (determined in $CHCl_3$ with a $CDCl_3$ insert by Evans method[5]), S = 2 corresponds to 4 unpaired electrons. Elem. analysis (%): calcd. for $C_{25}H_{22}Br_2FeNP$: C 51.50, H 3.80, N 2.40; found: C: 51.11, H 4.17, N 2.19. Single crystals of **1-Fe** suitable for X-ray diffraction analysis were obtained by layering the CH_2Cl_2 solution of **1-Fe** with hexanes at room temperature.

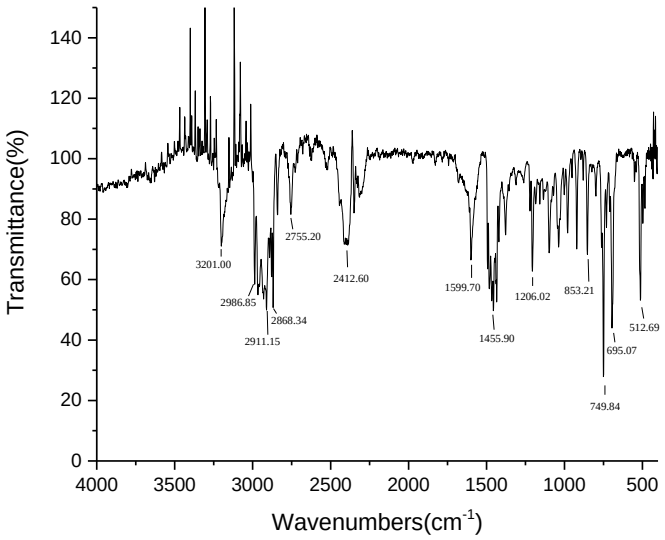


Figure S12. The IR spectrum of (PN^H)$FeBr_2$ (**1-Fe**) in nujol.

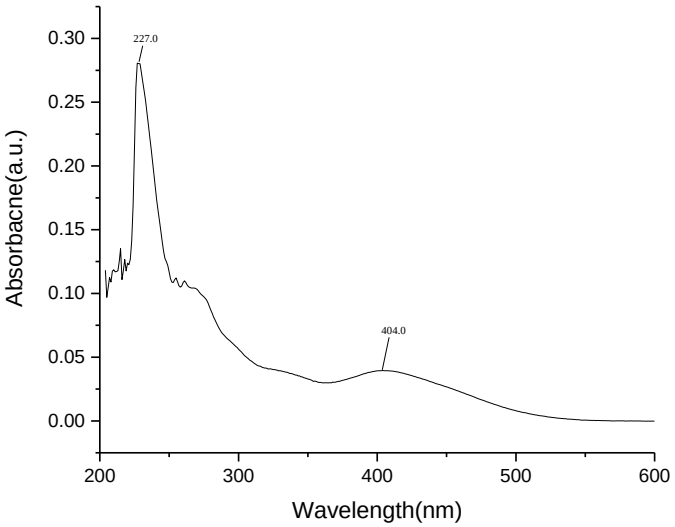


Figure S13. The UV-vis spectrum of (PN^H)$FeBr_2$ (**1-Fe**) in CH_2Cl_2.

*NMR scale reaction of cis-$FeBr_2(CO)_4$ with PN^H ligand **1***

A cold (-30 °C) solution of *N*-(2-(diphenylphosphanyl)benzyl)aniline ligand **1** (20 mg, 0.054 mmol) in 0.6 mL of CD_2Cl_2 was added to a solid *cis*-$FeBr_2(CO)_4$ (17 mg, 0.052 mmol) in a vial in a glovebox. Immediately after the addition of ligand **1**, the release of CO gas was observed, resulting in a dark brown solution, which was transferred to an NMR tube, and the progress of the reaction was monitored by NMR spectroscopy. After 20 min at room temperature, NMR analysis revealed the formation of a mixture of a paramagnetic complex **1-Fe** (minor component) and a diamagnetic low-spin derivative **1-Fe'** (major component), assigned to *cis-CO,cis-Br*-(PN^H)$FeBr_2(CO)_2$ based on the ligand field considerations and similarity with the related *cis-CO,cis-Br*-(PN^{Py})$FeBr_2(CO)_2$ complex, the preparation of which by the analogous reaction of *cis*-$FeBr_2(CO)_4$ with a PN^{Py} ligand was previously reported by Kirchner *et al.*[6] Overall, the reaction of *cis*-$FeBr_2(CO)_4$ with ligand **1** was monitored by NMR for 7 h at room temperature showing >90% decomposition of **1-Fe'** within 7 h (Figures S14-S15; approx. 50% decomposition of **1-Fe'** was observed in 2 h at room temperature) give **1-Fe**. An analogous result was also obtained when the reaction was repeated in the dark. The treatment of *cis*-$FeBr_2(CO)_4$ with ligand **1** was repeated in CH_2Cl_2 and after 20 min at room temperature the mixture was subjected to IR analysis, showing the presence of two non-equivalent CO ligands in **1-Fe'** (Figure S16). Due to the instability of **1-Fe'**, all attempts to isolate this complex by crystallization from the reaction mixture and or by performing the reaction at low temperatures were unsuccessful and led to mixtures of **1-Fe'** and **1-Fe**. Similarly, due to the instability of **1-Fe'** and rather long $^{13}C\{^1H\}$-NMR acquisition times, all attempts to observe ^{13}C-resonances for CO ligands of **1-Fe'** were unsuccessful. *cis-CO,cis-Br*-(PN^H)$FeBr_2(CO)_2$ (**1-Fe'**): ^1H-NMR (500 MHz; CD_2Cl_2; δ, ppm): 7.68–7.39 (m, 12 H aromatic), 7.35 (s, 1 H, aromatic), 7.23 (m, 3 H, aromatic), 7.11–6.99 (m, 1 H, aromatic), 6.87 (d, J = 7.1 Hz, 2 H, aromatic), 5.85 (br s, 1 H, N*H*), 4.92 (d, J = 12.9 Hz, 1 H, CH_2N), 4.39 (d, J = 12.1 Hz, 1 H, CH_2N). $^{31}P\{^1H\}$-NMR (202.5 MHz; CD_2Cl_2; δ, ppm): 60.14 (s, 1 P, PPh$_2$). IR (CH_2Cl_2; selected stretches): 2002 cm^{-1} (CO), 2050 cm^{-1} (CO).

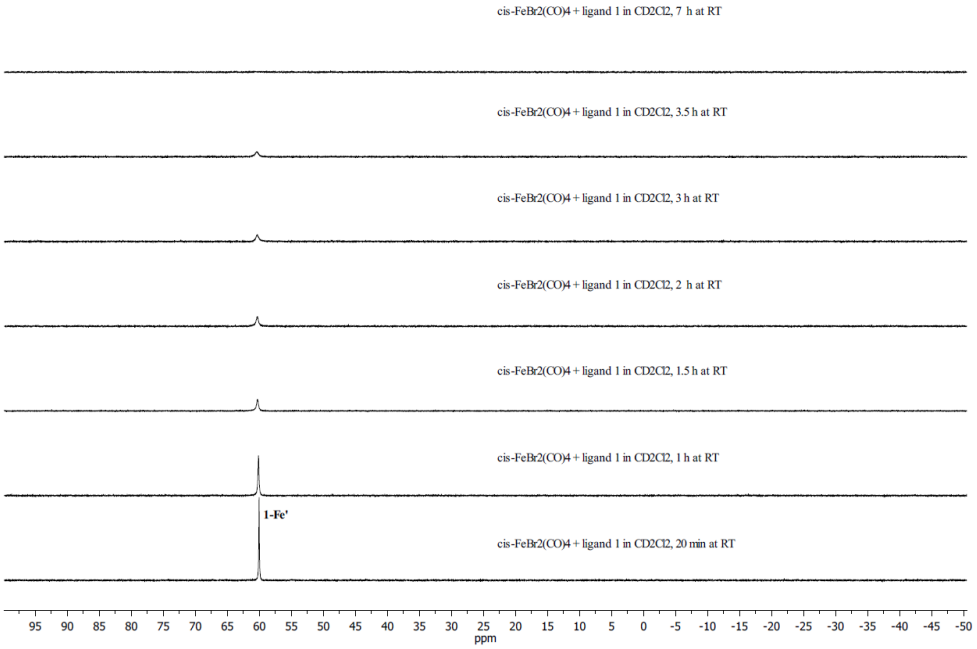
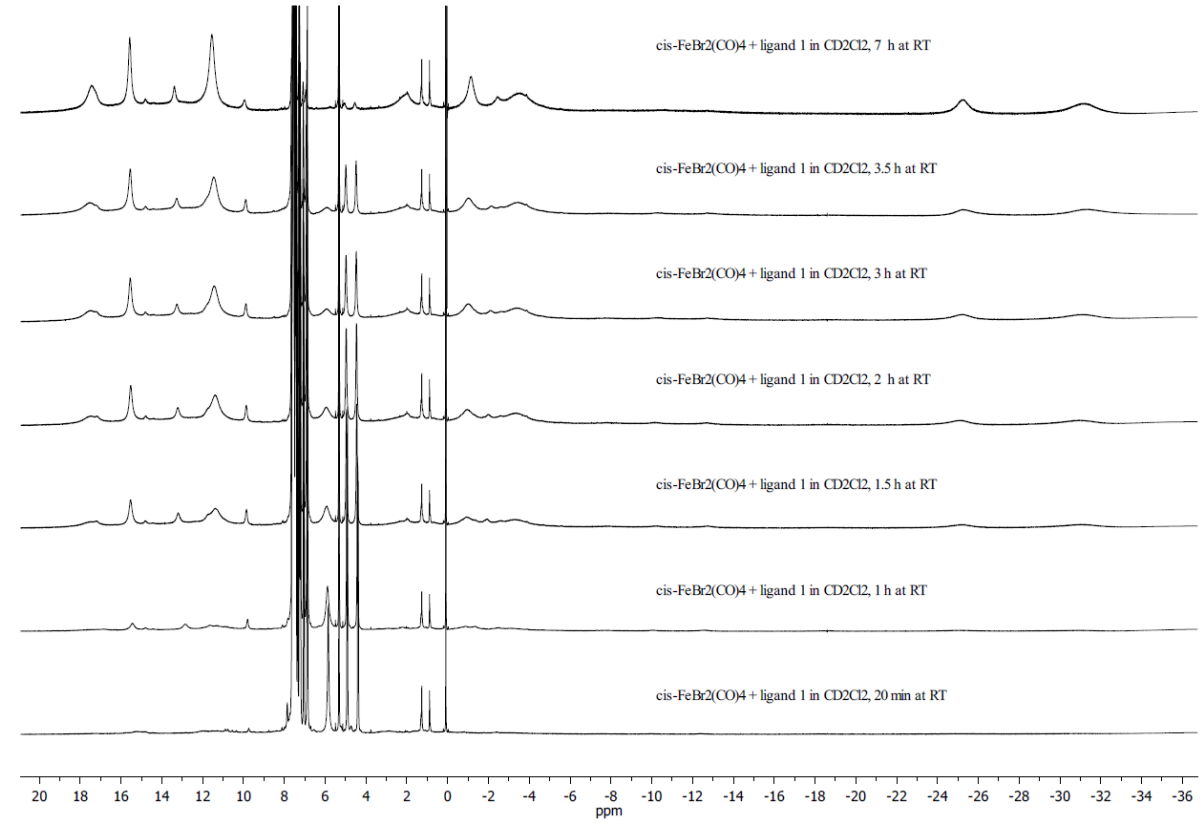


Figure S14. $^{31}P\{^1H\}$-NMR spectra for the reaction of *cis*-$FeBr_2(CO)_4$ with ligand **1** in CD_2Cl_2 at room temperature, showing the formation and decomposition of **1-Fe'**.

(**A**)



(**B**)

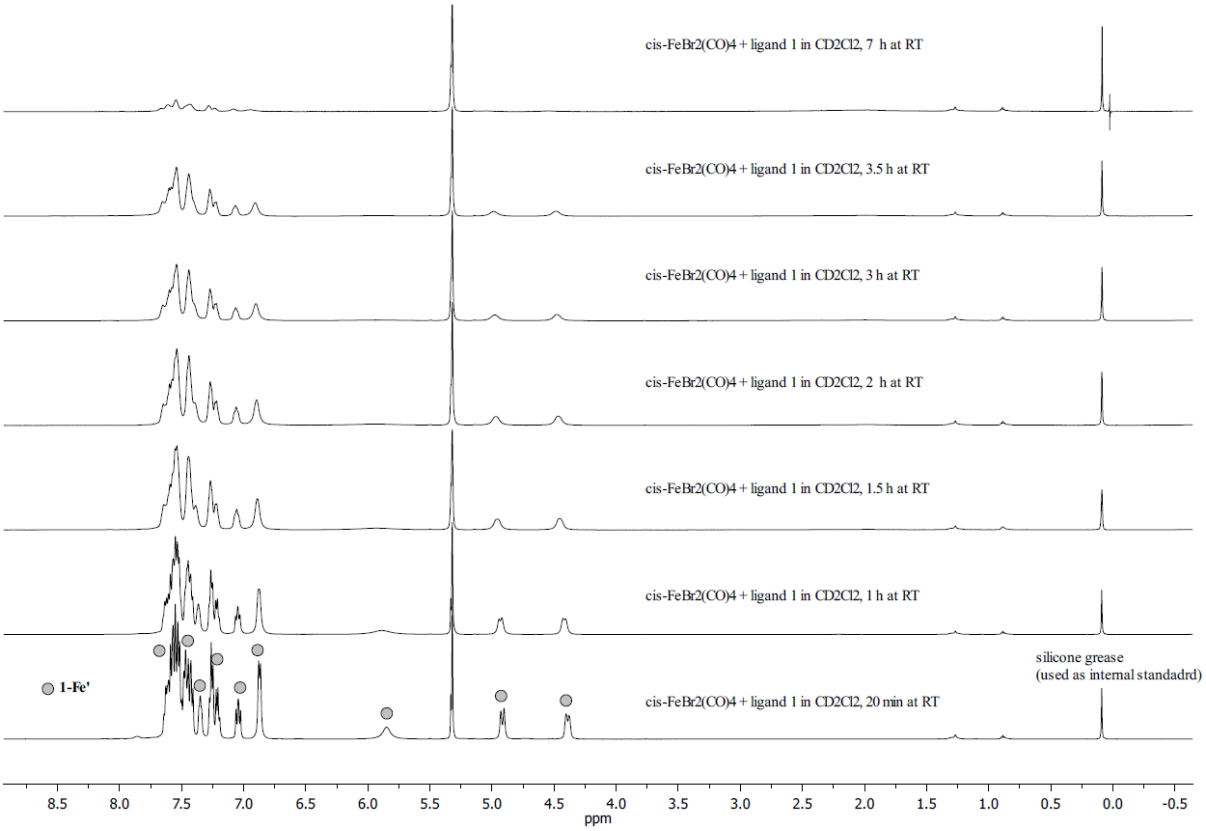


Figure S15. ^{1}H-NMR spectra for the reaction of *cis*-$FeBr_2(CO)_4$ with ligand **1** in CD_2Cl_2 at room temperature: (**A**) full spectra; (**B**) expanded spectra, showing the region for **1-Fe'**.

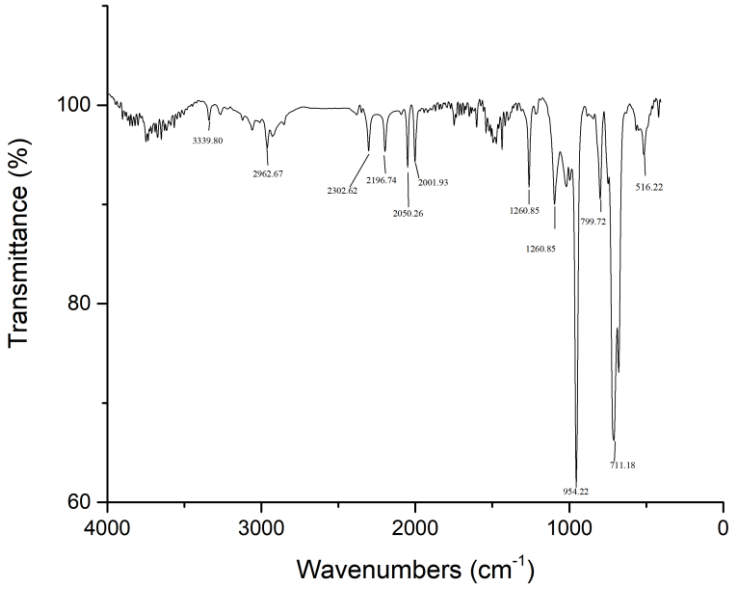


Figure S16. The IR spectrum in CH_2Cl_2 taken from the reaction of *cis*-$FeBr_2(CO)_4$ with ligand **1** after 20 min at room temperature.

*NMR scale reaction of cis-$FeBr_2(CO)_4$ with PN^{Me2} ligand **3***

The reaction was done analogously to the reaction of *cis*-$FeBr_2(CO)_4$ with ligand **1** (described above) using 13.8 mg (0.043 mmol) of 1-(2-(diphenylphosphanyl)phenyl)-N,N-dimethylmethanamine (PN^{Me2} ligand **3**) and 13.5 mg (0.041 mmol) of *cis*-$FeBr_2(CO)_4$. The initial formation of a mixture of a diamagnetic complex, akin to *cis-CO,cis-Br*-(PN^{Me2})$FeBr_2(CO)_2$ (**3-Fe'**), and a paramagnetic complex, akin to (PN^{Me2})$FeBr_2$ (**3-Fe**) was observed after 20 min at room temperature in CD_2Cl_2. However, the complete decomposition of **3-Fe'** to **3-Fe** *via* the release of CO was detected after 24 h at room temperature (Figures S17-S18). Similarly to **1-Fe'**, all attempts to isolate **3-Fe'** and/or obtain complex in analytically pure form by crystallization from the reaction mixture and/or by performing the reaction of *cis*-$FeBr_2(CO)_4$ with ligand **3** at low temperatures were unsuccessful and resulted in mixtures of **3-Fe'** with **3-Fe**. *cis-CO,cis-Br*-(PN^{Me2})$FeBr_2(CO)_2$ (**3-Fe'**): ^{1}H-NMR (500 MHz; CD_2Cl_2; δ, ppm): 7.86–7.12 (m, 13 H, aromatic), 6.79 (br s, 1 H, aromatic), 3.81 (br s, 2 H, *CH*$_2$N), 2.97 (s, 3 H, N*Me*$_2$), 2.78 (s, 3 H, N*Me*$_2$). ^{31}P{^{1}H}-NMR (202.5 MHz; CD_2Cl_2; δ, ppm): 58.67 (br s, 1 P, *P*Ph_2).

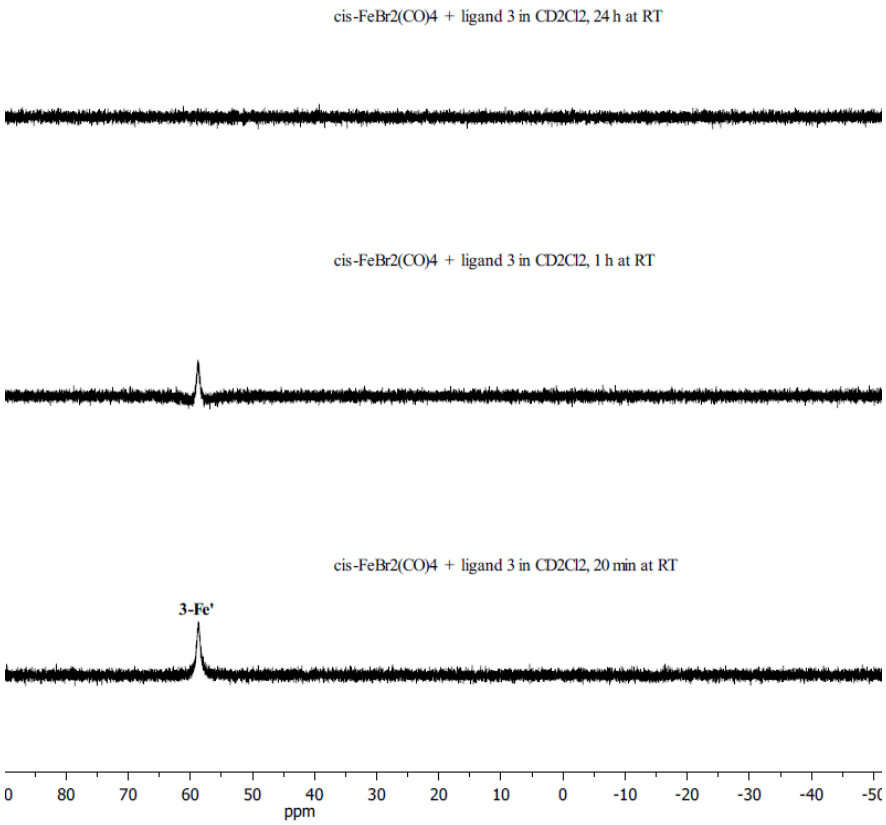
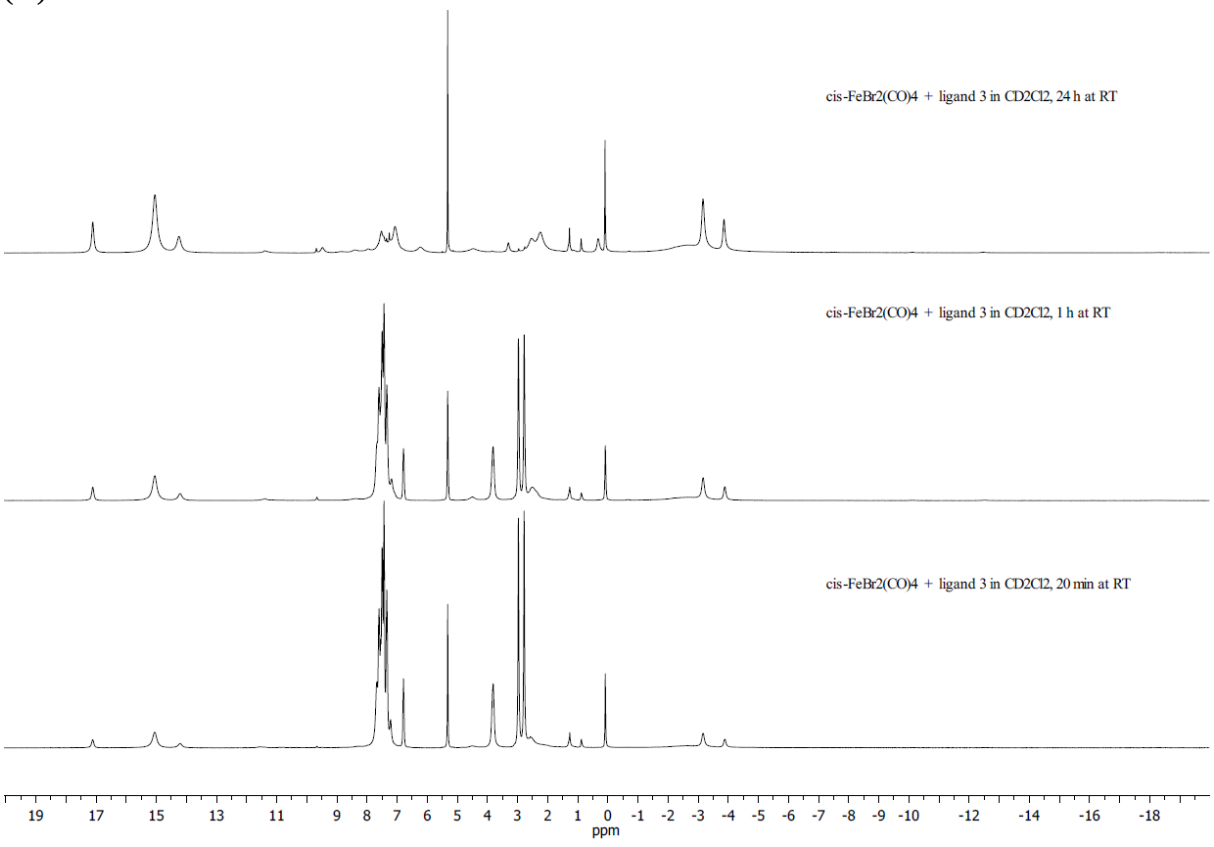


Figure S17. $^{31}P\{^{1}H\}$-NMR spectra for the reaction of *cis*-$FeBr_2(CO)_4$ with ligand **3** in CD_2Cl_2 at room temperature, showing the formation and decomposition of *cis-CO,cis-Br*-(PN^{Me2})$FeBr_2(CO)_2$ (**3-Fe'**).

(**A**)



(**B**)

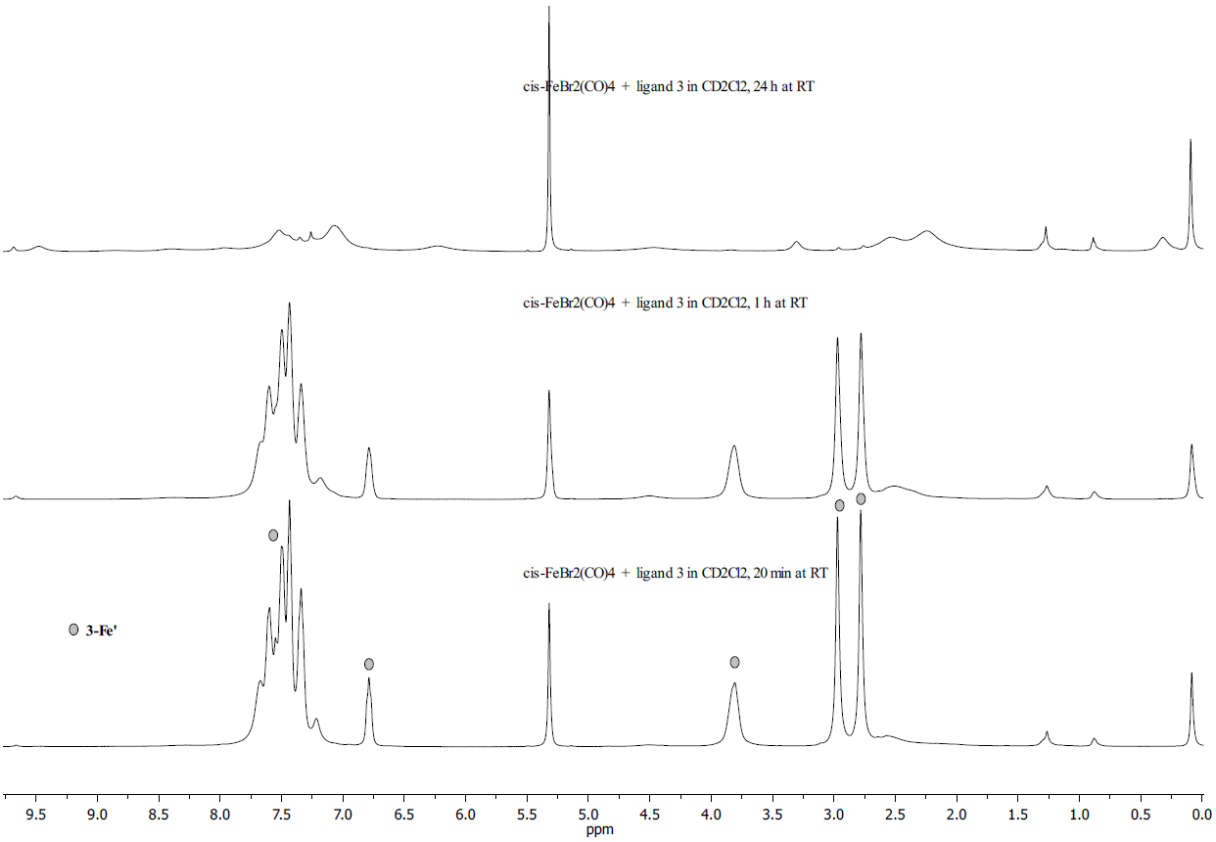


Figure S18. ^{1}H-NMR spectra for the reaction of *cis*-$FeBr_2(CO)_4$ with ligand **3** in CD_2Cl_2 at room temperature: (**A**) full spectra; (**B**) expanded spectra, showing the region for **3-Fe'**.

*Preparation of (PN^{DMP})$CoCl_2$ (**2-Co**)*

The reaction was done analogously to the preparation of **1-Co** above. A yellow solution of (2-diphenylphosphinobenzylidene)-2,6-dimethylphenylenamine (PN^{DMP}) ligand **2** (93.1 mg, 0.237 mmol) in 5 mL of THF was added at room temperature to anhydrous $CoCl_2$ (30.8 mg, 0.237 mmol). Immediately after mixing, the color of the reaction mixture turned green and then, within 10 min of stirring at room temperature, to dark blue. The resulting mixture was stirred at room temperature for 24 h. The solvent was pumped off, and the blue residue was dried in vacuum and recrystallized from CH_2Cl_2/hexanes to give blue crystals of **2-Co**. Yield: 69.5 mg, 56%. Elem. analysis (%): calcd. for $C_{27}H_{24}Cl_2CoNP$: C 61.97, H 4.62, N 2.68; found: C: 62.13, H 4.92, N 3.05. Single crystals of **2-Co** suitable for X-ray diffraction analysis were grown from CH_2Cl_2 solution at -28 °C.

*NMR scale dehydrogenation of ammonia borane (AB) in the presence of **1-Fe***

Reaction A: AB (3.2 mg, 0.1 mmol) and **1-Fe** (3 mg, 0.00514 mmol; 5 mol% to AB) were mixed in 0.6 mL of C_6D_6. The release of gas was observed upon mixing. The resulting mixture was transferred to an NMR tube, and the progress of the reaction was monitored by NMR spectroscopy first at room temperature for 21 h showing the formation of H_2 (Figure S19). After that, the mixture was heated at 60 °C for 6 h. During this time additional gas release was observed, and the color of the mixture turned dark with the formation of small amounts of black precipitate, which could be indicative of the decomposition of the iron complex. The mixture

was filtered, and the filtrate was analyzed by NMR spectroscopy, which revealed the formation of small amounts of cyclotriborazane (CTB; δ_B = -12.6 ppm) and unknown borate species (δ_B = -35.1 ppm, br s) (Figure S20). These observations, coupled with the ^{1}H-NMR and ^{31}P{^{1}H}-NMR spectra (Figures S21 and S22) recorded from the filtrate and showing the presence of the P-coordinated PN^{H} ligand **1**, suggest the decomposition of the iron complex and formation of the PN^{H}-borane adduct (by analogy with $Ph_3P{\cdot}BH_3$ species; δ_B = -38.2 ppm in $CDCl_3$ and δ_P = 20.4 ppm in $CDCl_3$[7]).

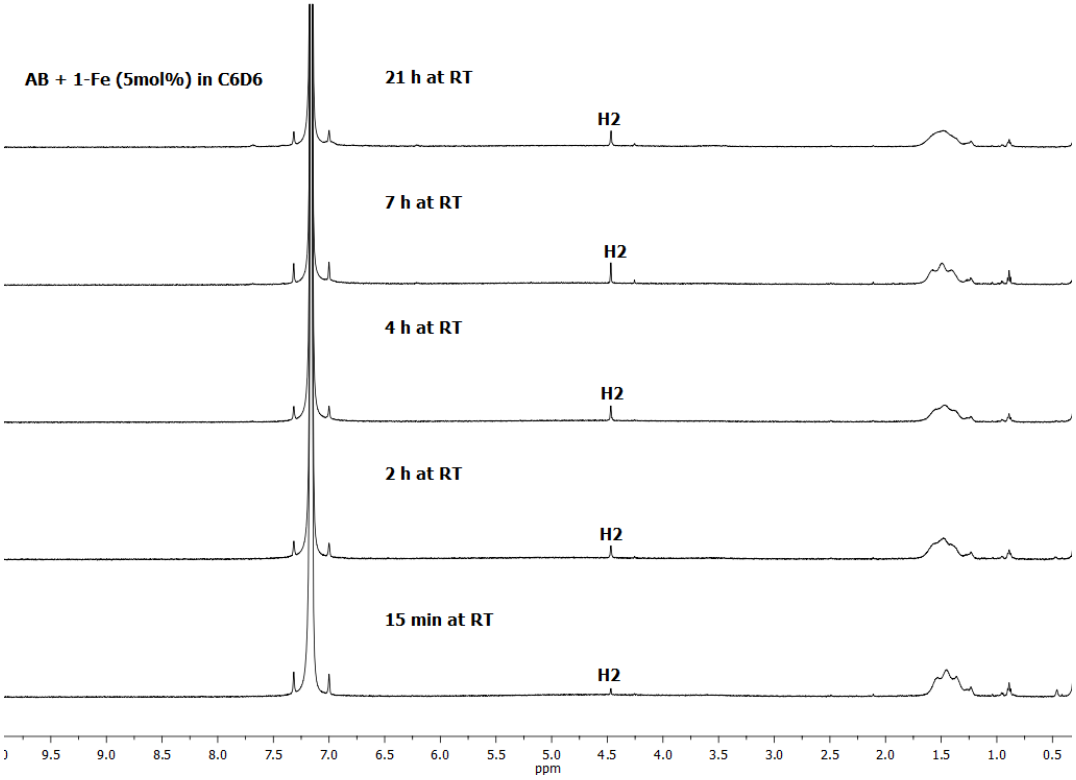


Figure S19. ^{1}H-NMR spectra taken directly from the reaction of AB with **1-Fe** (5 mol%) in C_6D_6 at room temperature showing the formation of H_2.

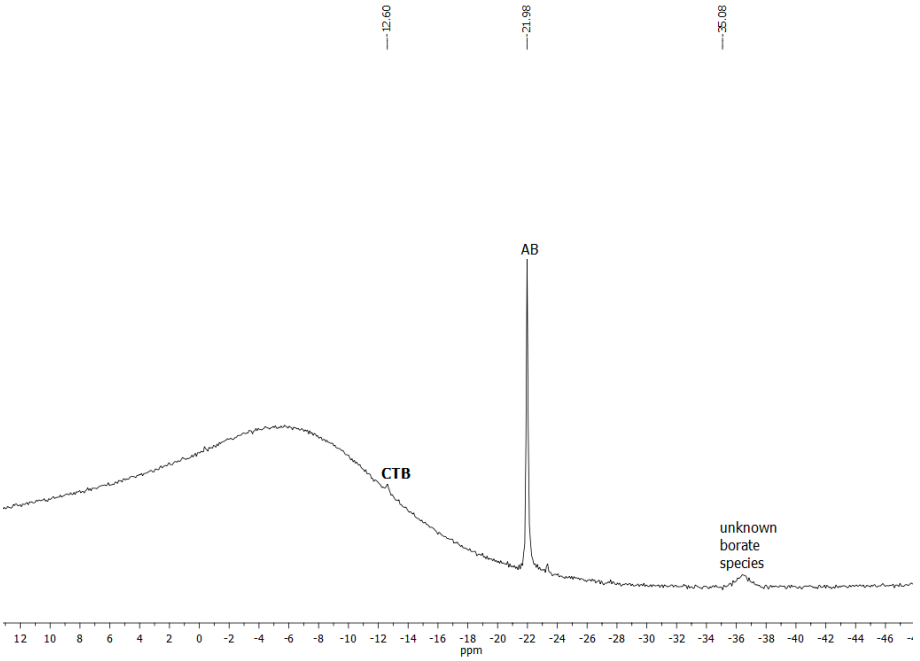


Figure S20. The ^{11}B{^{1}H}-NMR spectrum taken from the filtrate solution after heating the reaction of AB with **1-Fe** (5 mol%) in C_6D_6 at 60 °C for 6 h, followed by filtration.

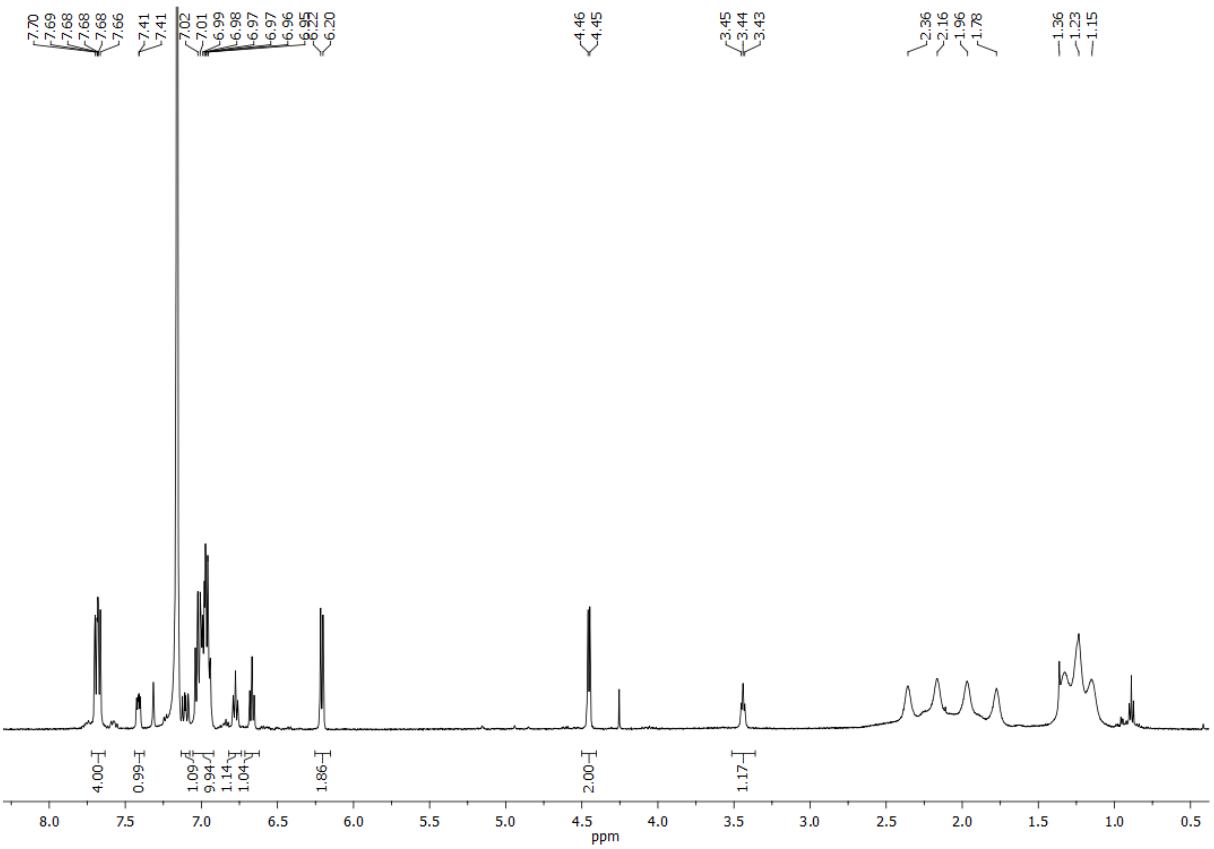


Figure S21. The ^{1}H-NMR spectrum taken from the filtrate solution after heating the reaction of AB with **1-Fe** (5 mol%) in C_6D_6 at 60 °C for 6 h, followed by filtration.

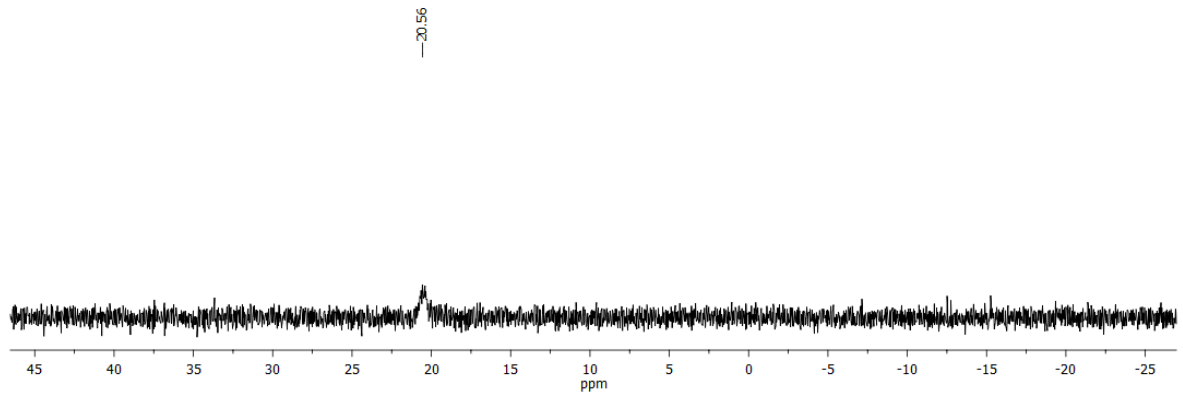


Figure S22. The ^{31}P{^{1}H}-NMR spectrum taken from the filtrate solution after heating the reaction of AB with **1-Fe** (5 mol%) in C_6D_6 at 60 °C for 6 h, followed by filtration.

The reaction was repeated with AB (20.4 mg, 0.726 mmol) and **1-Fe** (7 mg, 0.012 mmol; 1.65 mol% to AB) in 1 mL of C_6D_6 at 60 °C for 6 h. The ^{11}B{^{1}H}-NMR spectra recorded after that also revealed the formation of small amounts of μ-aminodiborane (ADB; δ_B = -27.5 ppm), cyclotriborazane (CTB; δ_B = -12.6 ppm), borazine ($B_3N_3H_6$; δ_B = 29.9 ppm) and the borate species, tentatively assigned to the PN^H-BH_3 adduct (*vide supra*) (Figure S23).

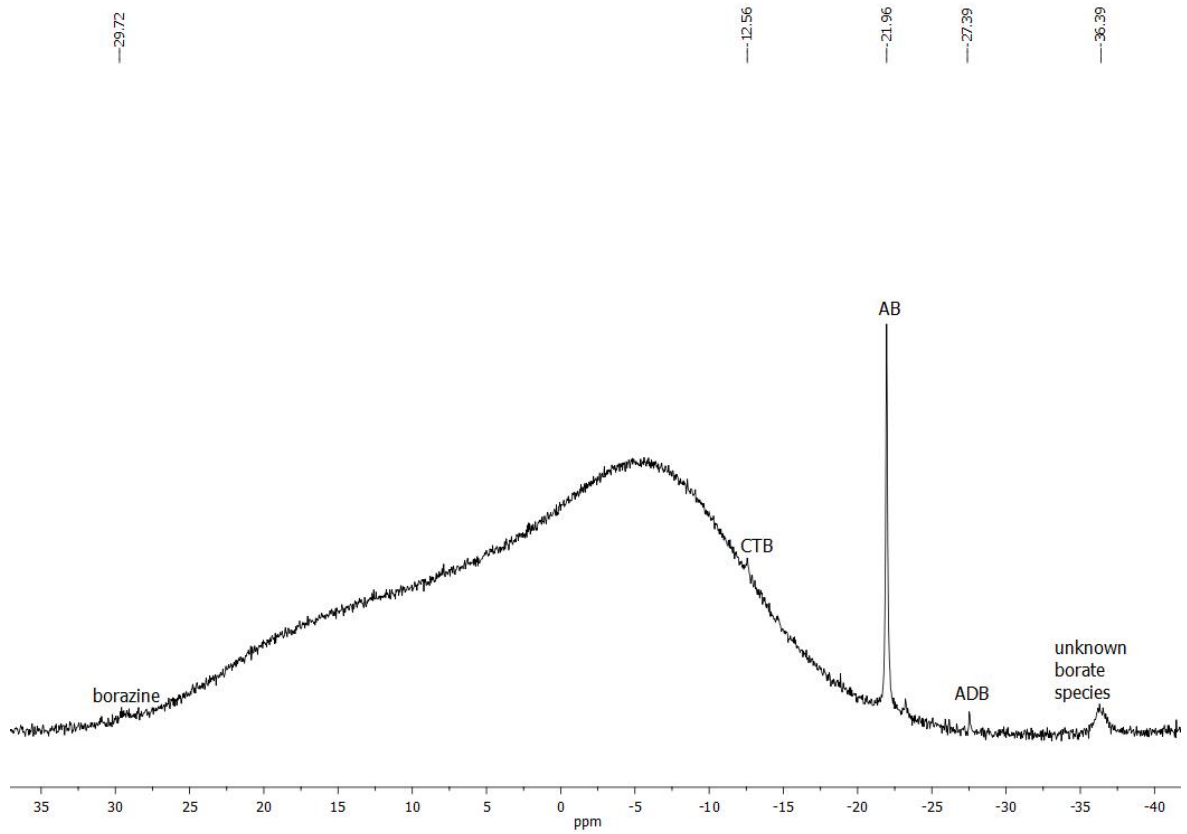
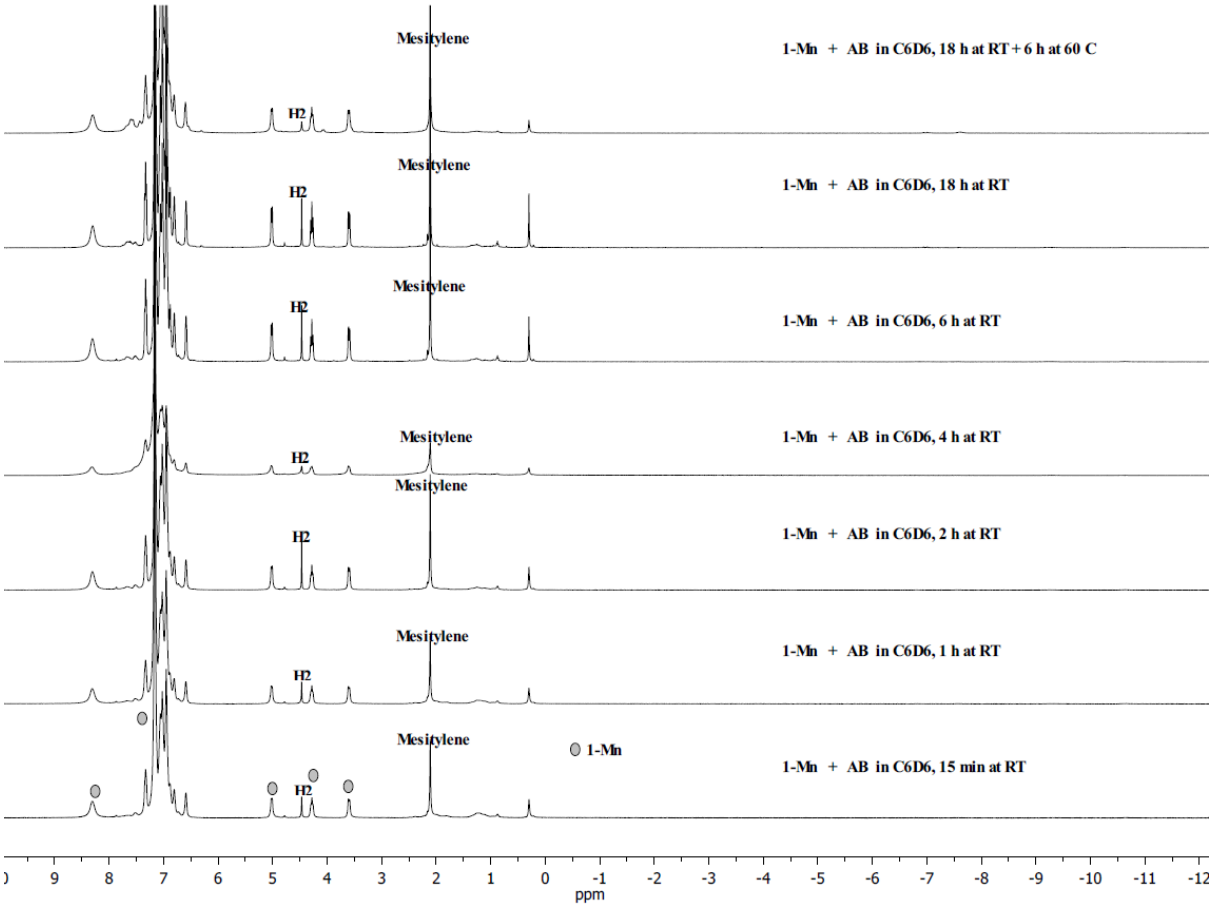


Figure S23. The $^{11}B\{^{1}H\}$-NMR spectrum taken from the filtrate solution after heating the reaction of AB with **1-Fe** (1.65 mol%) in C_6D_6 at 60 °C for 6 h, followed by filtration.

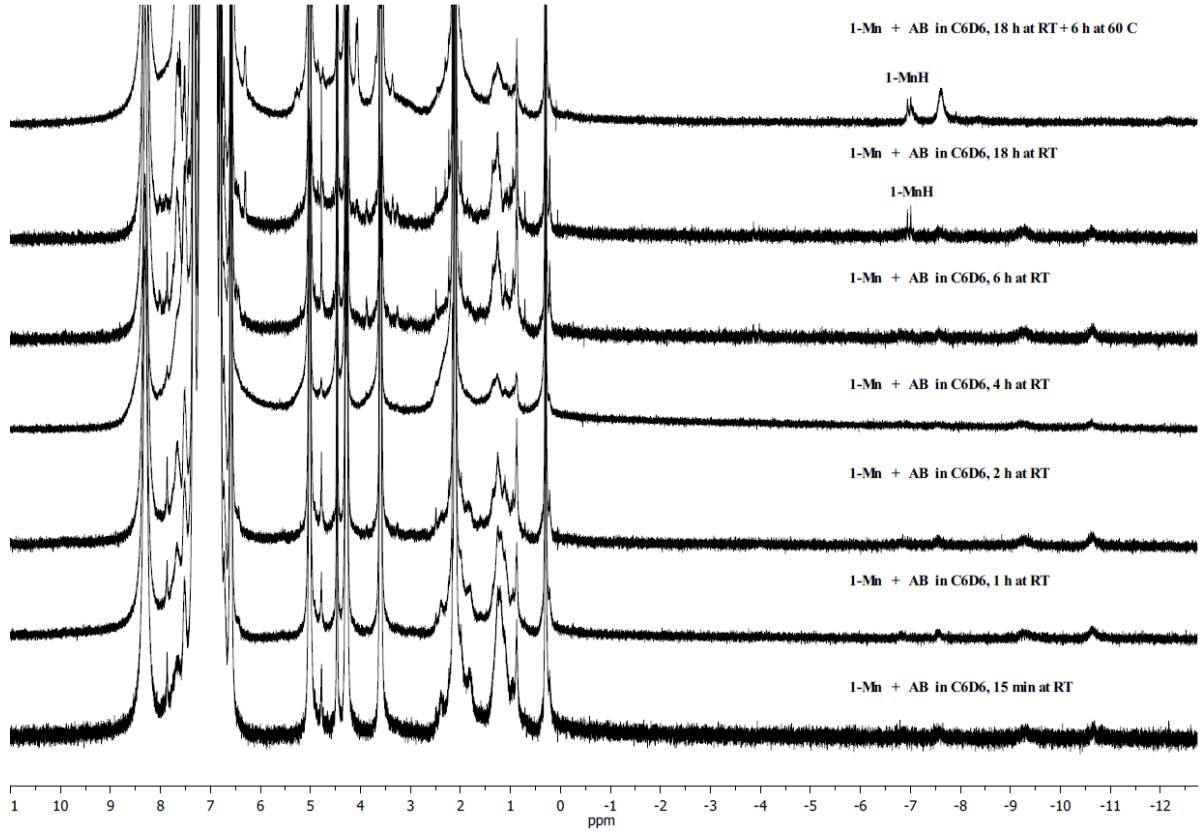
*NMR scale reaction of **1-Mn** with ammonia borane (AB)*

1-Mn (38 mg, 0.0648 mmol) and AB (2 mg, 0.0648 mmol) were mixed at room temperature in 0.7 mL of C_6D_6, and 1.8 µL of mesitylene was added to the mixture as an internal standard. Immediately after mixing **1-Mn** and AB the release of gas was observed. The resulting mixture was transferred to an NMR tube, and the progress of the reaction was monitored by NMR spectroscopy for 18 h at room temperature. After 18 h at room temperature, the mixture was heated at 60 °C for 6 h. The NMR spectra, showing the formation of H_2 and hydride species, including $(PN^{H})Mn(H)(CO)_3$ (**1-MnH**), as well as µ-aminodiborane (ADB; δ_B = -27.5 ppm) borazine ($B_3N_3H_6$; δ_B = 29.9 ppm) as the product of double dehydrogenation of AB are shown in Figures S24 and S25.

(A)


Mesitylene
H2
1-Mn + AB in C6D6, 18 h at RT + 6 h at 60 C
1-Mn + AB in C6D6, 18 h at RT
1-Mn + AB in C6D6, 6 h at RT
1-Mn + AB in C6D6, 4 h at RT
1-Mn + AB in C6D6, 2 h at RT
1-Mn + AB in C6D6, 1 h at RT
1-Mn + AB in C6D6, 15 min at RT
1-Mn
ppm

(B)


1-Mn + AB in C6D6, 18 h at RT + 6 h at 60 C
1-MnH
1-Mn + AB in C6D6, 18 h at RT
1-MnH
1-Mn + AB in C6D6, 6 h at RT
1-Mn + AB in C6D6, 4 h at RT
1-Mn + AB in C6D6, 2 h at RT
1-Mn + AB in C6D6, 1 h at RT
1-Mn + AB in C6D6, 15 min at RT
ppm

(**C**)

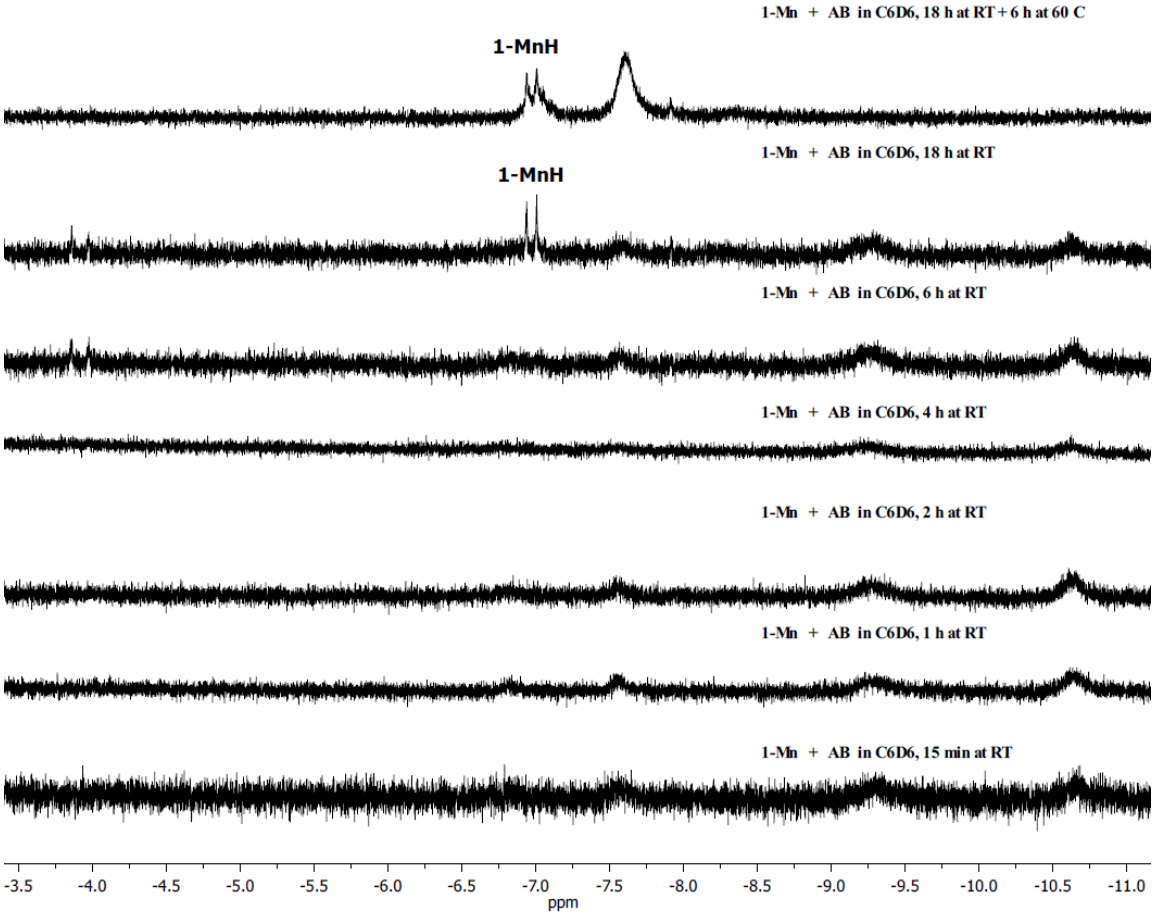


Figure S24. ^{1}H-NMR spectra for the reaction of **1-Mn** with AB in C_6D_6.

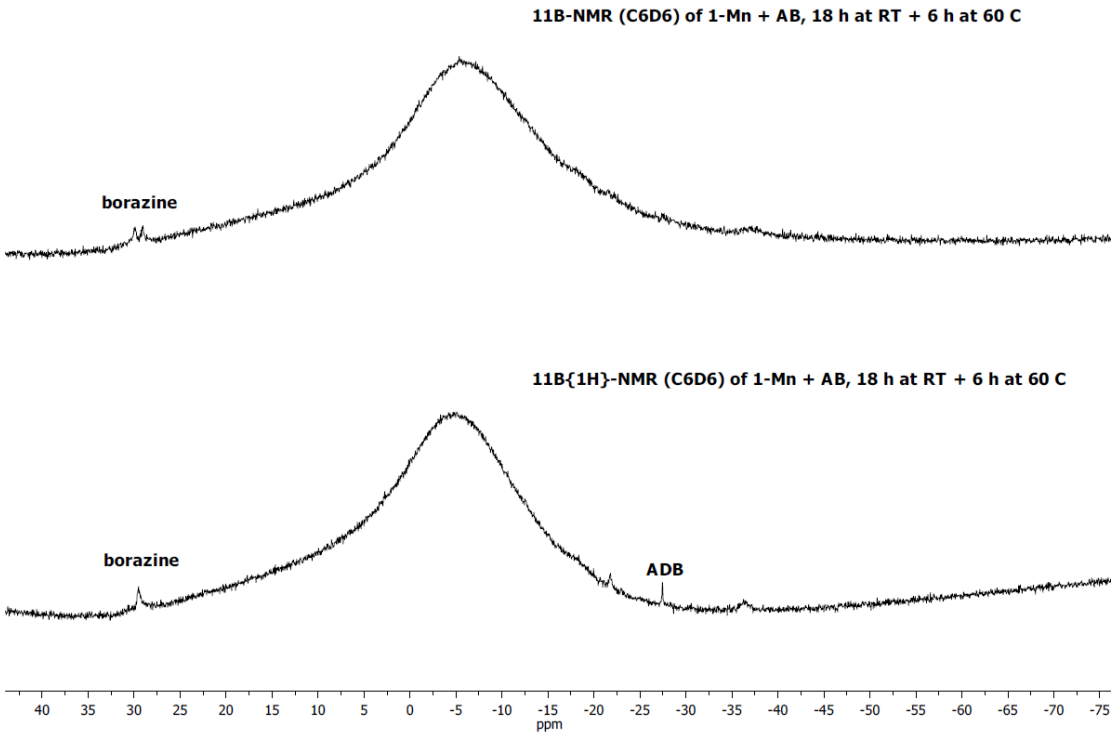
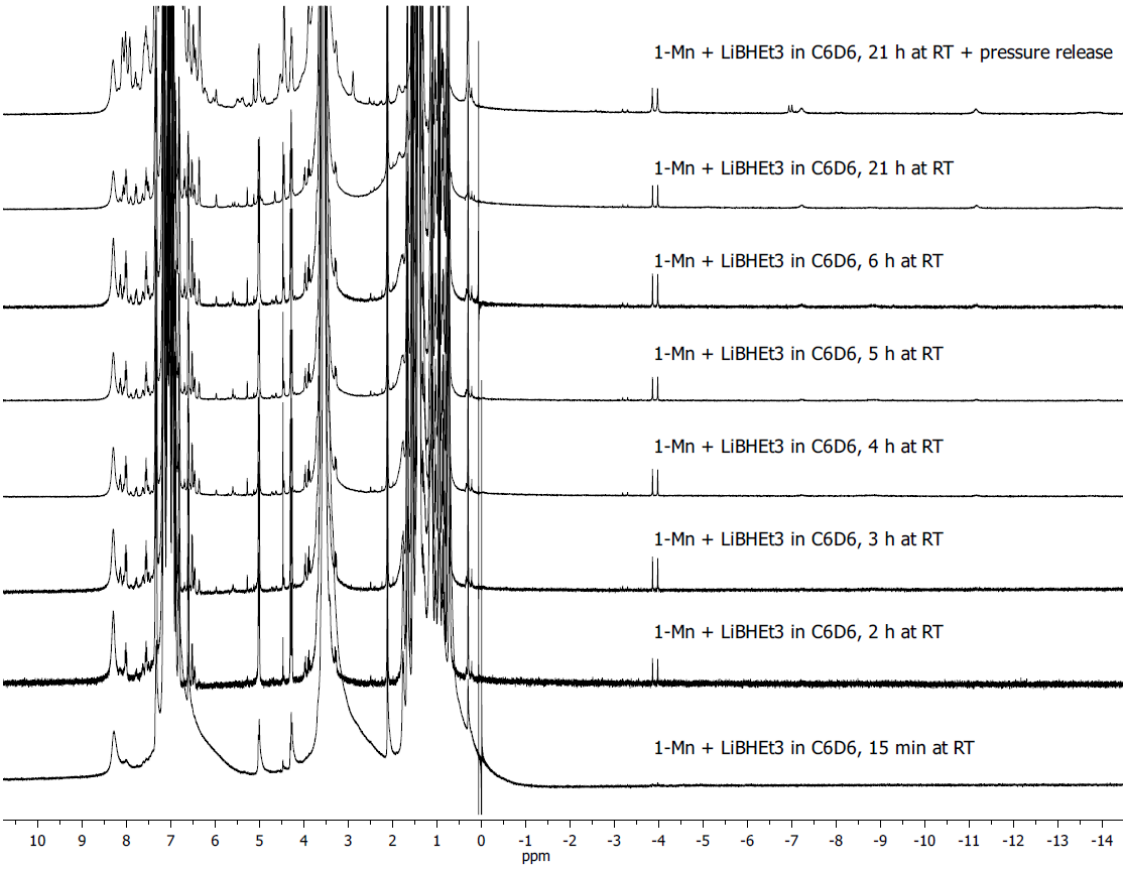


Figure S25. ^{11}B-NMR (top) and ^{11}B{^{1}H}-NMR (bottom) spectra taken from the reaction of **1-Mn** with AB in C_6D_6 after 18 h at room temperature, followed by heating at 60 °C for 6 h.

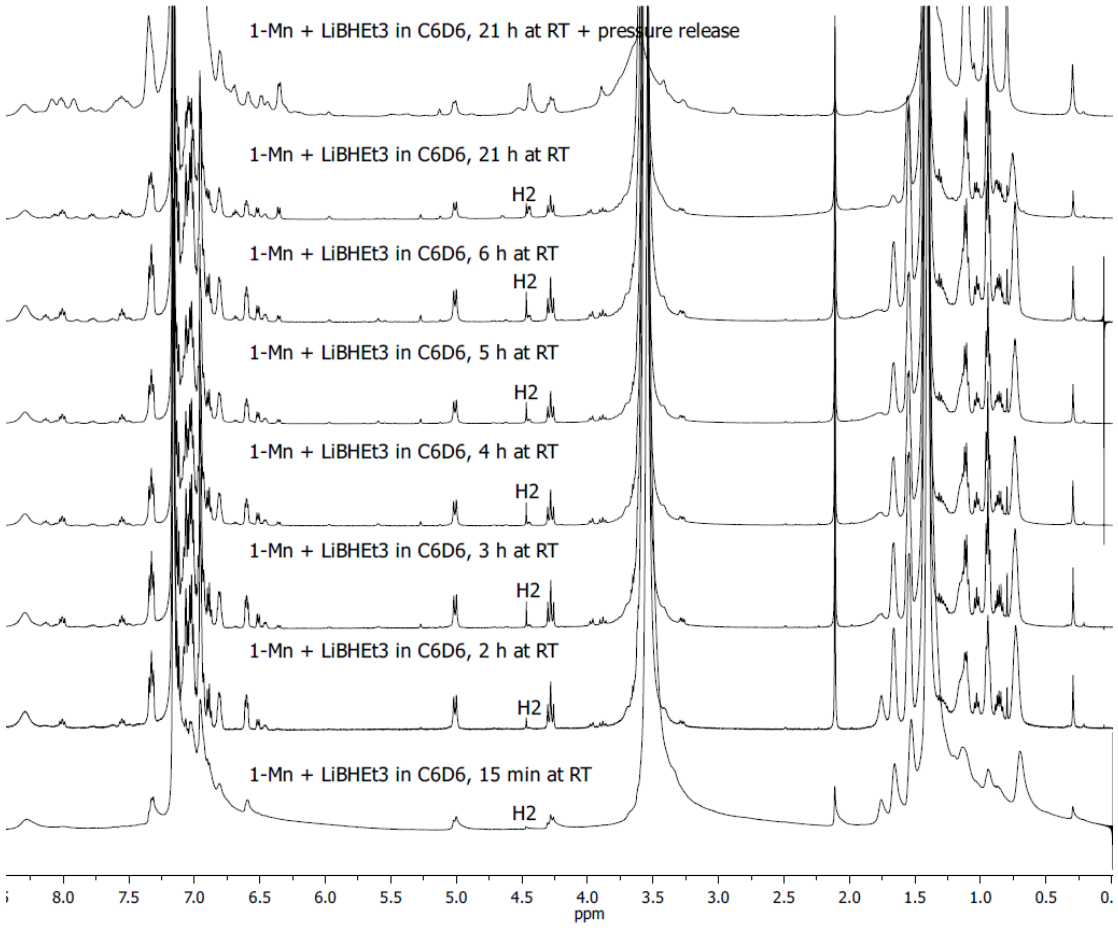
*NMR scale reaction of **1-Mn** with $LiBHEt_3$*

A solution of $LiBHEt_3$ in THF (25 µL, 1 mol/L, 0.025 mmol) was added *via* syringe to **1-Mn** (14.7 mg, 0.025 mmol) in 0.6 mL of C_6D_6. Immediately after the addition of $LiBHEt_3$, the release of gas was observed. The resulting mixture was transferred to an NMR tube, and the progress of the reaction was monitored by NMR spectroscopy for 21 h at room temperature. The NMR analysis (Figures S26 and S27) showed the formation of several hydride species within 6 h at room temperature. However, compared to the reaction of **1-Mn** with AB (*vide supra*), the major product herein gave rise to a slightly downfield shifted hydride resonance at δ_H -3.93 ppm (d, $^2J_{H\text{-}P}$ = 59.1 Hz) in the ^{1}H-NMR spectrum, coupled to the ^{31}P-resonance at δ_P 63.1 ppm in the $^{31}P\{^1H\}$-NMR spectrum. The formation of BEt_3 (δ_B 85.8 ppm)[8] was also detected by $^{11}B\{^1H\}$-NMR. Leaving the reaction of **1-Mn** with $LiBHEt_3$ for 21 h at room temperature and releasing the H_2 pressure resulted in the generation of the hydride complex **1-MnH** (δ_H 6.97 ppm, d, $^2J_{H\text{-}P}$ = 33.9 Hz), previously observed upon the treatment of **1-Mn** with AB (*vide supra*). Notably, the decomposition process *via* the release of the PN^H ligand was also suggested based on the $^{31}P\{^1H\}$-NMR analysis of the reaction mixture (see Figure S27). Interestingly, the formation of **1-MnH** was also detected in the ^{1}H-NMR spectra recorded directly from the reaction mixture during **1-Mn**-catalyzed TH of PhCN with AB in C_6D_6 at 60 °C (see Figure S28).

(**A**)



(**B**)



(**C**)

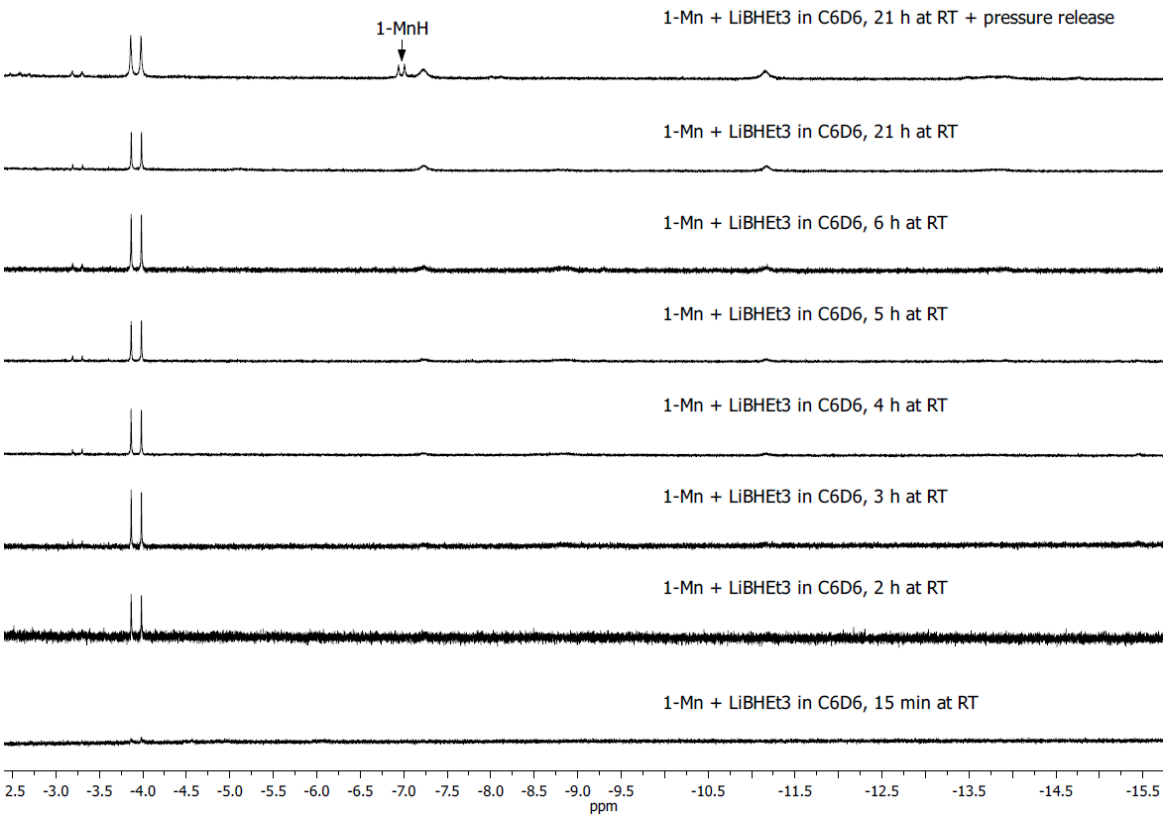


Figure S26. ^{1}H-NMR spectra for the reaction of **1-Mn** with $LiBHEt_3$ in C_6D_6.

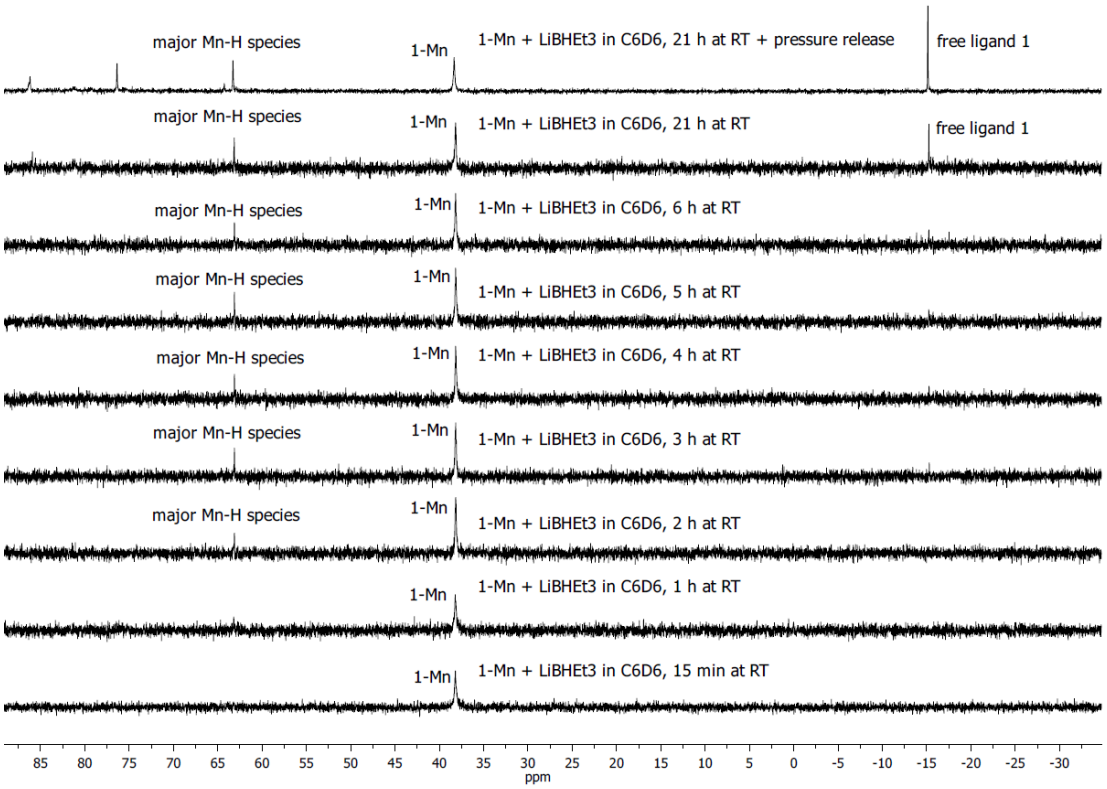


Figure S27. $^{31}P\{^{1}H\}$-NMR spectra for the reaction of **1-Mn** with $LiBHEt_3$ in C_6D_6.

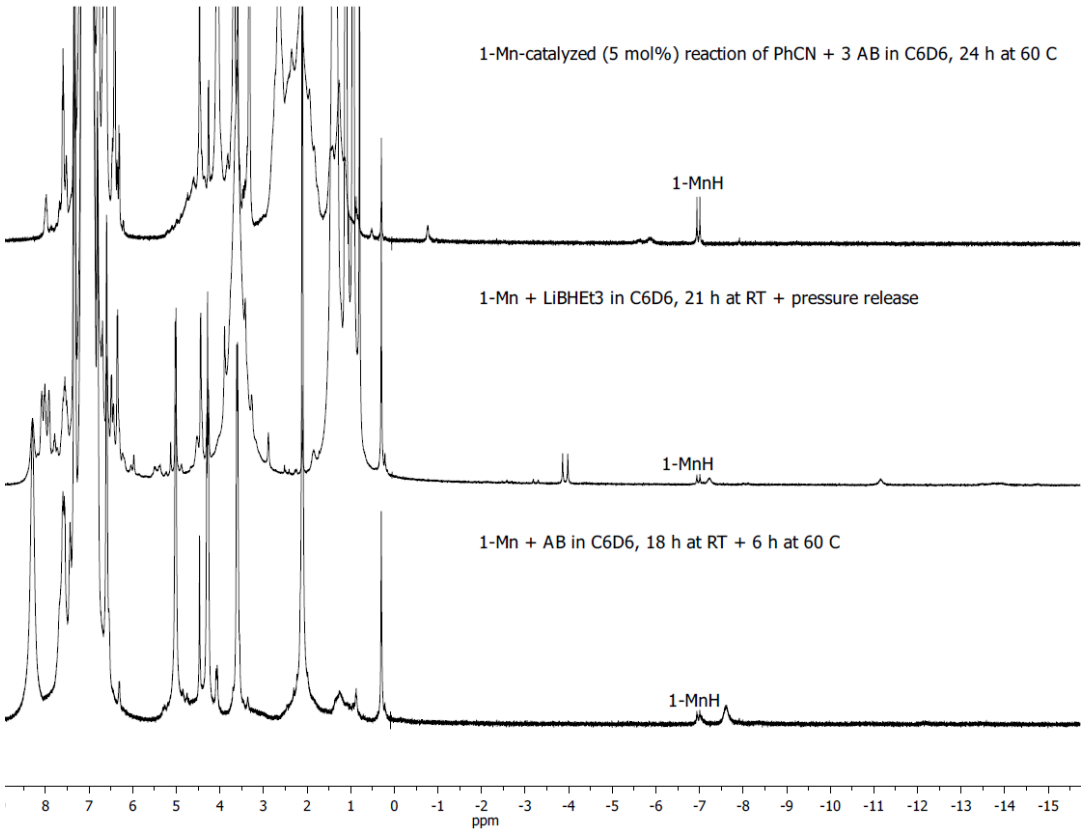


Figure S28. Comparison of the hydride regions of the ^{1}H-NMR spectra (in C_6D_6) taken from the reaction of **1-Mn** with AB (bottom), the reaction of **1-Mn** with $LiBHEt_3$ (middle), and the **1-Mn**-catalyzed (5 mol%) reaction of PhCN with AB (24 h at 60 °C, top), showing the formation of the same **1-MnH** hydride species.

General procedure for catalytic TH reactions

In a typical procedure, AB (22.2 mg, 0.72 mmol; 3 equiv. to the substrate) and the chosen metal catalyst (either **1-Mn**, **1-Fe** or **1-Co**) catalyst (0.012 mmol; 5 mol% to the substrate) were weighed in a 10 mL Supelco headspace vial. A nitrile substrate (0.24 mmol) in a corresponding solvent (PhMe, C_6D_6, hexanes, or ^{i}PrOH) was added to the vial to achieve a 0.12 mol/L reaction mixture. The vial was equipped with a magnetic stirring bar and sealed under argon with a magnetic screw cap having PTFE-faced butyl septa. Depending on the substrate and the solvent choice, the resulting mixture was left with stirring for 24 h either at 60 °C, 80 °C, or 100 °C (oil bath). After that, mesitylene (0.1-0.2 equiv. to the substrate) was added as an internal standard, and the mixture was transferred to an NMR tube and submitted for ^{1}H-NMR analysis. Conversions of substrates were calculated (where possible) by the integration of substrate resonances against those for mesitylene (internal standard). Then, the reaction mixture was quenched by the addition of methanol (5 mL) and left to stir for 3 hours at room temperature (this step was omitted for reactions performed in ^{i}PrOH). The obtained solution was filtered through a Celite pad, and the solvent was pumped off. The residue was dissolved in Et_2O (5 mL), and HCl (1.0 mol/L in Et_2O, 1 mL) was added. After continuous stirring for 3 h at room temperature, the formed precipitate was allowed to settle at the bottom of the flask. The solvent was decanted, and the precipitate was washed with Et_2O (3 x 5 mL), dried in vacuum weighed, and dissolved in D_2O. The resulting solution was submitted for NMR analysis using CH_3COONa (0.5 mol/L in D_2O, 240 μL; 0.12 mmol) as an internal standard. Yields of the produced amine hydrochlorides were determined by ^{1}H-NMR by integration of product resonances against those for CH_3COONa (internal standard). The reactions with lower/higher loadings of AB and/or the pre-catalyst and control experiment at lower temperatures (down to room temperature) and/or in the absence of a metal pre-catalyst were performed analogously. Conversions of substrates and yields of the hydrochloride salts can be found in Table 2 and Scheme 4 in the manuscript. NMR data for amine hydrochlorides and the corresponding NMR spectra can be found in sections 3 and 4, respectively.

*TH of PhCN with AB by in situ generated **1-Fe** pre-catalyst*

The reaction was performed using 38.5 μL (0.374 mmol) of PhCN and 34.6 mg (1.121 mmol) of AB in PhMe (4 mL) at 60 °C for 24 h analogously to the typical procedure for TH reactions described above. However, instead of introducing 5 mol% of **1-Fe**, $FeBr_2$ (4.0 mg, 0.0187 mmol, 5 mol% to PhCN) and the PN^H ligand **1** (7.0 mg, 0.019 mmol, 5.1 mol% to PhCN) were introduced to the reaction, allowing to generate the pre-catalyst **1-Fe** *in situ*. The ^{1}H-NMR analysis of the reaction mixture after 24 h at 60 °C revealed complete conversion of PhCN. The ^{1}H-NMR analysis of the isolated benzylamine hydrochloride salt in D_2O in the presence of NaOAc (0.24 mmol) as an internal standard revealed an 85% yield of the reduction product (Figure S29).

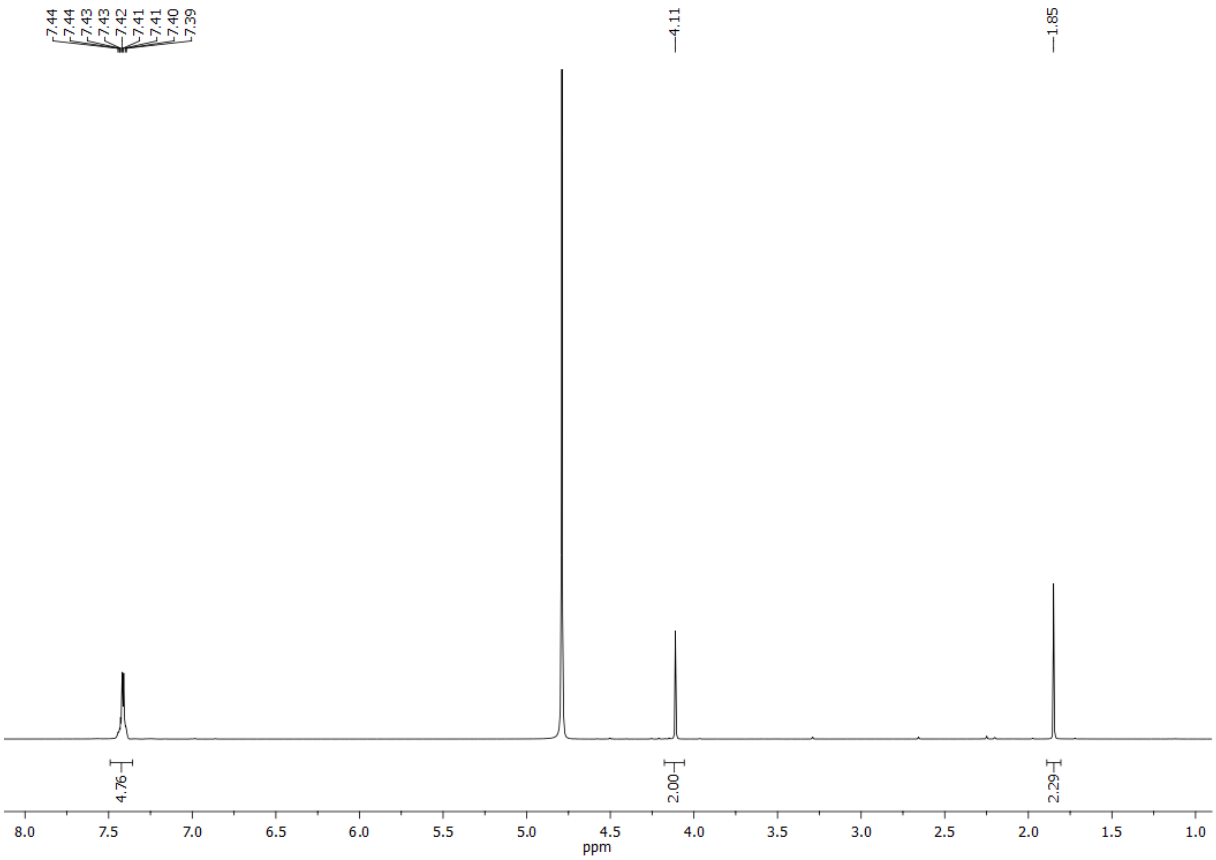


Figure S29. The ^{1}H-NMR spectrum (in D_2O) of $PhCH_2NH_3Cl$ obtained by the TH of PhCN with AB in the presence of $FeBr_2$ (5 mol%) and PN^{H} ligand **1** (5.1 mol%) during 24 h at 60 °C (the resonance at δ_H 1.85 ppm corresponds to NaOAc used as an internal standard).

*TH of PhCN with AB and $FeBr_2$ and PN^{Me2} (**3**)*

The reaction was performed using 44.3 µL (0.43 mmol) of PhCN, 39.8 mg (1.29 mmol) of AB and 12 µL (0.086 mmol, 0.2 equiv. to PhCN) of mesitylene (internal standard) in PhMe (4 mL) at 60 °C for 24 h analogously to the typical procedure for TH reactions described above. However, $FeBr_2$ (4.6 mg, 0.0214 mmol, 5 mol% to PhCN) and the PN^{Me2} ligand **3** (7.0 mg, 0.022 mmol, 5.1 mol% to PhCN) were introduced to the reaction, allowing to generate the iron complex $(PN^{Me2})FeBr_2$ *in situ*. The ^{1}H-NMR analysis of the reaction mixture after 24 h at 60 °C revealed only a small conversion of PhCN. The ^{1}H-NMR analysis of the isolated benzylamine hydrochloride salt in D_2O in the presence of NaOAc (0.12 mmol) as an internal standard revealed only a 3% yield of the reduction product (Figure S30).

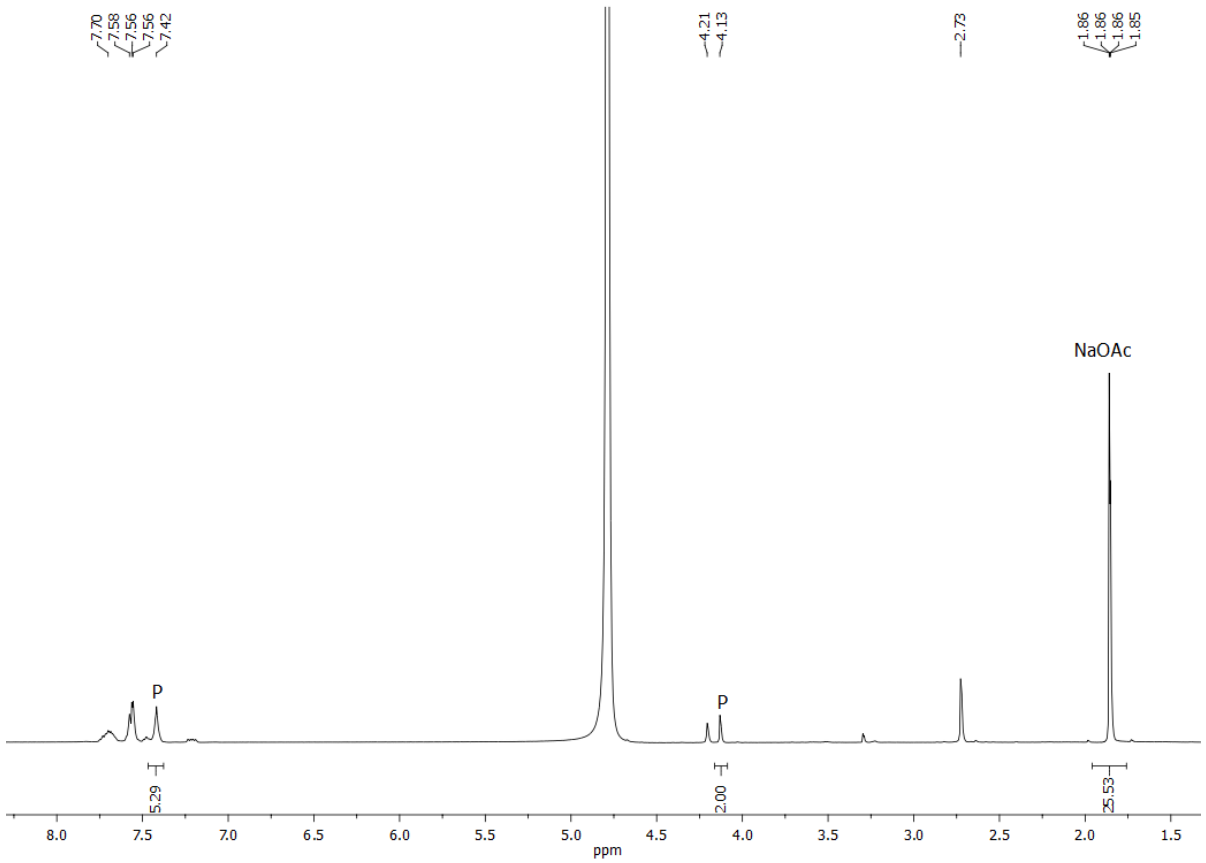


Figure S30. The ^{1}H-NMR spectrum (in D_2O) of $PhCH_2NH_3Cl$ obtained by the TH of PhCN with AB in the presence of $FeBr_2$ (5 mol%) and PN^{Me2} ligand **3** (5.1 mol%) during 24 h at 60 °C (P = product).

Reduction of PhN=CH$_2$Ph with AB

The reduction of $PhN=CH_2Ph$ (21.8 mg, 0.12 mmol) with AB (7.41 mg, 0.24 mmol) in hexanes (1 mL) at 60 °C for 24 h was performed in a Supelco headspace vial under both catalyst-free and **1-Fe**-catalyzed (5 mol%) conditions. The reduction product was subjected to the same workup procedure as for products of the TH of nitriles (*vide supra*), resulting in the corresponding amine hydrochloride salt ($PhN(CH_2Ph)H_2Cl$) in 25% yield (determined by ^{1}H-NMR in D_2O in the presence of 0.12 mmol of NaOAc as an internal standard) (Figure S31). Considering that primary imine intermediates, formed during TH of nitriles, are typically more reactive compared to secondary imines (akin to $PhN=CH_2Ph$ tested herein), these observations suggest that the reduction of intermediate imine products in the TH of nitriles with AB does not necessarily require the catalyst and can occur under catalyst-free conditions.

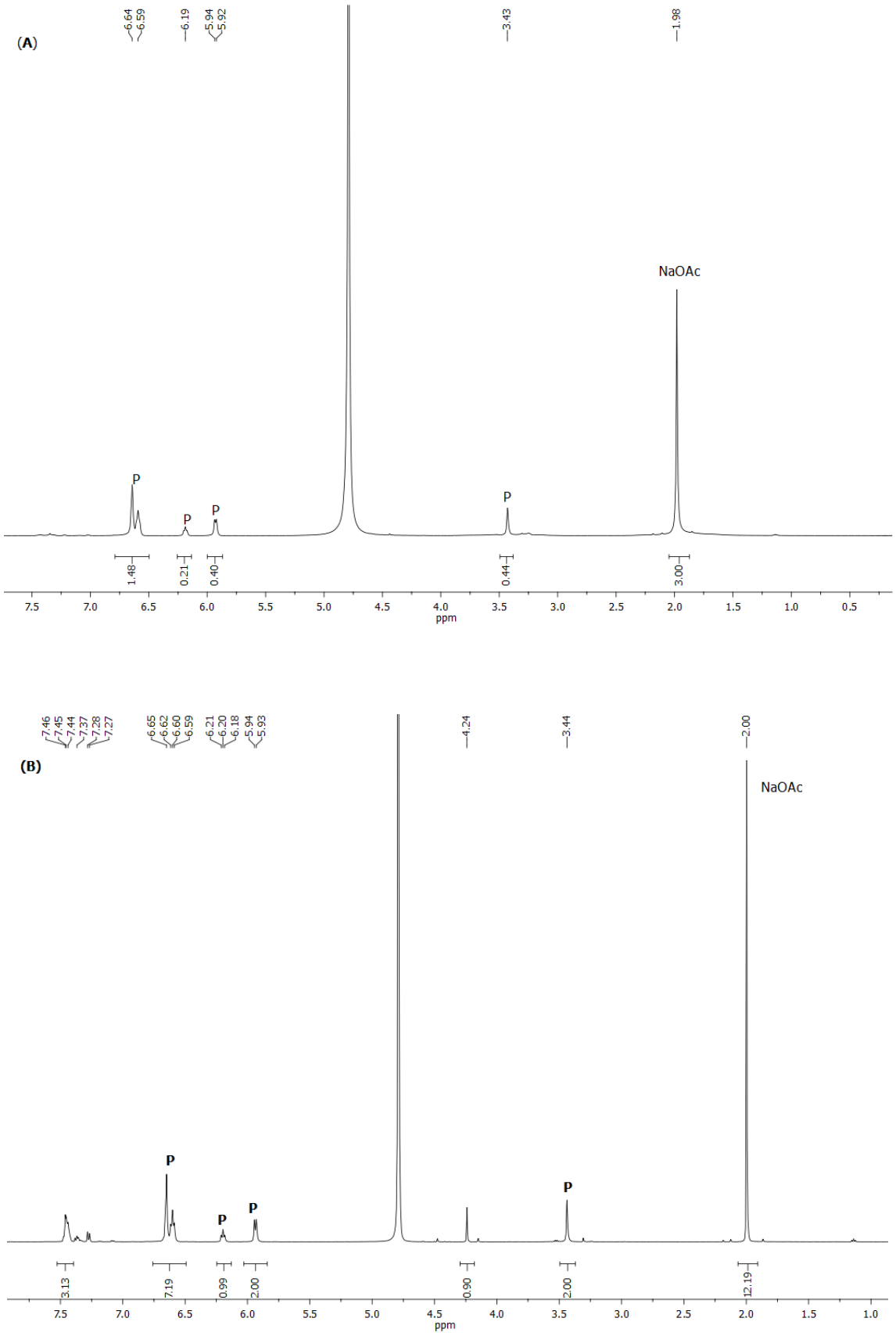


Figure S31. ^{1}H-NMR spectra (in D_2O) of the hydrochloride salt of the product of the reduction of PhN=CH_2Ph with AB in hexanes (24 h at 60 °C): (**A**) in the presence of 5 mol% of **1-Fe**; (**B**) catalyst-free (P = PhN(CH_2Ph)H_2Cl).

NMR scale reaction of benzylamine with AB

Benzylamine (26.2 µL, 0.24 mmol) in 2 mL of hexanes was added at room temperature to a mixture of solid AB (22.2 mg, 0.72 mmol) and **1-Fe** (7 mg, 0.012 mmol; 5 mol% to benzylamine) in a Supelco headspace vial. The vial was sealed, and the mixture was stirred at 60 °C for 24 h. After the reaction completion, 6 µL (0.043 mmol) of mesitylene (as an internal standard) was added to the vial, and the mixture was transferred to an NMR tube for ^{1}H-NMR analysis, which revealed the complete conversion of benzylamine and formation of the borylamine species (Figure S32A), previously observed during the **1-Fe**-catalyzed TH of benzonitrile in hexanes after 24 h at 60 °C (Figure S32C). Similar borylamines have been recently reported by Kirchner et al.[9] The analogous reaction of benzylamine with AB in hexanes at 60 °C in the absence of the pre-catalyst **1-Fe** also showed a complete conversion of benzylamine to borylamine products (Figure S32B). The ^{11}B-NMR spectra (Figure S33) are also in agreement with the formation of borylamine species (the ^{11}B-resonances of the obtained species are within the δ_B range of 21-27 ppm, observed in our group previously for related borylamines produced during Co-catalyzed hydroboration of nitriles[10] and nitro compounds[11] with HBPin).

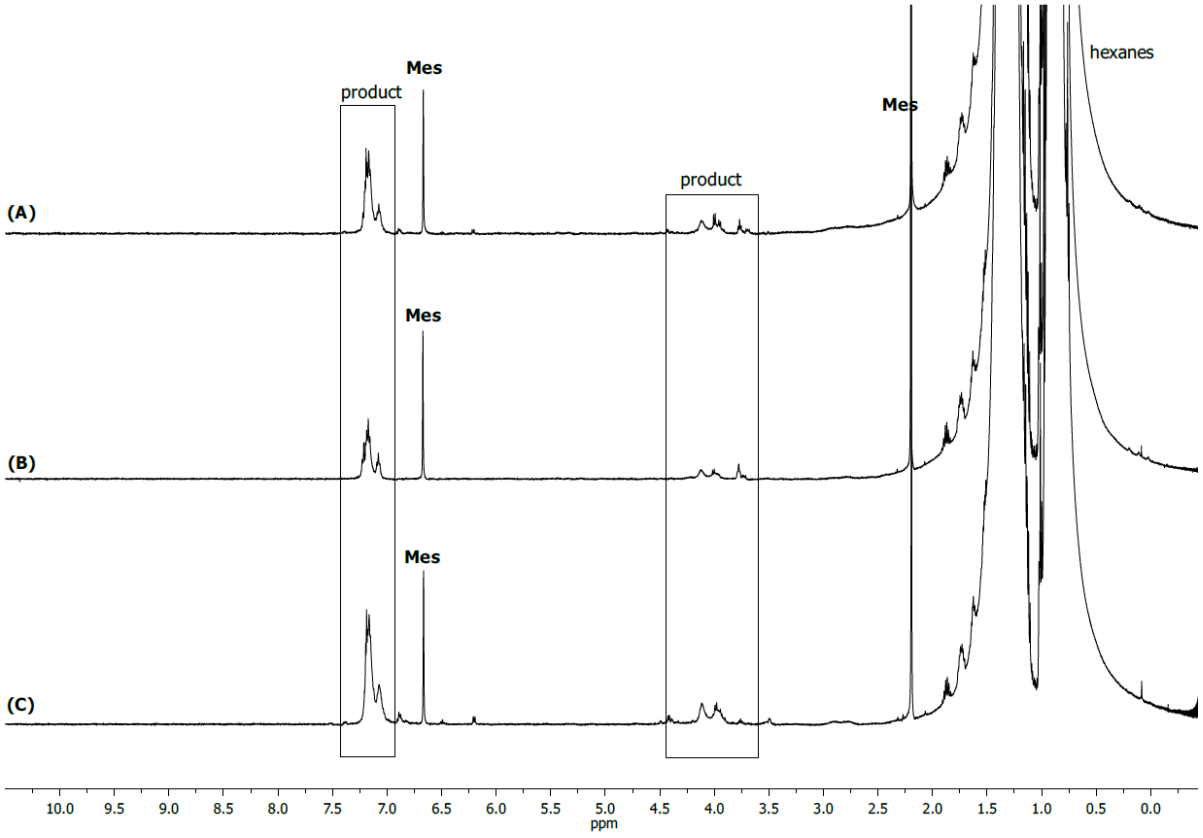


Figure S32. ^{1}H-NMR spectra (in hexanes) of the products of the reaction (24 h, 60 °C in hexanes) of $PhCH_2NH_2$ with AB in the presence of **1-Fe** (**A**), in the absence of **1-Fe** (**B**) and **1-Fe**-catalyzed TH of PhCN with AB (**C**) (24 h, 60 °C in hexanes).

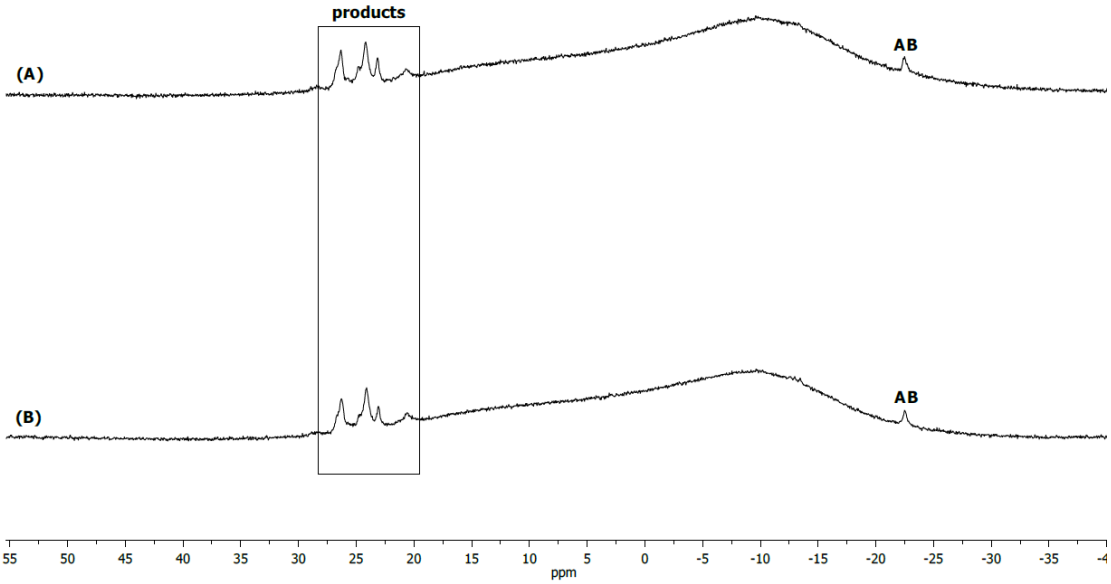
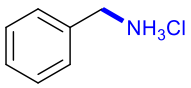


Figure S33. $^{11}B\{^{1}H\}$-NMR spectra (in hexanes) of the products of the reaction (24 h, 60 °C in hexanes) of $PhCH_2NH_2$ with AB in the presence of **1-Fe** (**A**) and in the absence of **1-Fe** (**B**).

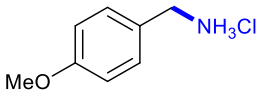
3. NMR data for products of transfer hydrogenation reactions

NMR spectra were recorded in D_2O using the samples from precipitated hydrochloride salts (see the general procedure above). Yields of isolated products were confirmed by ^{1}H-NMR using EtOAc as an internal standard. NMR yields of hydrochloride salts are listed below (only the best yields are shown) and in Scheme 4 in the manuscript. Conversions of the nitrile substrates (shown in parentheses in Scheme 4 in the manuscript) were calculated (where possible) by the integration of ^{1}H-NMR spectra taken directly from the reaction mixtures in the presence of mesitylene as an internal standard. NMR spectra for products of **1-Fe**-catalyzed TH reactions are shown in Section 4.



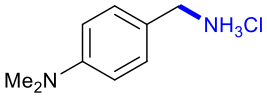
4, 97%

^{1}H-NMR (500 MHz; D_2O; δ, ppm): 7.45-7.38 (m, 5 H, *Ph*); 4.11 (s, 2 H, *CH*$_2$). ^{13}C{^{1}H}-NMR (126 MHz; D_2O; δ, ppm): 133.1 (s, *Ph*); 129.2 (s, *Ph*); 129.1 (s, *Ph*); 128.8 (s, *Ph*); 43.2 (s, *CH*$_2$). NMR data are similar to those previously reported in the literature.[12]



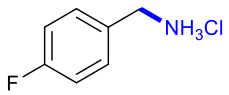
5, >99%

^{1}H-NMR (500 MHz; D_2O; δ, ppm): 7.35 (br s, 2 H. aromatic); 6.99 (br s, 2 H, aromatic); 4.07 (s, 2 H, *CH*$_2$); 3.78 (s, 3 H, O*CH*$_3$). ^{13}C{^{1}H}-NMR (126 MHz; D_2O; δ, ppm): 159.4 (s); 130.6 (s); 125.2 (s); 114.6 (s); 55.4 (s); 42.6 (s). NMR data are similar to those previously reported in the literature.[12]



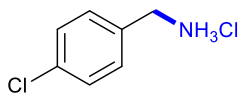
6, 54%

^{1}H-NMR (500 MHz; D_2O; δ, ppm): 7.43 (d, *J* = 8.6 Hz, 1 H, aromatic); 7.28 (d, *J* = 8.6 Hz, 1 H, aromatic).; 4.09 (s, 2 H, *CH*$_2$); 3.01 (s, 6 H, *NMe*$_2$). ^{13}C{^{1}H}-NMR (126 MHz; D_2O; δ, ppm): 147.3 (s); 130.5 (s); 128.4 (s); 118.1 (s); 43.4 (s); 42.5 (s). NMR data are similar to those previously reported in the literature.[13]



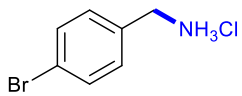
7, 98%

^{1}H-NMR (500 MHz; D_2O; δ, ppm): 7.42 (br s, 1 H, aromatic); 7.15 (br s, 1 H, aromatic); 4.10 (s, 2 H, *CH*$_2$). ^{13}C{^{1}H}-NMR (126 MHz; D_2O; δ, ppm): 162.8 (d, *J* = 244.9 Hz, *i*-C (C-F) of *C*$_6$*H*$_4$); 130.9 (d, *J* = 8.3 Hz, *m*-C of *C*$_6$*H*$_4$); 129.5 (s, *i*-C (C-CH$_2$) of *C*$_6$*H*$_4$); 115.9 (d, *J* = 22.0 Hz, *o*-C of *C*$_6$*H*$_4$), 42.6 (s, *CH*$_2$). ^{19}F- NMR (471 MHz; D_2O; δ, ppm): -113.13 (s). NMR data are similar to those previously reported in the literature.[12]



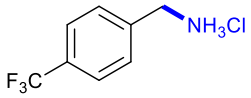
8, 71%

^{1}H-NMR (500 MHz; D_2O; δ, ppm): 7.42 (br s, 2 H, aromatic); 7.37 (br s, 2 H, aromatic); 4.10 (s, 2 H, *CH*$_2$). ^{13}C{^{1}H}-NMR (126 MHz; D_2O; δ, ppm): 134.3 (s); 132.0 (s); 130.3 (s); 129.1 (s); 42.6 (s). NMR data are similar to those previously reported in the literature.[12]



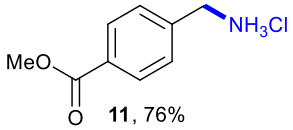
9, 10%

^{1}H-NMR (500 MHz; D_2O; δ, ppm): 7.61 (br s, 2 H, aromatic); 7.34 (br s, 2 H, aromatic); 4.12 (s, 2 H, *CH*$_2$). ^{13}C{^{1}H}-NMR (126 MHz; D_2O; δ, ppm): 132.2 (s); 132.1 (s); 130.7 (s); 122.7 (s); 42.6 (s). NMR data are similar to those previously reported in the literature.[14]



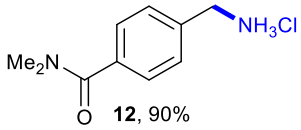
10, 69%

^{1}H-NMR (500 MHz; D_2O; δ, ppm): 7.73 (br s, 2 H, aromatic); 7.56 (br s, 2 H, aromatic); 4.18 (s, 2 H, *CH*$_2$). ^{13}C{^{1}H}-NMR (126 MHz; D_2O; δ, ppm): 138.3 (s); 130.1 (q, J = 32.3 Hz); 129.0 (br s); 126.0 (m); 125.1 (s); 123.0 (s); 42.9 (s). ^{19}F- NMR (471 MHz; D_2O; δ, ppm): -62.44 (s). NMR data are similar to those previously reported in the literature.[12]



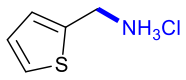
11, 76%

^{1}H-NMR (500 MHz; D_2O; δ, ppm): 8.00 (d, J = 8.2 Hz, 2 H, aromatic); 7.51 (d, J = 8.3 Hz, 2 H, aromatic); 4.21 (s, 2 H, *CH*$_2$N); 3.88 (s, 3 H, O*CH*$_3$). ^{13}C{^{1}H}-NMR (126 MHz; D_2O; δ, ppm): 168.9 (s); 138.5 (s); 130.09 (s); 129.97 (s); 128.8 (s); 52.7 (s); 42.7 (s). NMR data are similar to those previously reported in the literature.[15]



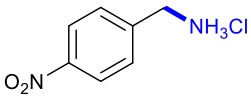
12, 90%

^{1}H-NMR (500 MHz; D_2O; δ, ppm): 7.50 (d, J = 6.7 Hz, 2 H, aromatic); 7.45 (d, J = 6.7 Hz, 2 H, aromatic); 4.19 (s, 2 H, *CH*$_2$); 3.06 (s, 3 H, *NMe*$_2$); 2.95 (s, 3 H, *NMe*$_2$). ^{13}C{^{1}H}-NMR (126 MHz; D_2O; δ, ppm): 173.0 (s); 135.6 (s); 134.7 (s); 129.1 (s); 127.4 (s); 42.7 (s); 39.6 (s); 35.3 (s). NMR data are similar to those previously reported in the literature.[16]



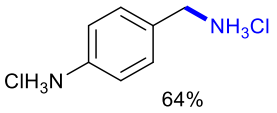
13, 98%

^{1}H-NMR (500 MHz; D_2O; δ, ppm): 7.48 (d, J = 5.1 Hz, 1 H); 7.21 (d, J = 3.3 Hz, 1 H); 7.05–7.10 (m, 1 H); 4.37 (s, 2 H, *CH*$_2$). ^{13}C{^{1}H}-NMR (126 MHz; D_2O; δ, ppm): 133.8 (s); 129.6 (s); 128.0 (s); 127.7 (s); 37.4 (s). NMR data are similar to those previously reported in the literature.[17]



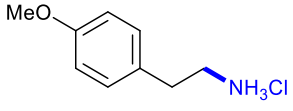
14, 21%

^{1}H-NMR (500 MHz; D_2O; δ, ppm): 8.20 (d, J = 7.6 Hz, 2 H, aromatic); 7.59 (d, J = 7.6 Hz, 2 H, aromatic); 4.24 (s, 2 H, *CH*$_2$N). ^{13}C{^{1}H}-NMR (126 MHz; D_2O; δ, ppm): 148.0 (s); 139.8 (s); 129.8 (s); 124.2 (s); 42.3 (s). NMR data are similar to those previously reported in the literature.[18]



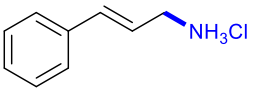
64%

^{1}H-NMR (500 MHz; D_2O; δ, ppm): 7.23 (d, J = 7.1 Hz, 2 H, aromatic); 6.86 (d, J = 7.1 Hz, 2 H, aromatic); 4.01 (s, 2 H, *CH*$_2$N). ^{13}C{^{1}H}-NMR (126 MHz; D_2O; δ, ppm): 134.1 (s); 130.3 (s); 124.2 (s); 117.2 (s); 42.7 (s). NMR data are similar to those previously reported in the literature.[11,12]



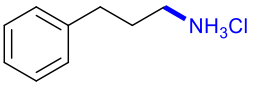
15, 87%

^{1}H-NMR (500 MHz; D_2O; δ, ppm): 7.21 (br d, J = 5.1 Hz, 2 H, aromatic); 6.93 (br d, J = 5.1 Hz, 2 H, aromatic); 3.76 (s, 3 H, *OMe*); 3.17 (s, 2 H, *CH*$_2$); 2.88 (s, 2 H, *CH*$_2$). ^{13}C{^{1}H}-NMR (126 MHz; D_2O; δ, ppm): 157.9 (s); 130.1 (s); 129.1 (s); 114.5 (s); 55.4 (s); 40.7 (s); 31.9 (s). NMR data are similar to those previously reported in the literature.[19]



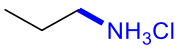
16, 29%

^{1}H-NMR (500 MHz; D_2O; δ, ppm): 7.48 (d, J = 7.3 Hz, 2 H, *o*-H, *Ph*); 7.38 (t, J = 7.4 Hz, 2 H, *m*-H, *Ph*); 7.34 (m, 1 H, *p*-H, *Ph*); 6.77 (d, J = 16.0 Hz, 1 H, Ph*CH*=); 6.42–6.22 (m, 1 H, PhCH=*CH*-); 3.72 (d, J = 6.8 Hz, 2 H, CH_2N). ^{13}C{^{1}H}-NMR (126 MHz; D_2O; δ, ppm): 135.8 (s); 135.7 (s); 129.0 (s); 128.7 (s); 126.7 (s); 120.6 (s); 41.3 (s). NMR data are similar to those previously reported in the literature.[20]



17, 69%

^{1}H-NMR (500 MHz; D_2O; δ, ppm): 7.34 (d, J = 7.3 Hz, 2 H, *o*-H, *Ph*); 7.29-7.23 (m, 3 H, *m*-H and *o*-H, *Ph*); 3.01–2.90 (m, 2 H, CH_2N); 2.68 (t, J = 7.7 Hz, 2 H, PhCH_2); 1.98–1.90 (m, 2 H, PhCH$_2CH_2$CH$_2$N). ^{13}C{^{1}H}-NMR (126 MHz; D_2O; δ, ppm): 141.0 (s); 128.8 (s); 128.5 (s); 126.4 (s); 39.0 (s); 31.8 (s); 28.5 (s). NMR data are similar to those previously reported in the literature.[18,21]



18, 82%

^{1}H-NMR (500 MHz; D_2O; δ, ppm): 2.91 (br t, J = 6.9 Hz, 2 H, CH_2N); 1.68-1.55 (m, 2 H, CH_3CH_2), 0.92 (br t, J = 7.0 Hz, 3 H, CH_3CH_2). ^{13}C{^{1}H}-NMR (126 MHz; D_2O; δ, ppm): 41.4 (s); 20.6 (s); 10.4 (s). NMR data are similar to those previously reported in the literature.[14]

4. NMR spectra for products of transfer hydrogenation reactions

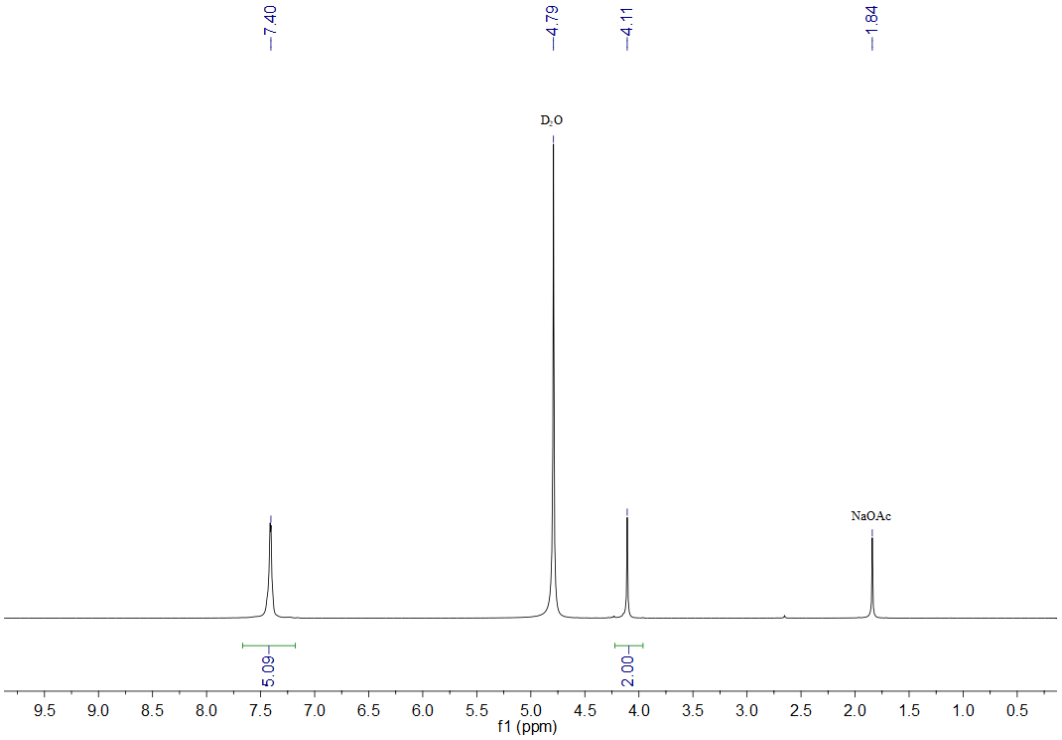


Figure S34. The ^{1}H-NMR spectrum (in D_2O) of $PhCH_2NH_3Cl$ (**4**).

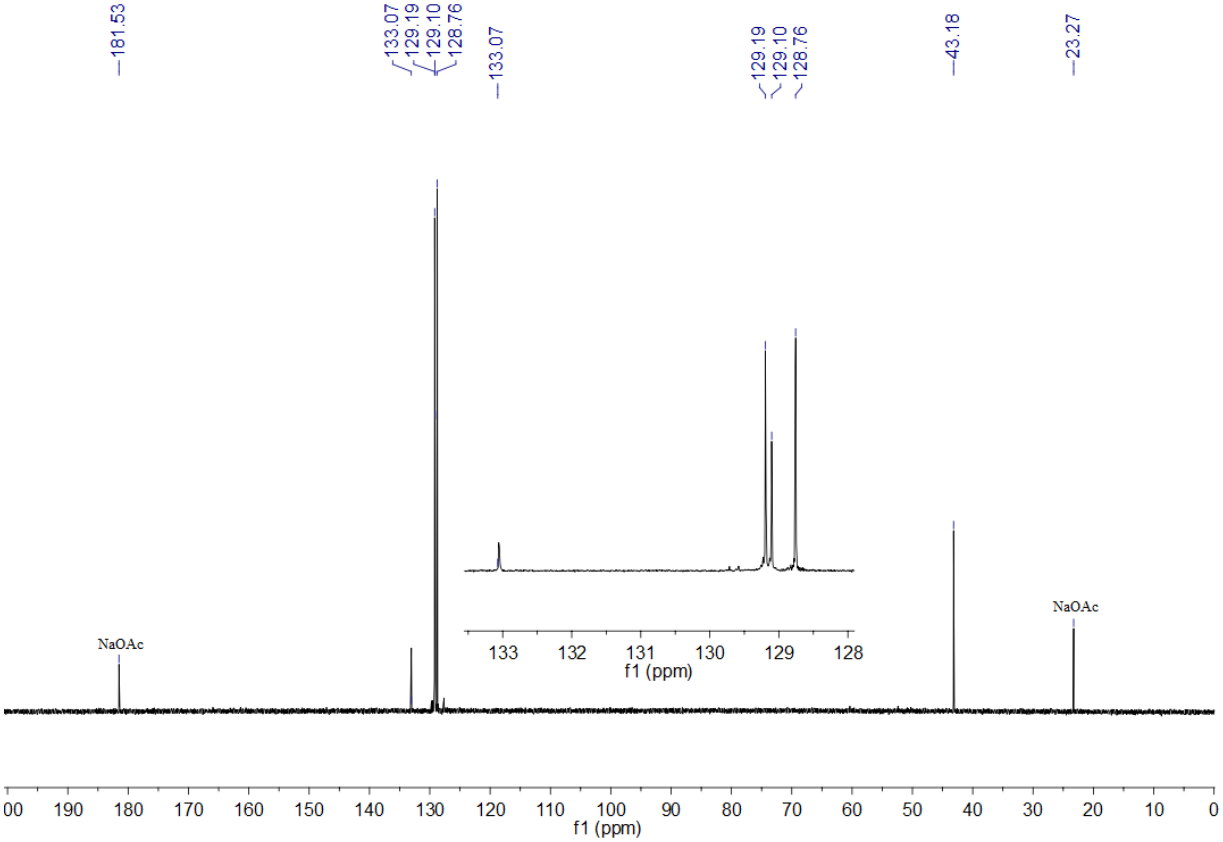


Figure S35. The ^{13}C{^{1}H}-NMR spectrum (in D_2O) of $PhCH_2NH_3Cl$ (**4**).

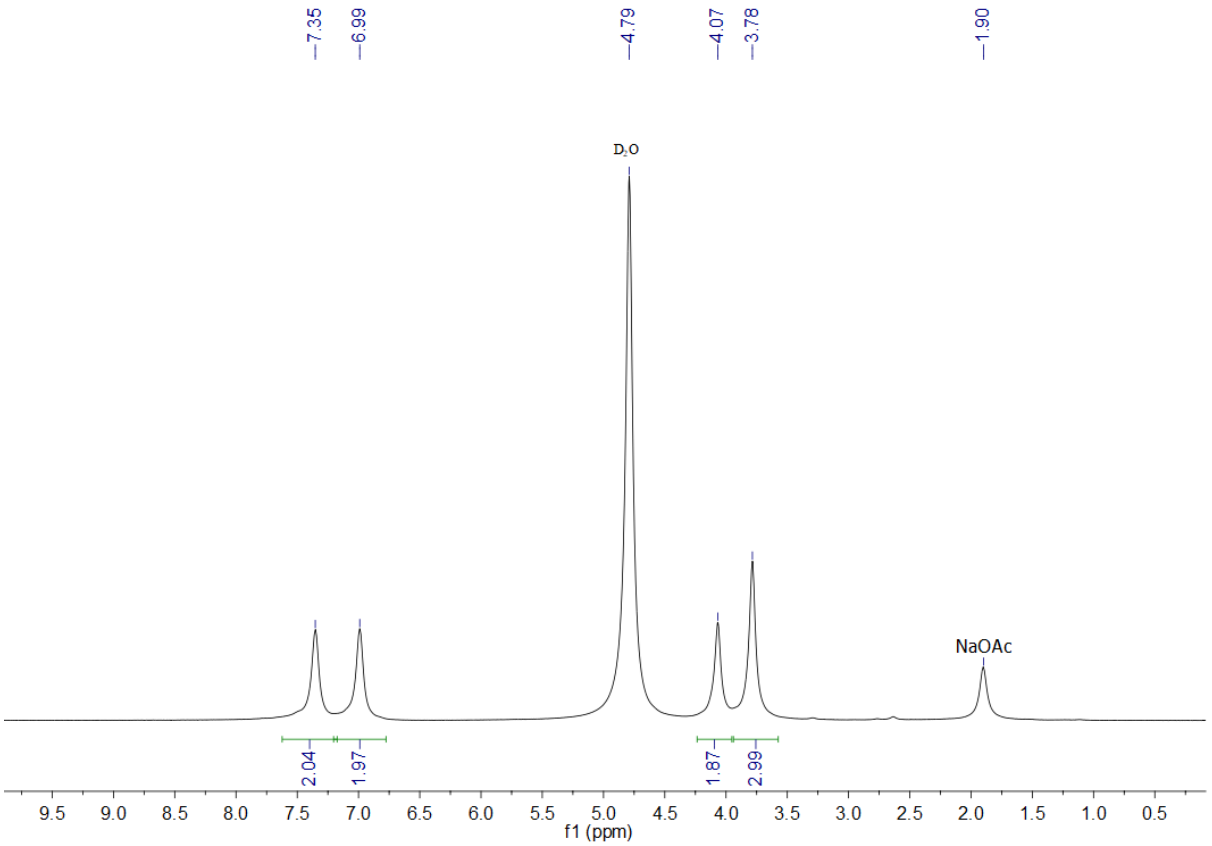


Figure S36. The ^{1}H-NMR spectrum (in D_2O) of *p*-MeO-C_6H_4-CH_2NH_3Cl (**5**).

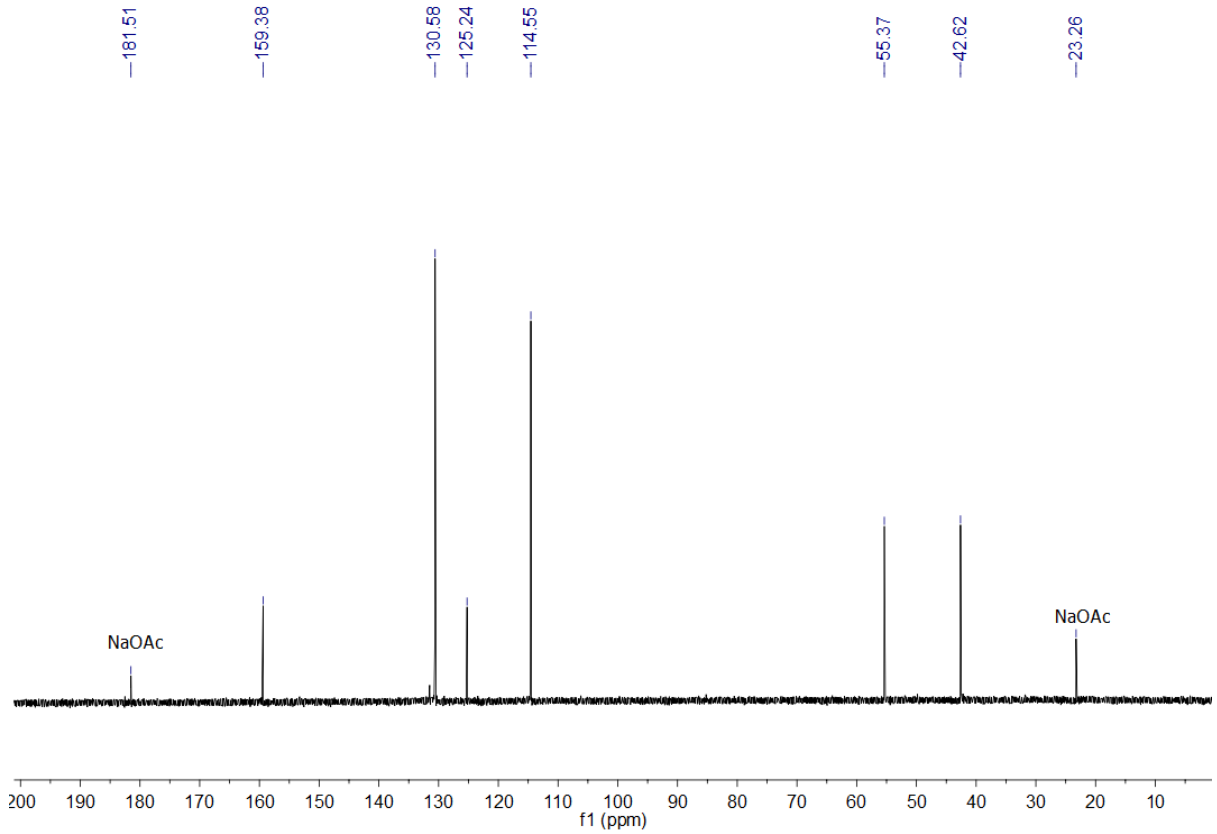


Figure S37. The ^{13}C{^{1}H}-NMR spectrum (in D_2O) of *p*-MeO-C_6H_4-CH_2NH_3Cl (**5**).

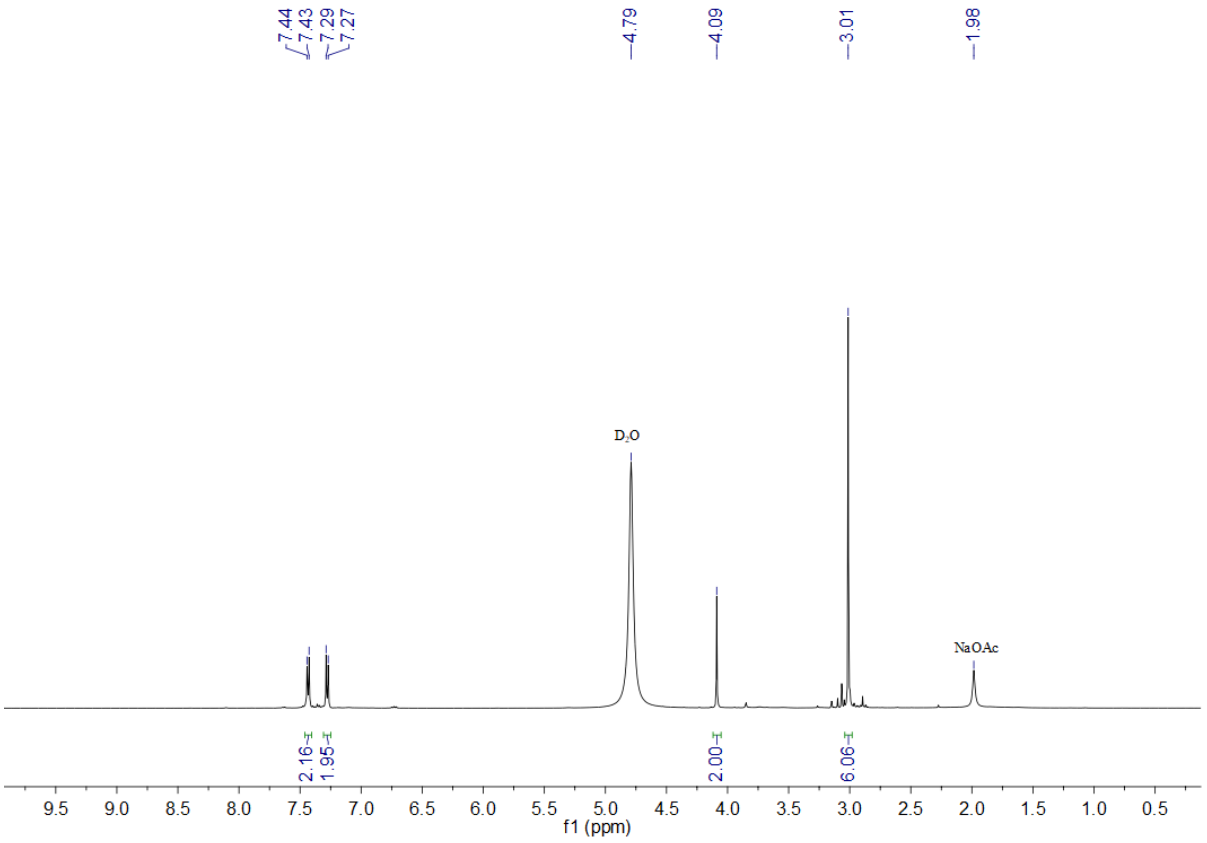


Figure S38. The ^{1}H-NMR spectrum (in D_2O) of *p*-Me_2N-C_6H_4-CH_2NH_3Cl (**6**).

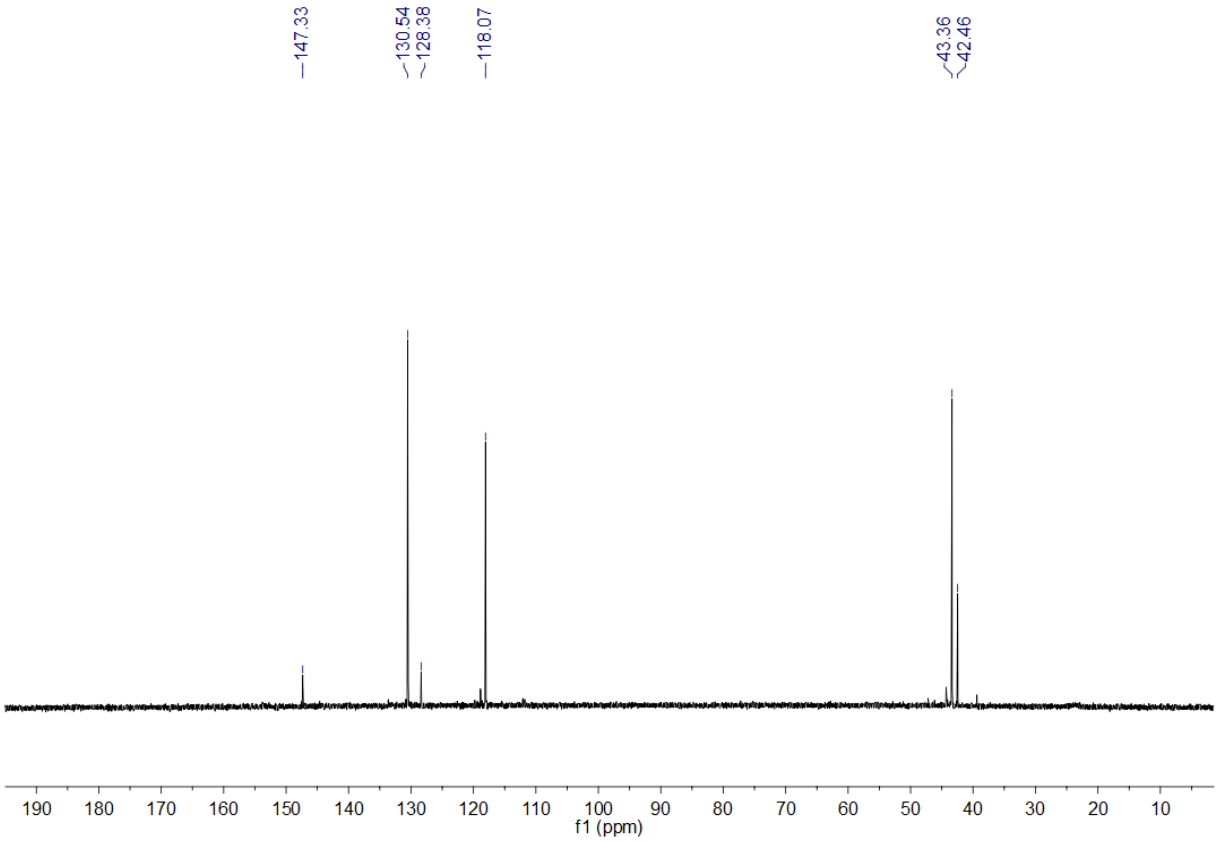


Figure S39. The ^{13}C{^{1}H}-NMR spectrum (in D_2O) of *p*-Me_2N-C_6H_4-CH_2NH_3Cl (**6**).

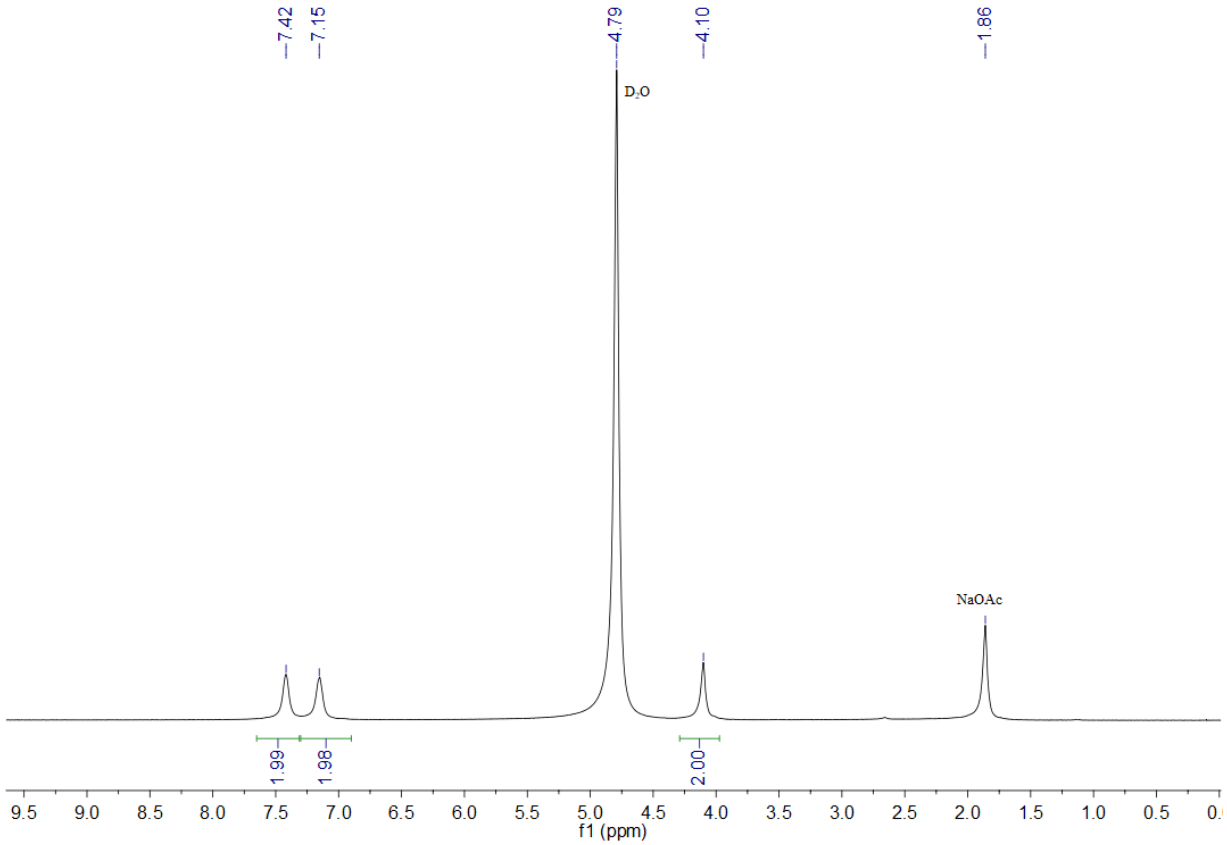


Figure S40. The ^{1}H-NMR spectrum (in D_2O) of *p*-F-C_6H_4-CH_2NH_3Cl (**7**).

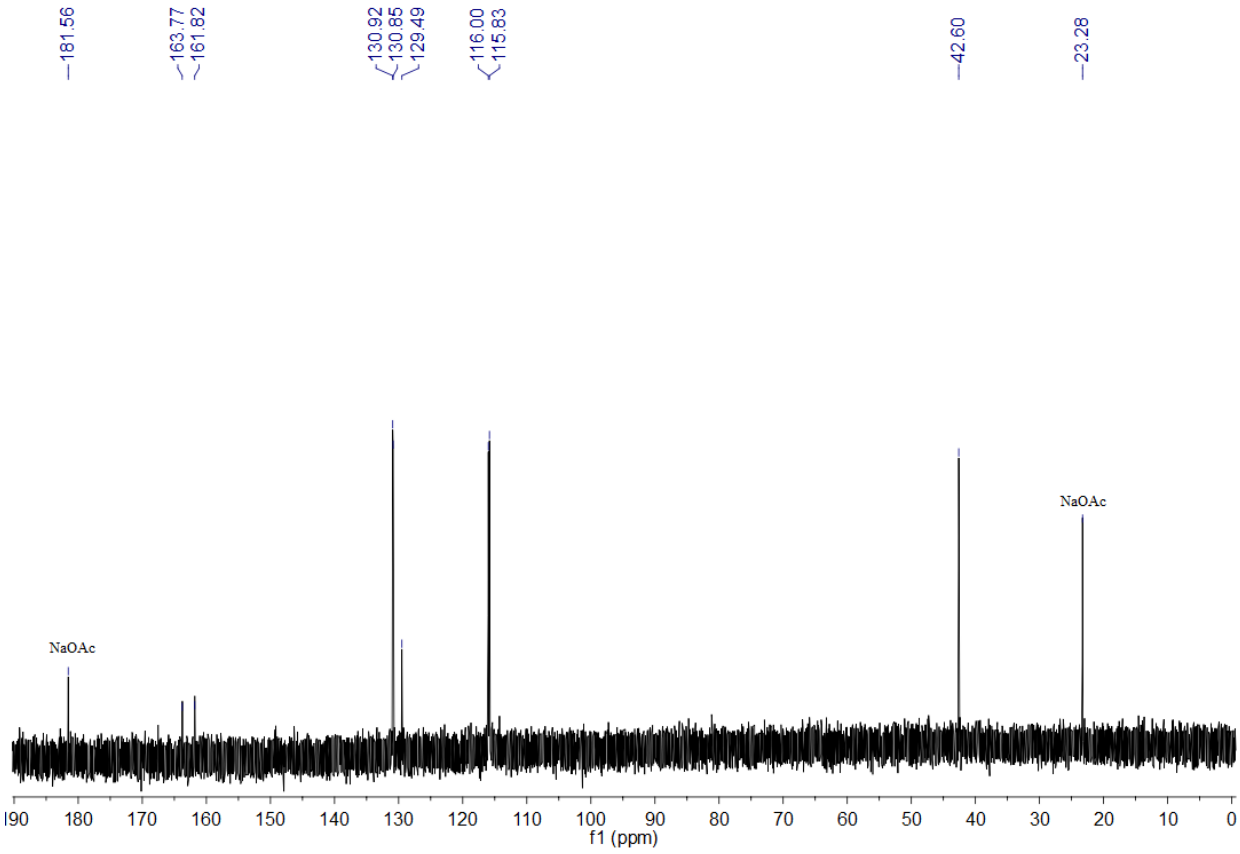


Figure S41. The ^{13}C{^{1}H}-NMR spectrum (in D_2O) of *p*-F-C_6H_4-CH_2NH_3Cl (**7**).

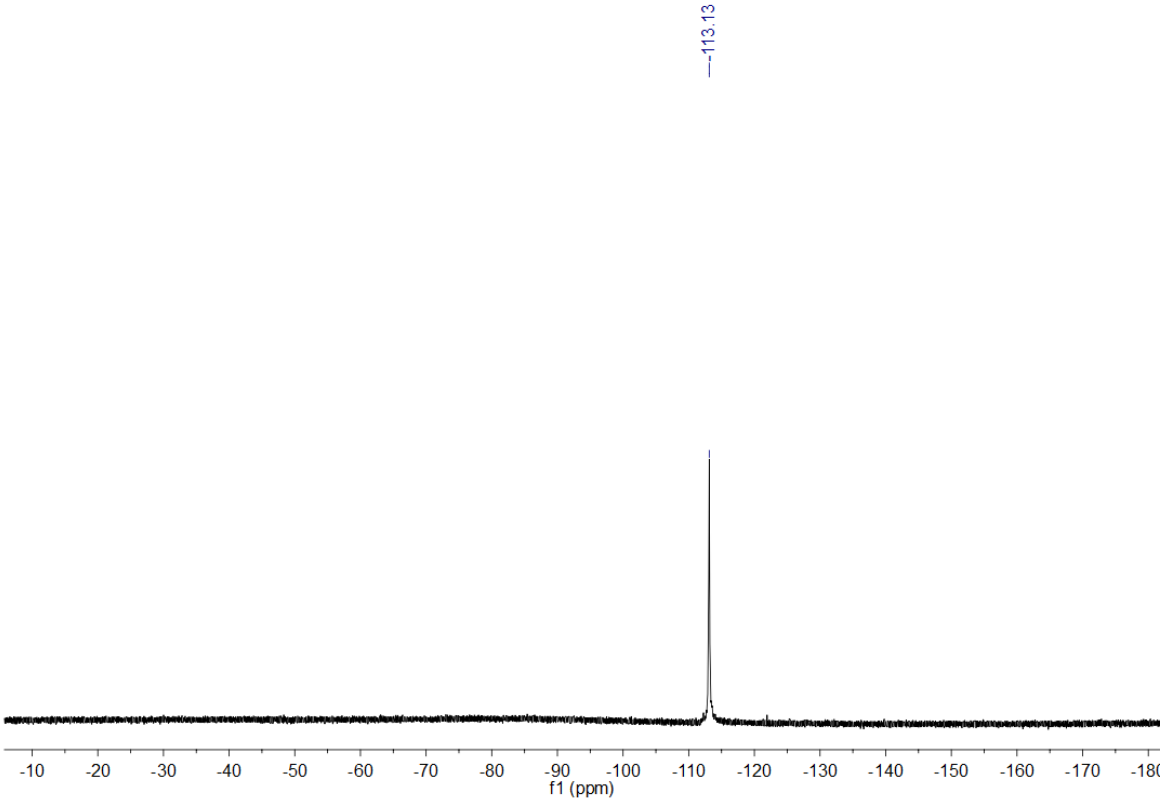


Figure S42. The ^{19}F-NMR spectrum (in D_2O) of *p*-F-C_6H_4-CH_2NH_3Cl (**7**).

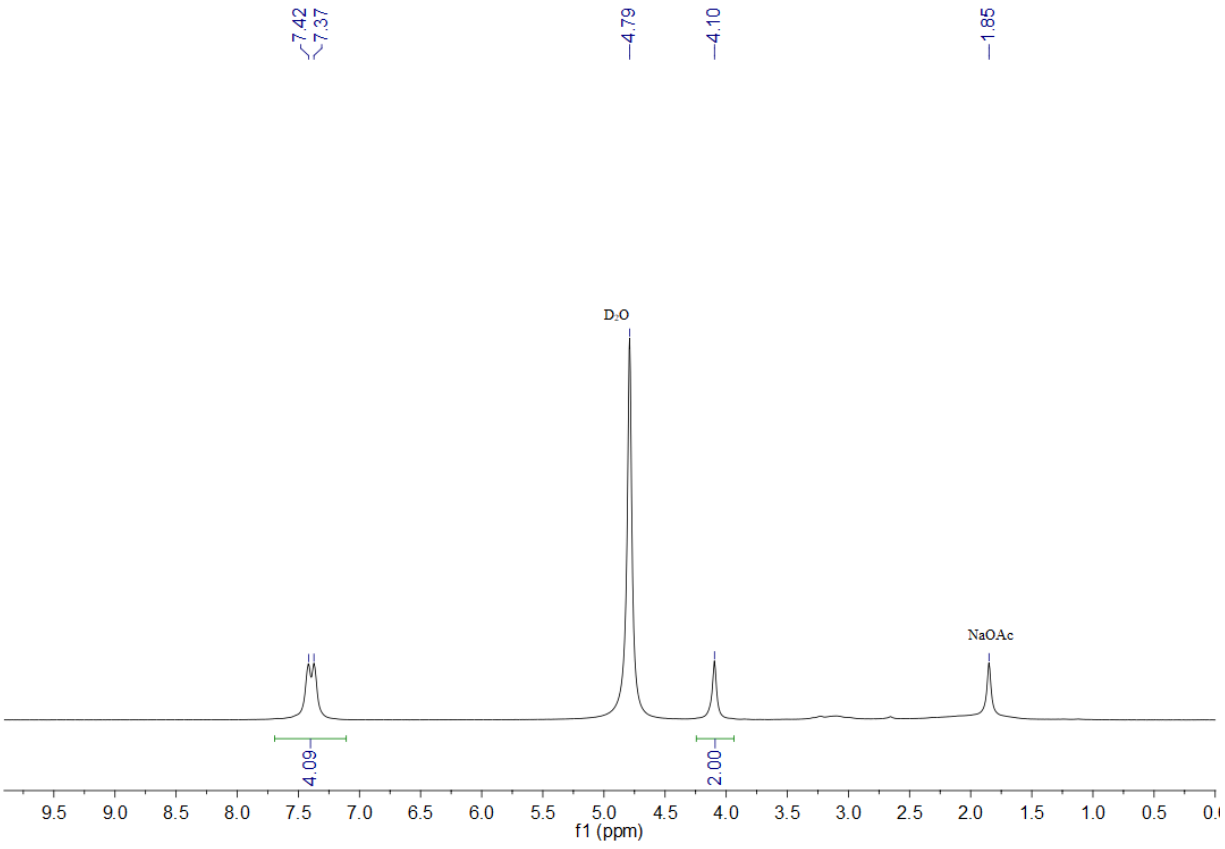


Figure S43. The ^{1}H-NMR spectrum (in D_2O) of *p*-Cl-C_6H_4-CH_2NH_3Cl (**8**).

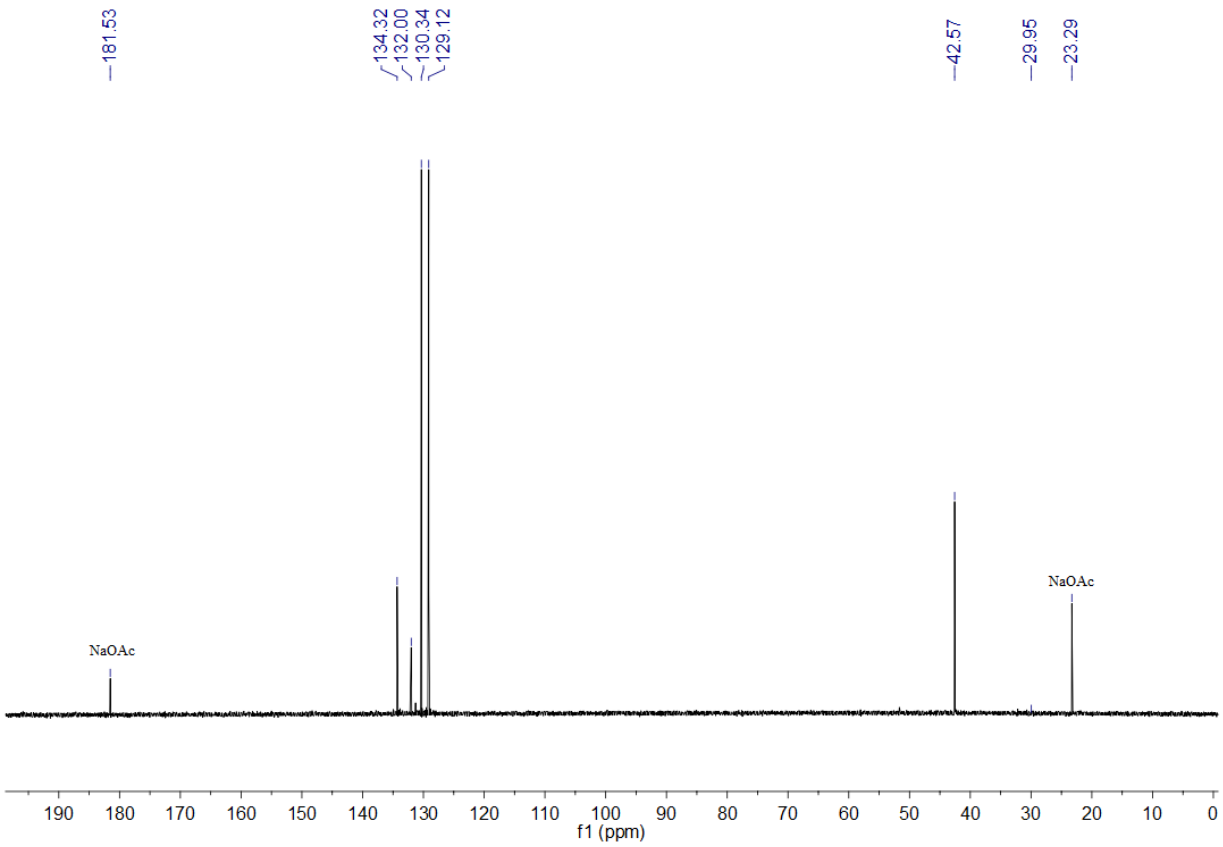


Figure S44. The $^{13}C\{^{1}H\}$-NMR spectrum (in D_2O) of *p*-Cl-C_6H_4-CH_2NH_3Cl (**8**).

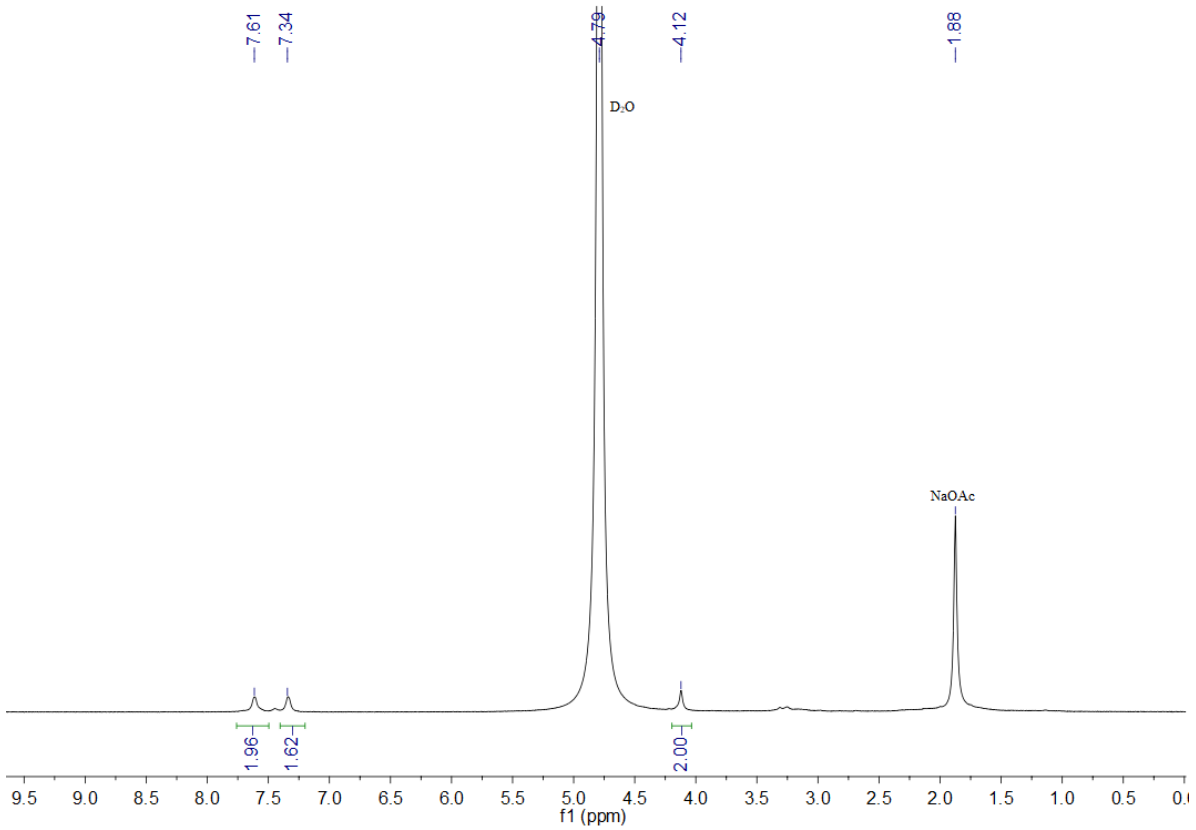


Figure S45. The ^{1}H-NMR spectrum (in D_2O) of *p*-Br-C_6H_4-CH_2NH_3Cl (**9**).

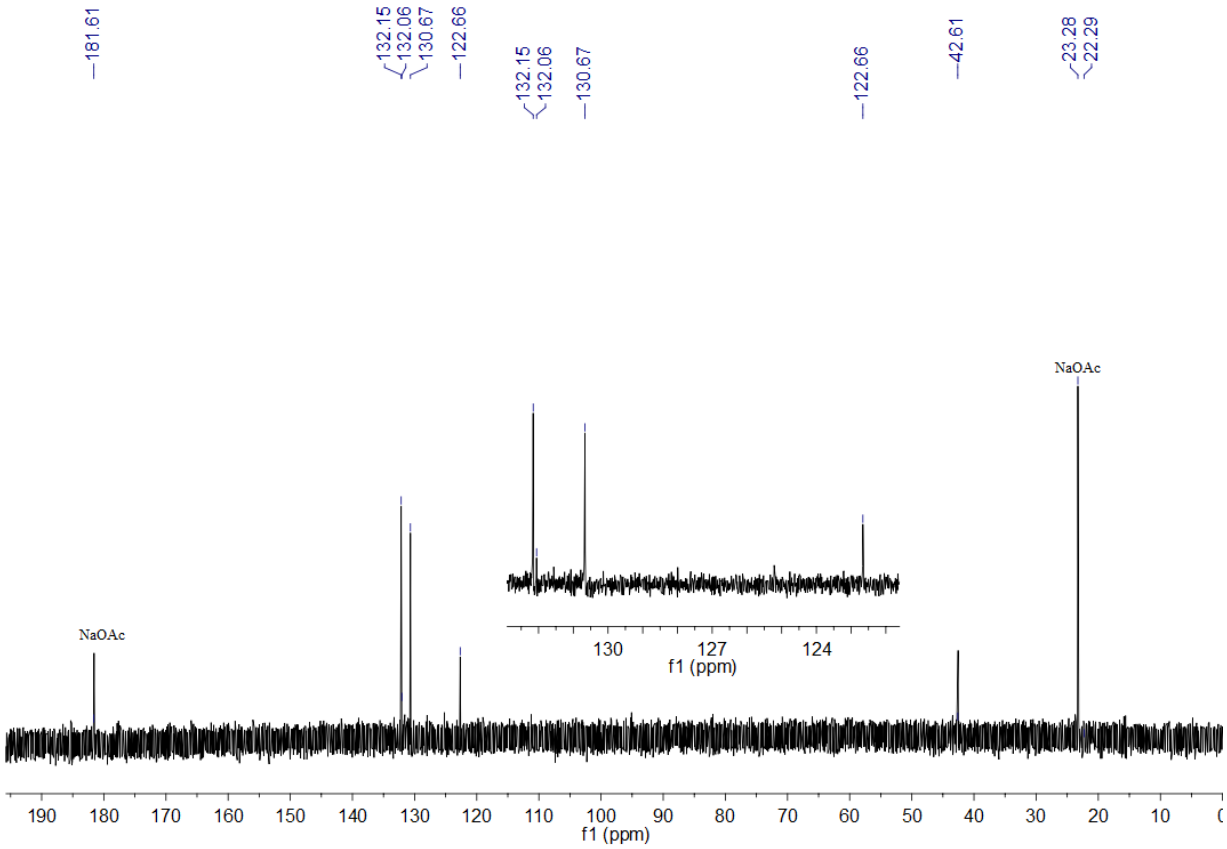


Figure S46. The $^{13}C\{^{1}H\}$-NMR spectrum (in D_2O) of *p*-Br-C_6H_4-CH_2NH_3Cl (**9**).

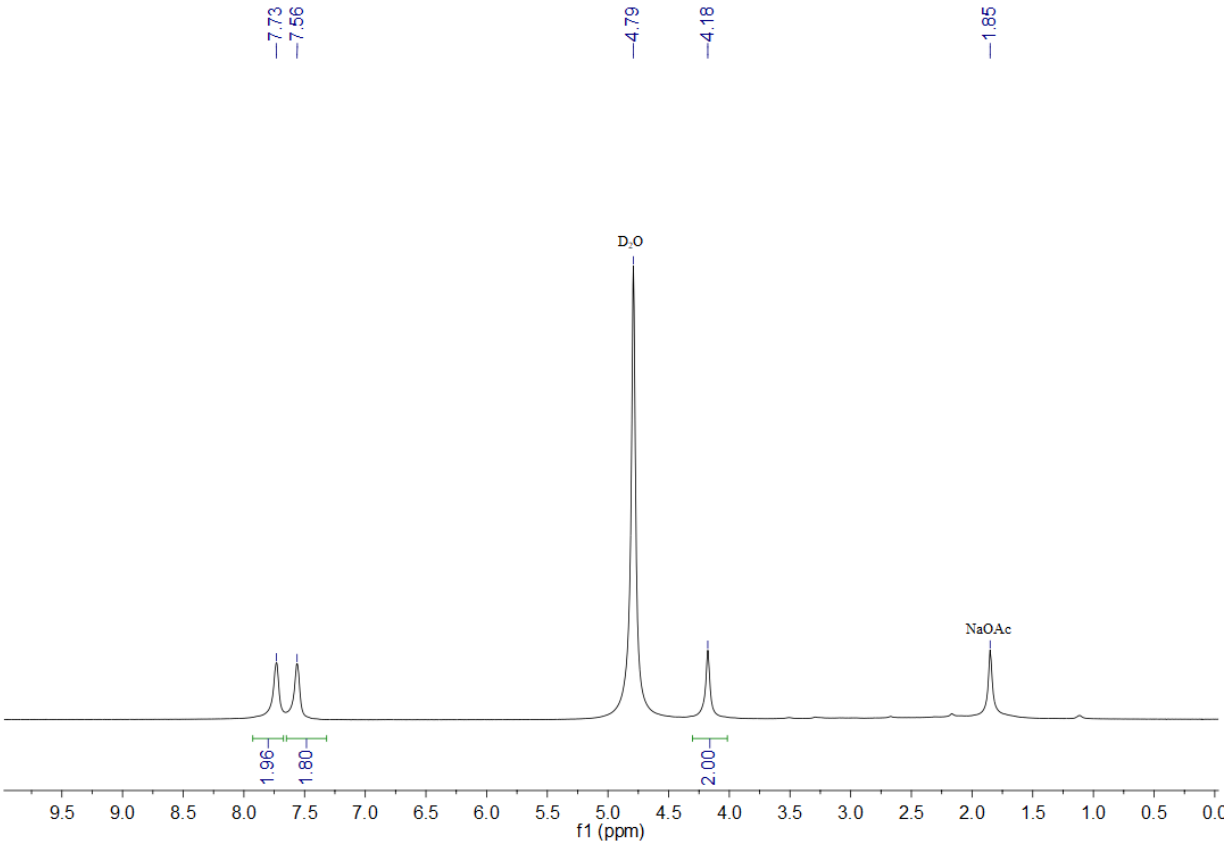


Figure S47. The ^{1}H-NMR spectrum (in D_2O) of *p*-CF_3-C_6H_4-CH_2NH_3Cl (**10**).

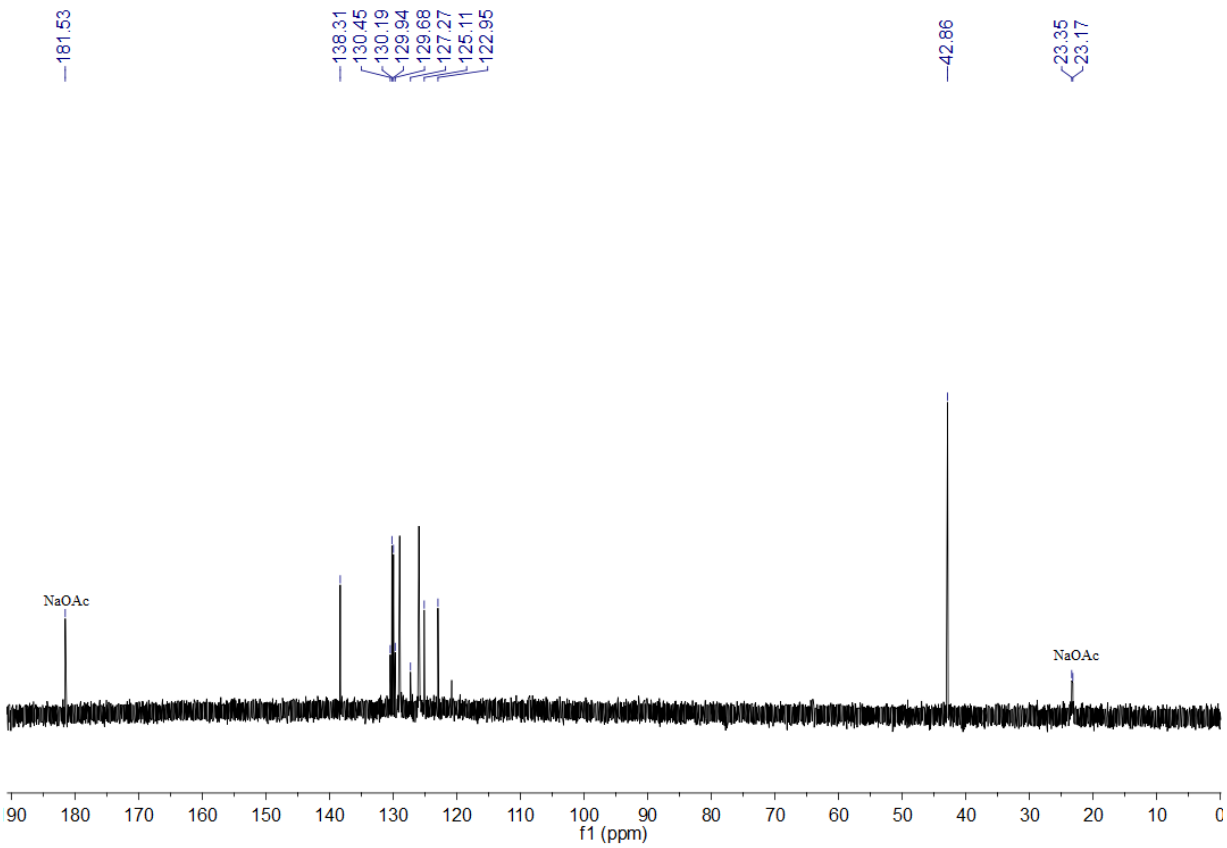


Figure S48. The $^{13}C\{^{1}H\}$-NMR spectrum (in D_2O) of *p*-CF_3-C_6H_4-CH_2NH_3Cl (**10**).

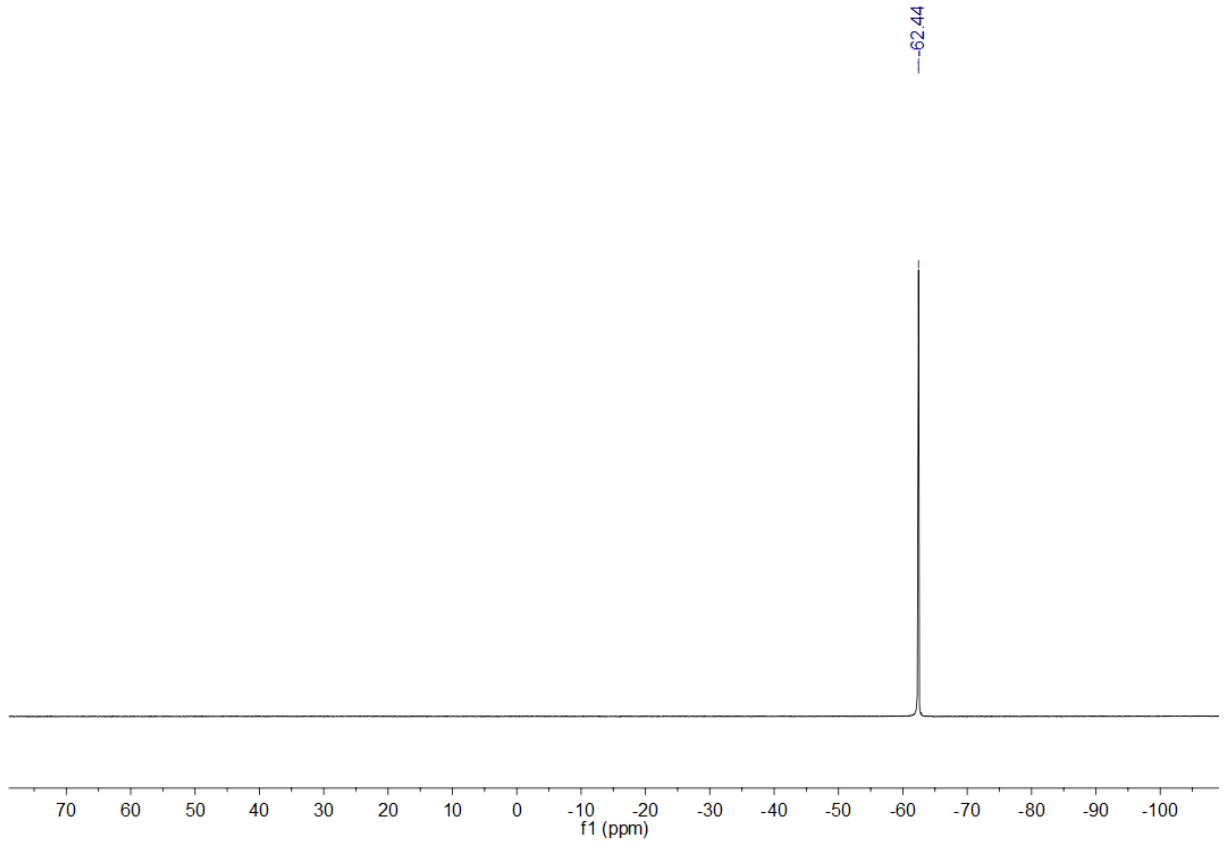


Figure S49. The ^{19}F-NMR spectrum (in D_2O) of *p*-CF_3-C_6H_4-CH_2NH_3Cl (**10**).

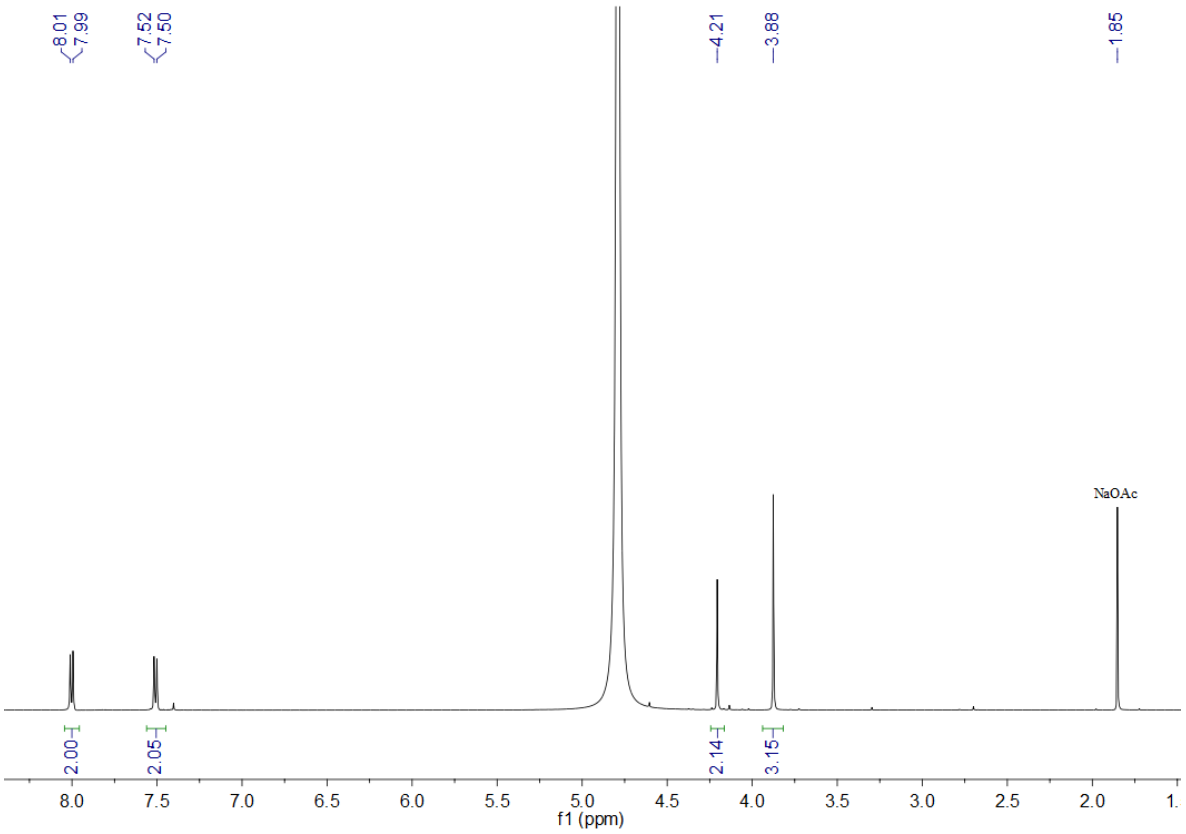


Figure S50. The ^{1}H-NMR spectrum (in D_2O) of *p*-MeOC(O)-C_6H_4-CH_2NH_3Cl (**11**).

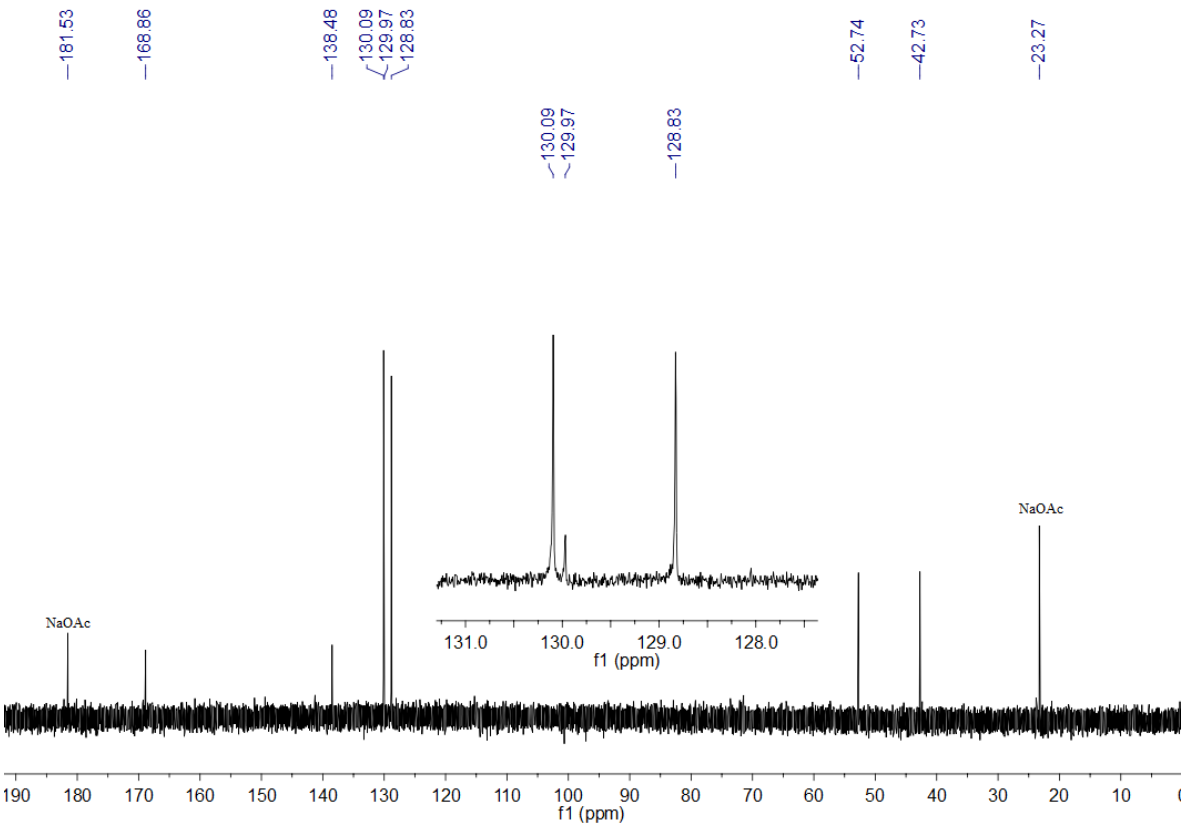


Figure S51. The ^{13}C{^{1}H}-NMR spectrum (in D_2O) of *p*-MeOC(O)-C_6H_4-CH_2NH_3Cl (**11**).

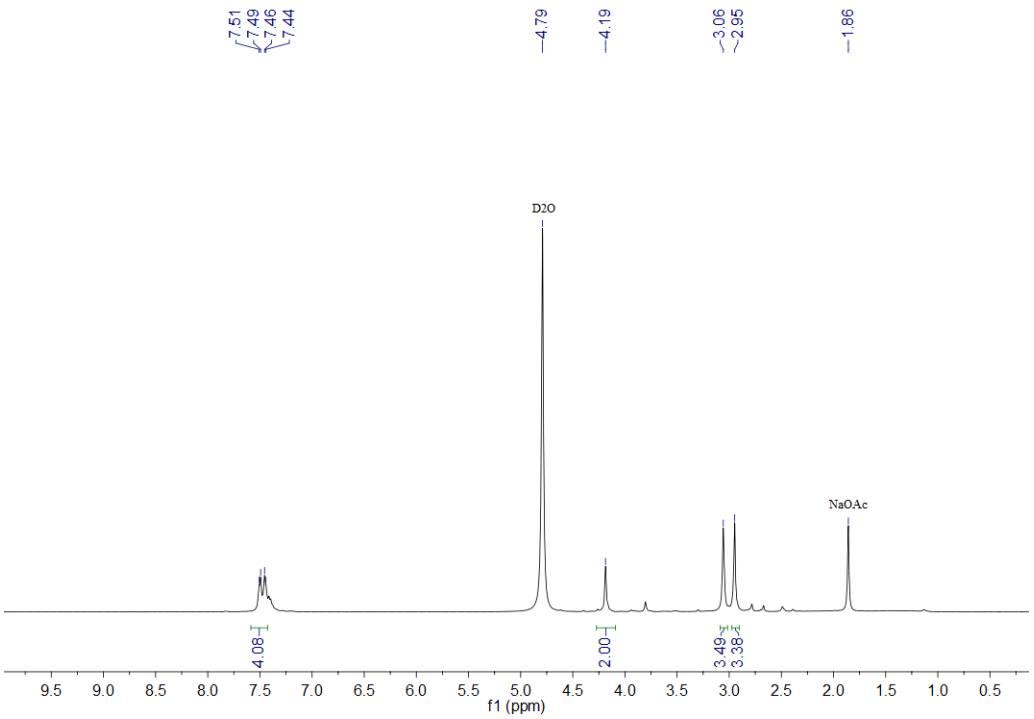


Figure S52. The ^{1}H-NMR spectrum (in D_2O) of *p*-$Me_2NC(O)$-C_6H_4-CH_2NH_3Cl (**12**).

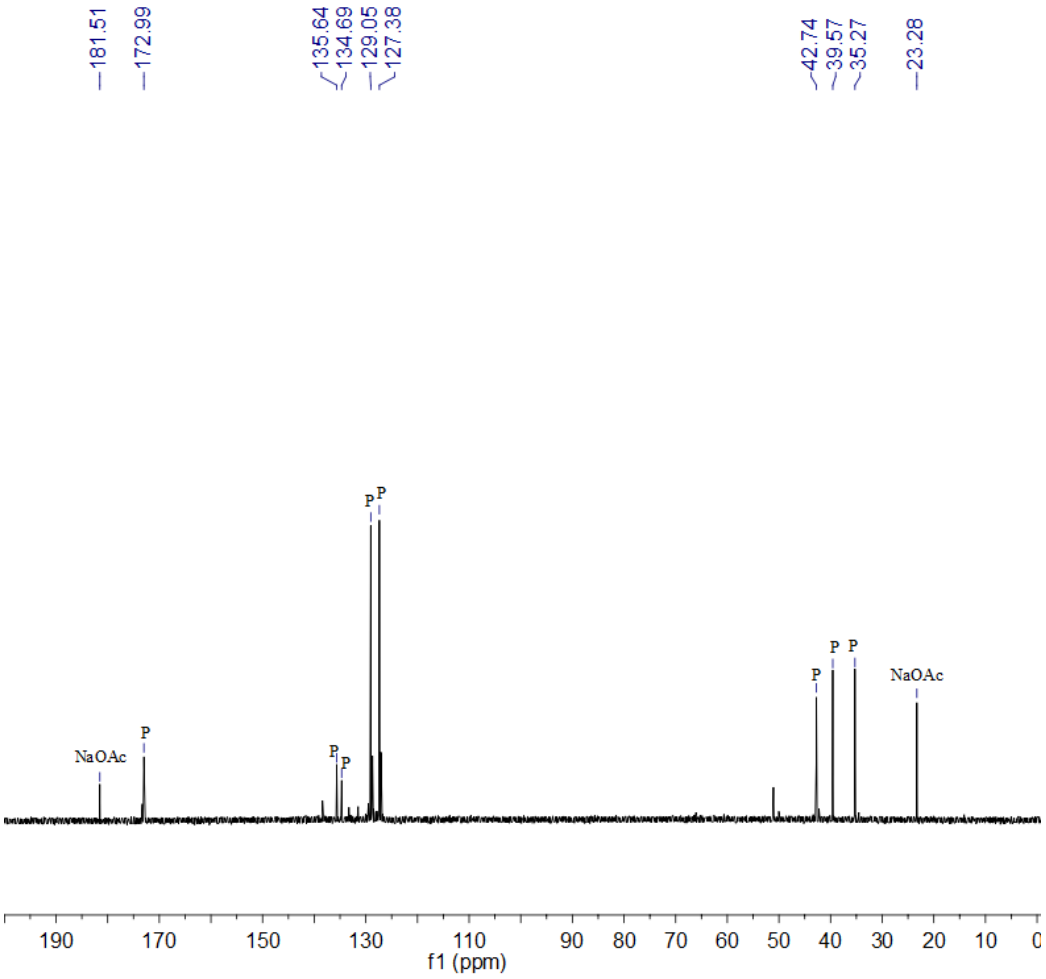


Figure S53. The ^{13}C{^{1}H}-NMR spectrum (in D_2O) of *p*-$Me_2NC(O)$-C_6H_4-CH_2NH_3Cl (**12**) (marked as P).

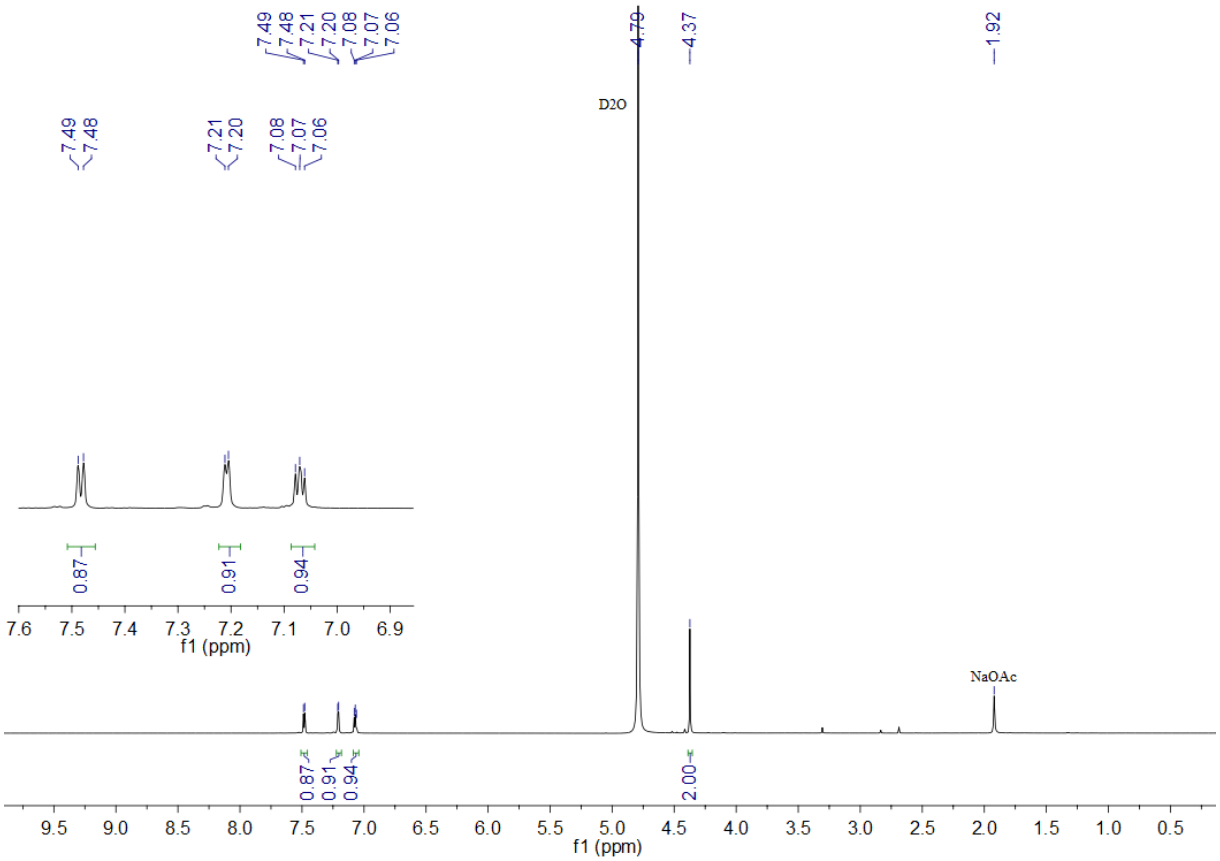


Figure S54. The ^{1}H-NMR spectrum (in D_2O) of 2-thiophenemethylamine hydrochloride (**13**).

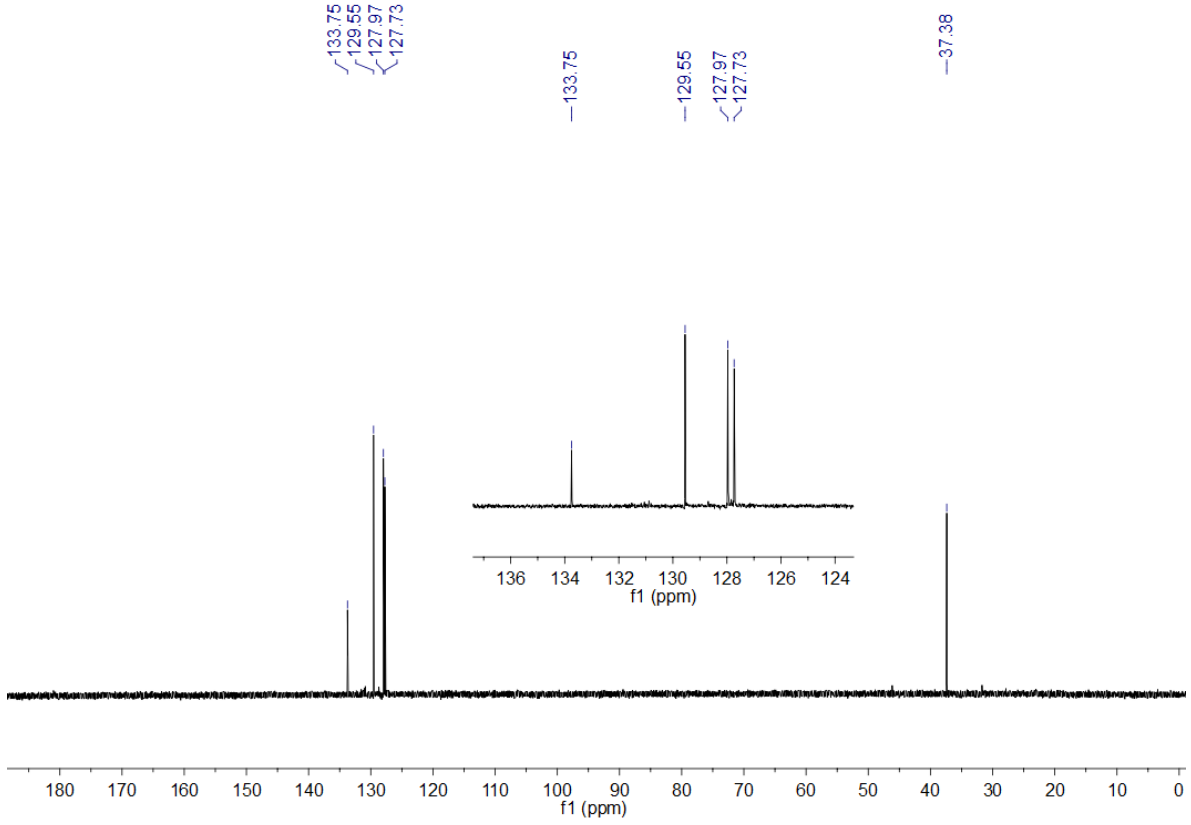
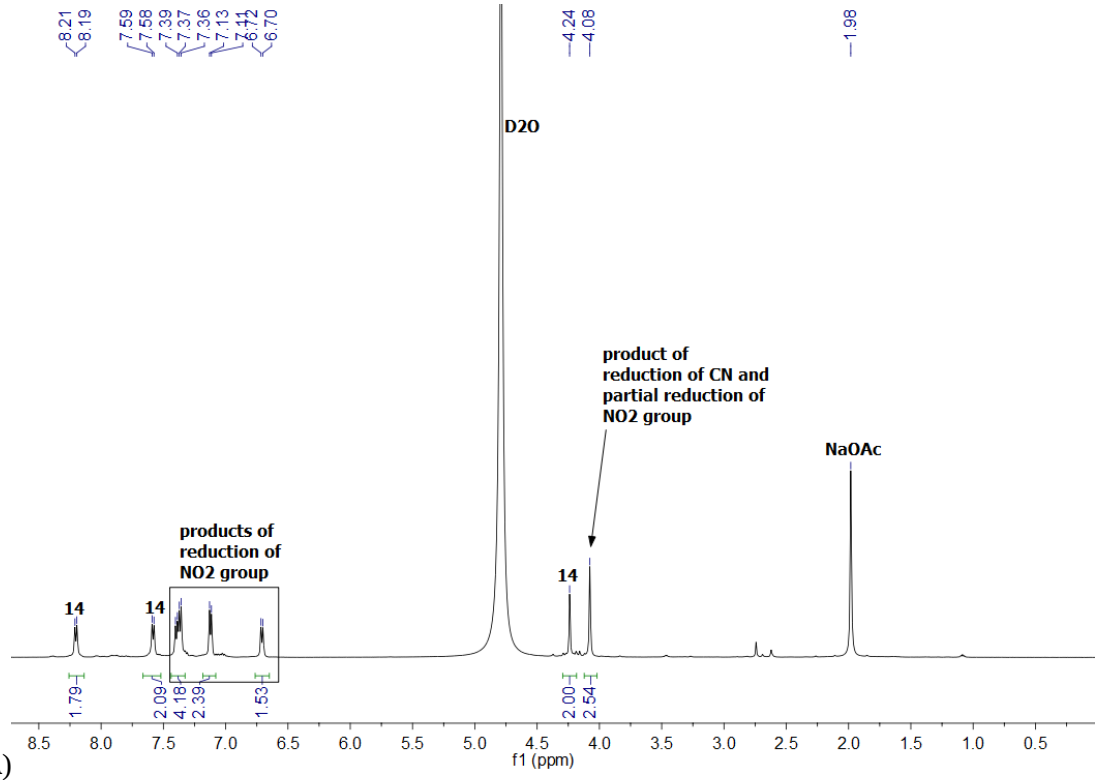
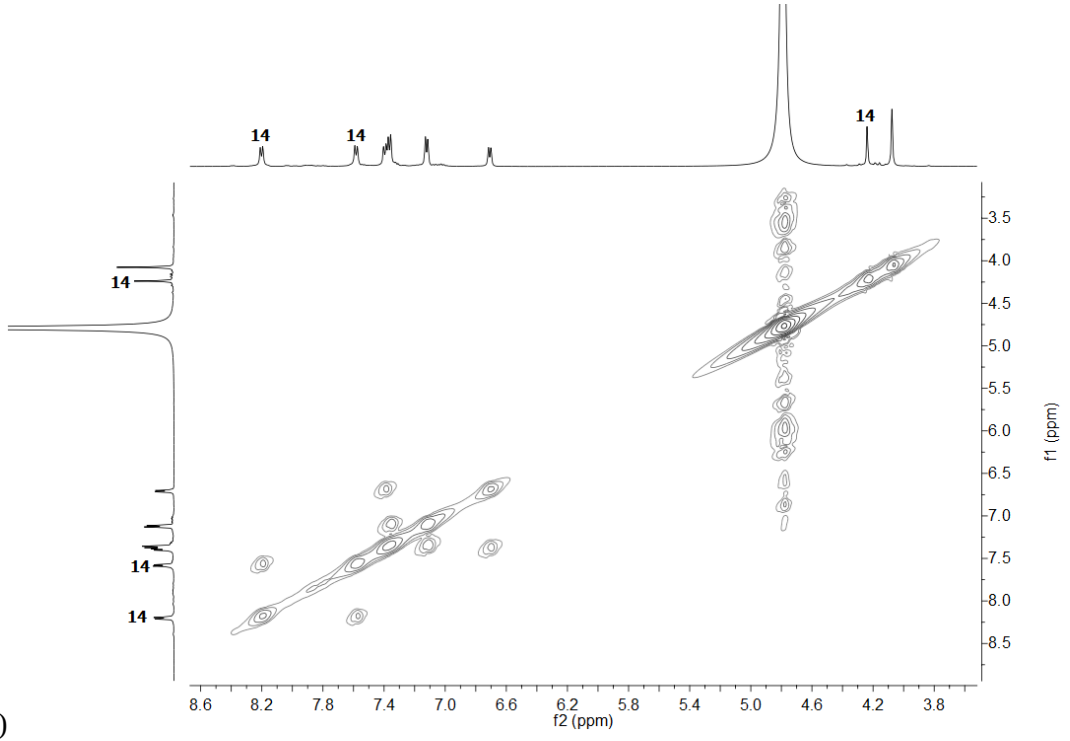


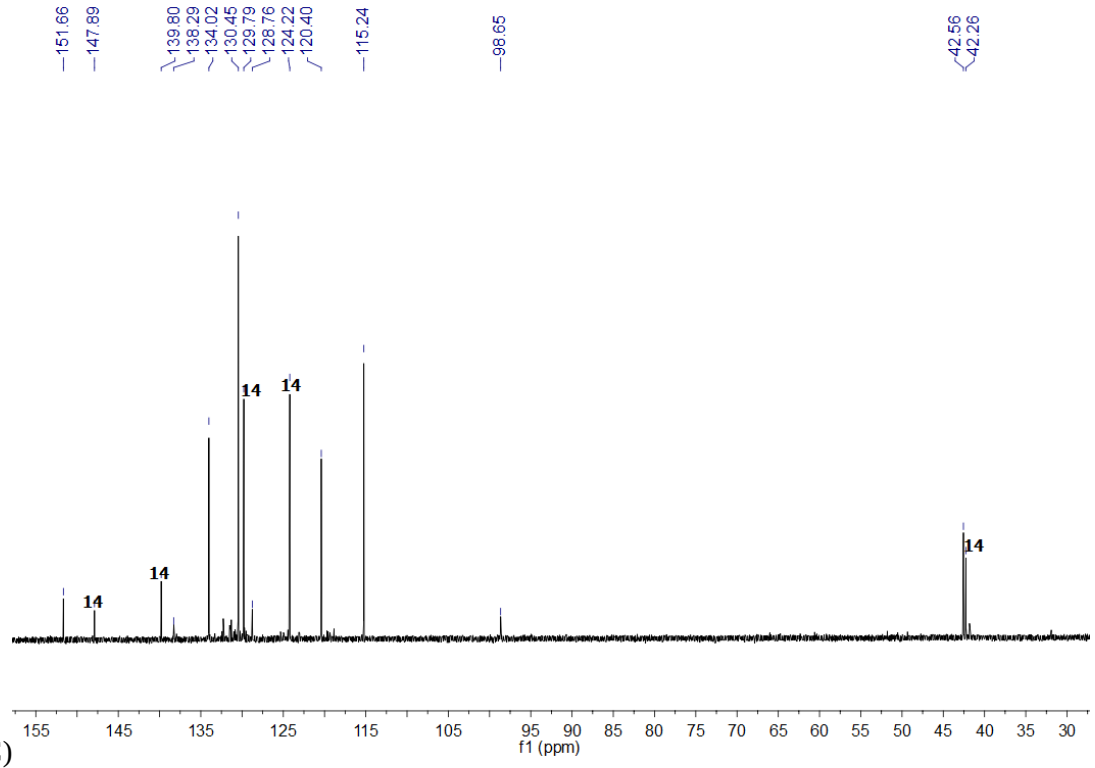
Figure S55. The ^{13}C{^{1}H}-NMR spectrum (in D_2O) of 2-thiophenemethylamine hydrochloride (**13**).


8.21
8.19
7.59
7.58
7.39
7.37
7.36
7.13
6.72
6.70
4.24
4.08
1.98
D2O
product of reduction of CN and partial reduction of NO2 group
NaOAc
products of reduction of NO2 group
14
14
14
14
1.79
2.09
4.18
2.39
1.53
2.00
2.54
f1 (ppm)

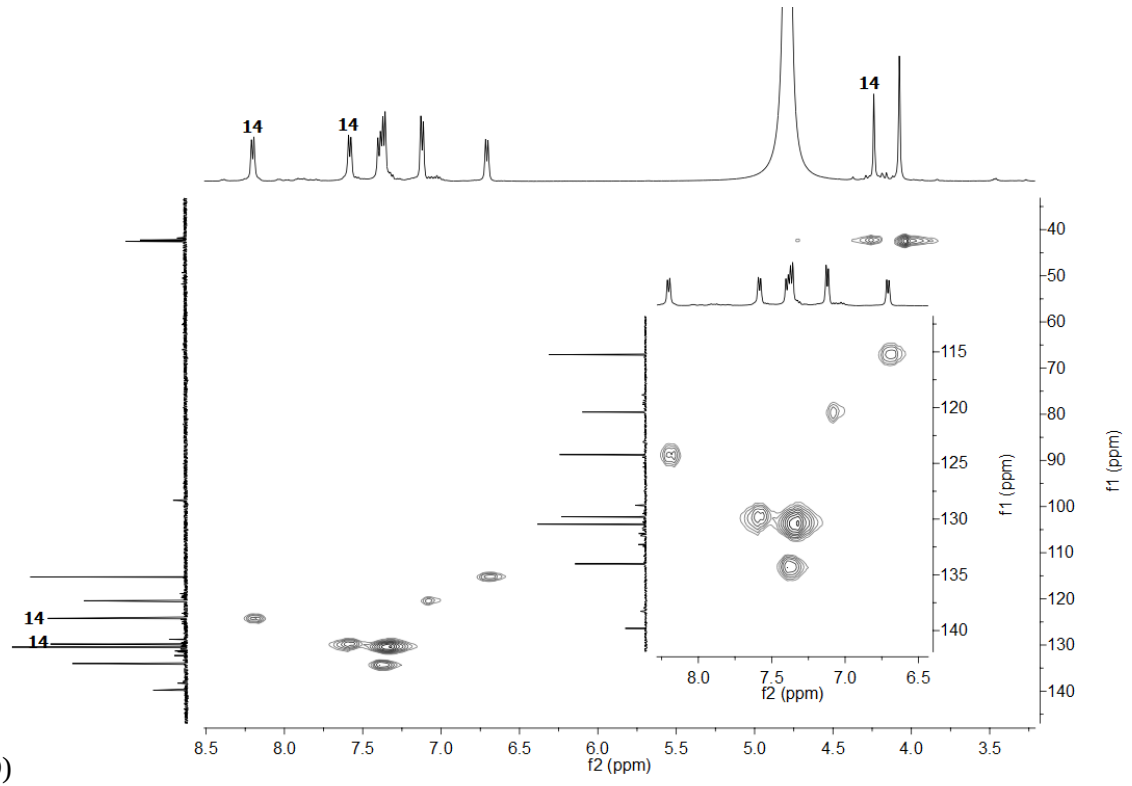
(**A**)


14
14
14
14
14
14
f2 (ppm)
f1 (ppm)

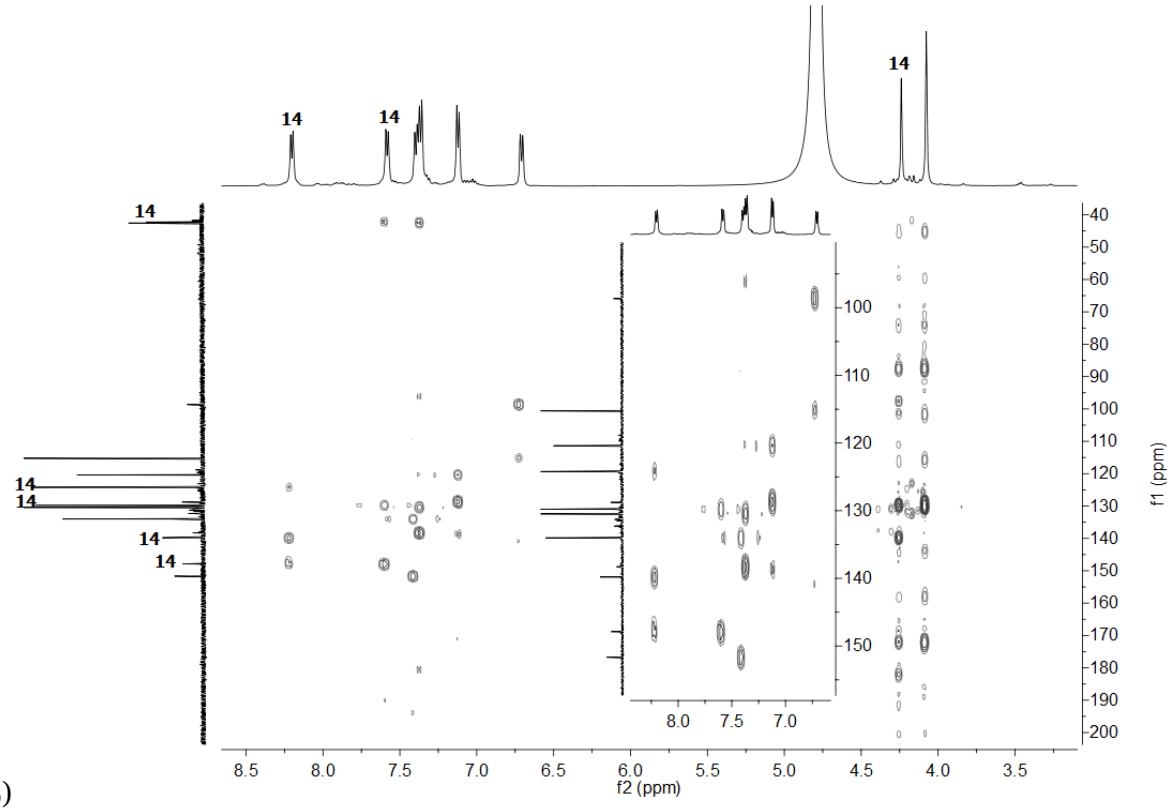
(**B**)


151.66
147.89
139.80
138.29
134.02
130.45
129.79
128.76
124.22
120.40
115.24
98.65
42.56
42.26
14
f1 (ppm)

(**C**)

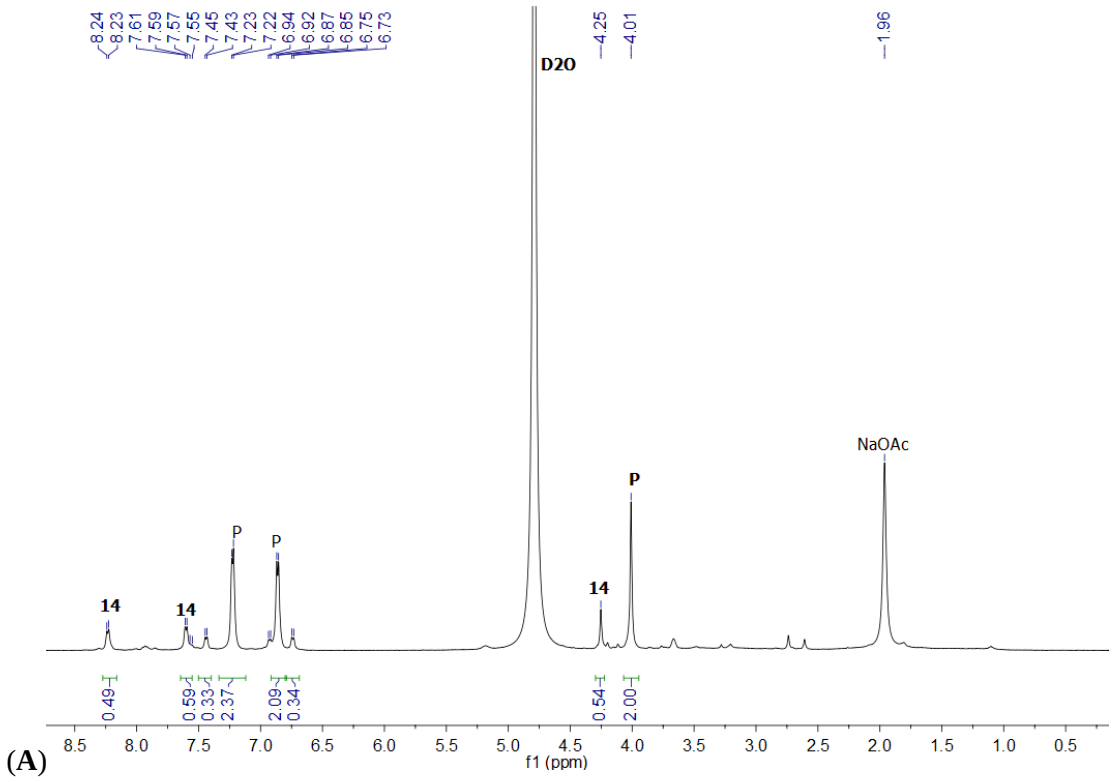

14
f2 (ppm)
f1 (ppm)

(**D**)

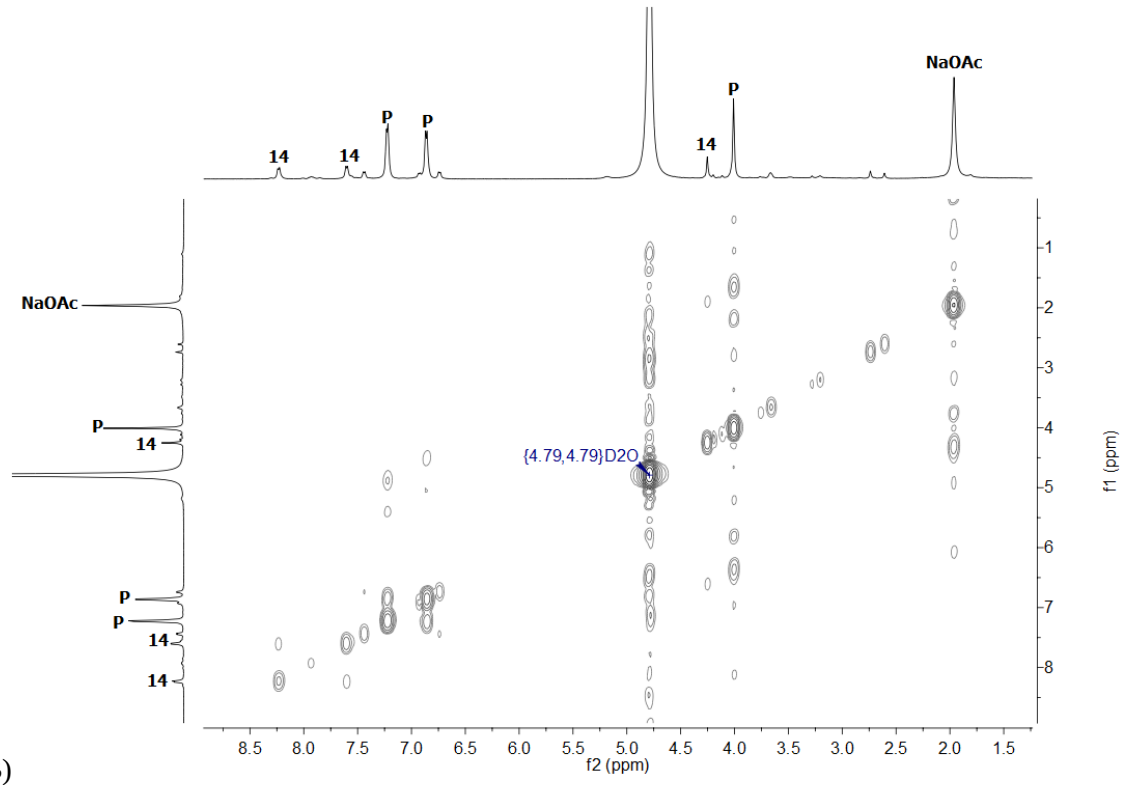


(**E**)

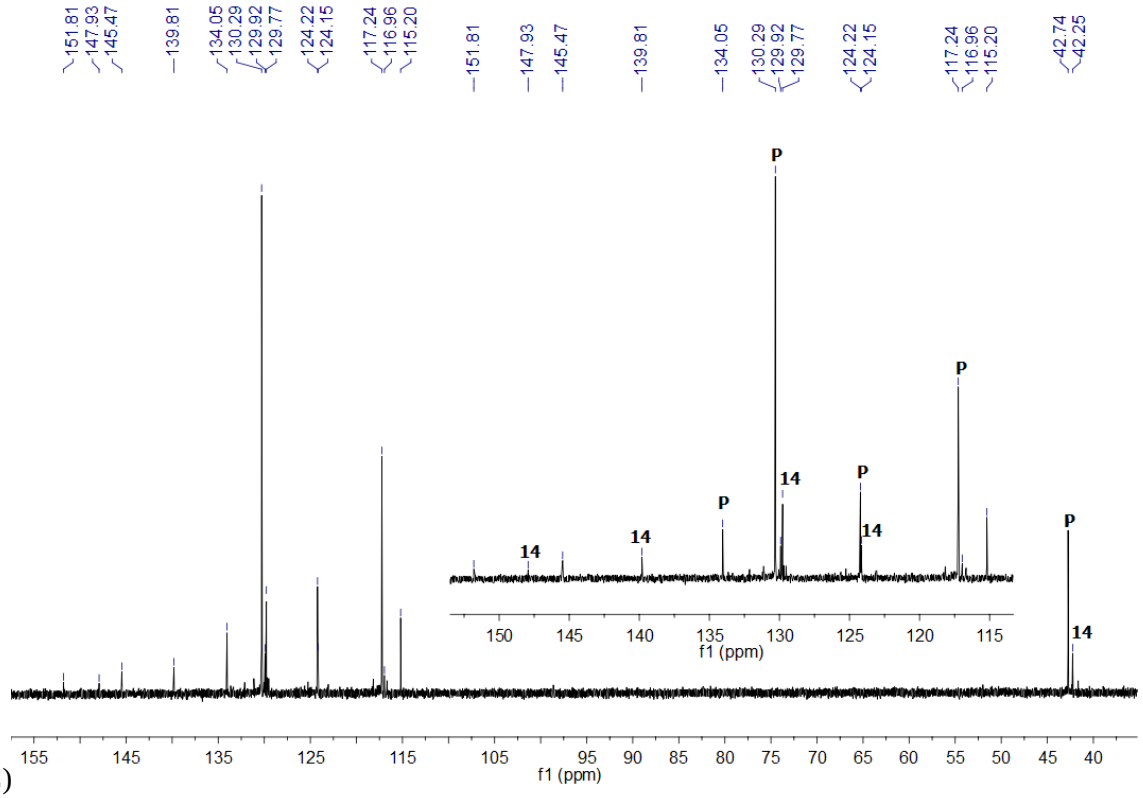
Figure S56. NMR spectra (in D_2O; **A** – ^1H; **B** – ^1H-^1H COSY; **C** – $^{13}C\{^1H\}$; **D** – ^1H-^{13}C HSQC; **E** – ^1H-^{13}C HMBC) for the outcome of the **1-Fe**-catalyzed reaction of 4-nitrobenzonitrile with 3 equiv. of AB for 24 h at 100 °C, showing the formation of 21% of *p*-NO_2-$C_6H_4CH_2NH_3Cl$ (**14**) in a mixture with the products of the nitro group reduction.



(**A**)


NaOAc
P
14
{4.79,4.79}D2O
f1 (ppm)
f2 (ppm)

(B)


151.81
147.93
145.47
139.81
134.05
130.29
129.92
129.77
124.22
124.15
117.24
116.96
115.20
42.74
42.25
P
14
f1 (ppm)

(C)

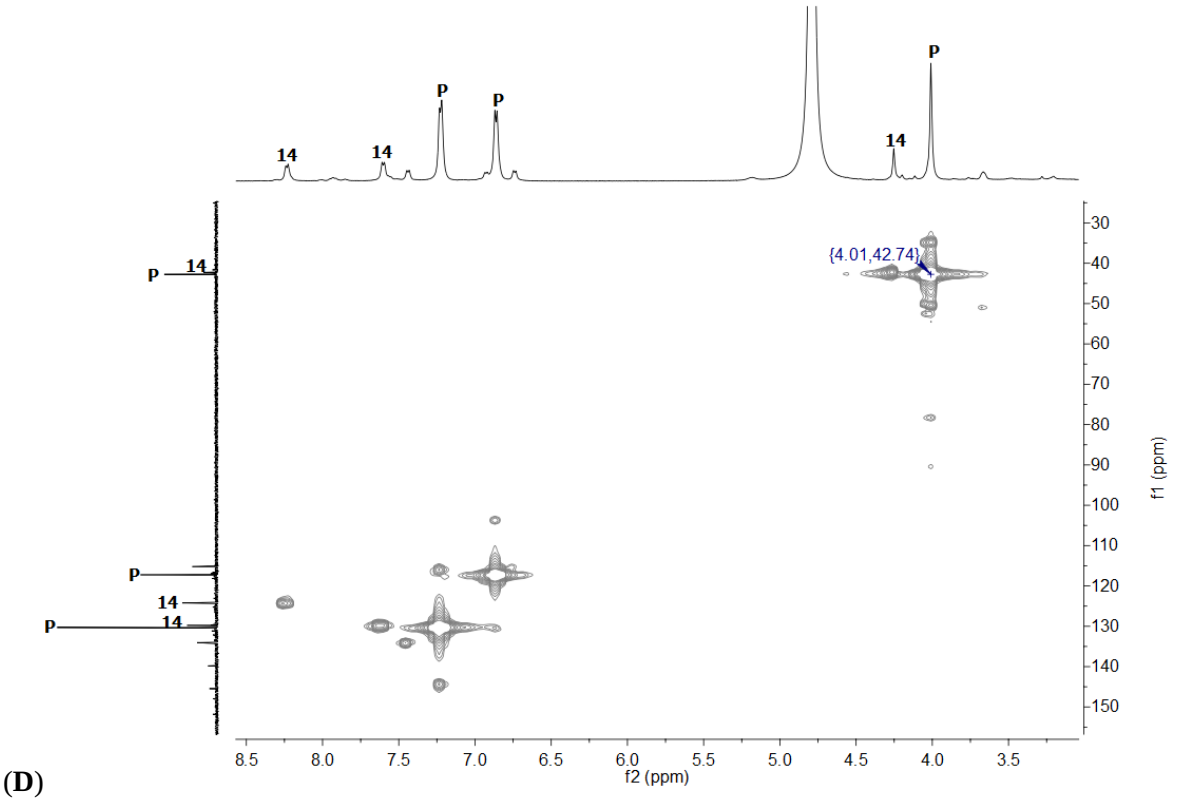


Figure S57. NMR spectra (in D_2O; **A** – ^{1}H; **B** – ^{1}H-^{1}H COSY; **C** – $^{13}C\{^{1}H\}$; **D** – ^{1}H-^{13}C HSQC; **E** – ^{1}H-^{13}C HMBC) for the outcome of **1-Fe**-catalyzed reaction of 4-nitrobenzonitrile with 6 equiv. of AB for 24 h at 100 °C, showing the formation of *p*-$ClH_3NC_6H_4CH_2NH_3Cl$ (marked as P) as the major product (64%) and 4-nitrobenzylamine hydrochloride (**14**) as the minor product (20%).

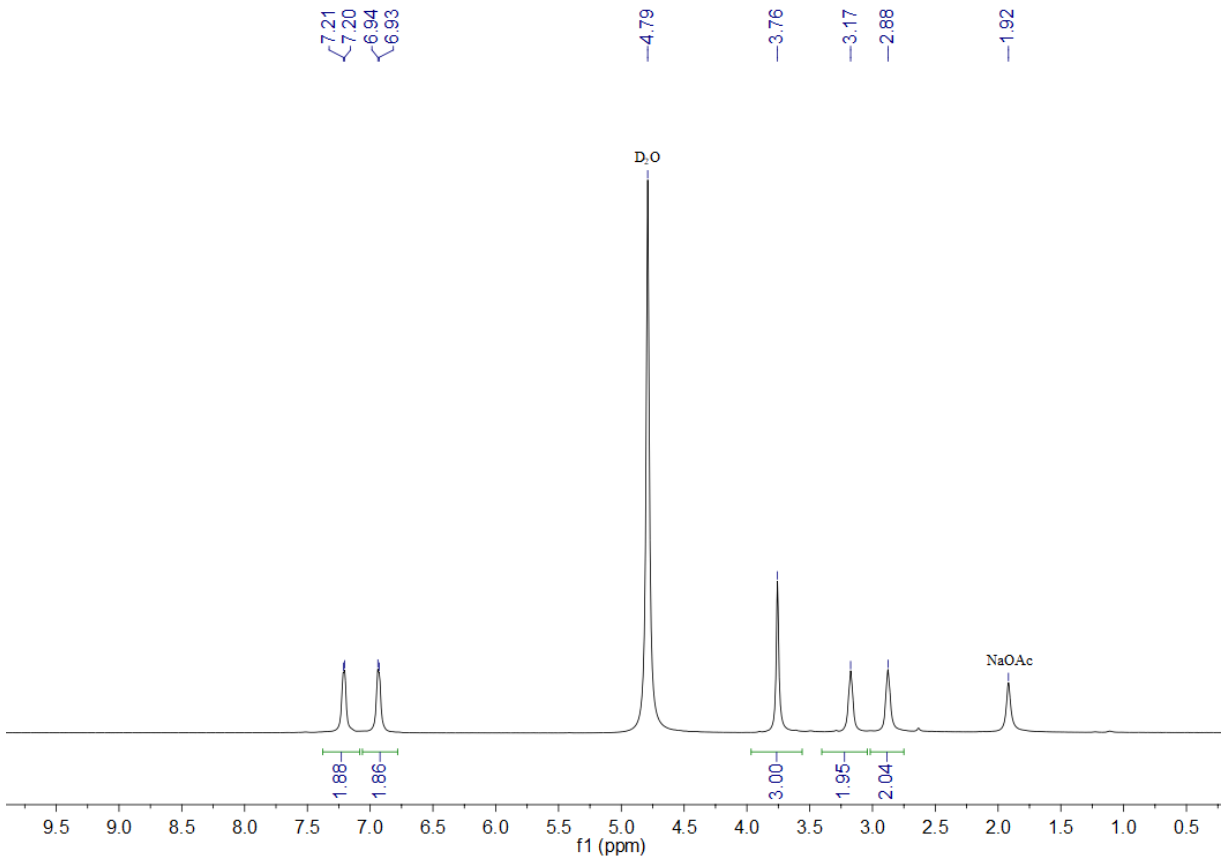


Figure S58. The ^{1}H-NMR spectrum (in D_2O) of *p*-MeO-C_6H_4-$CH_2CH_2NH_3Cl$ (**15**).

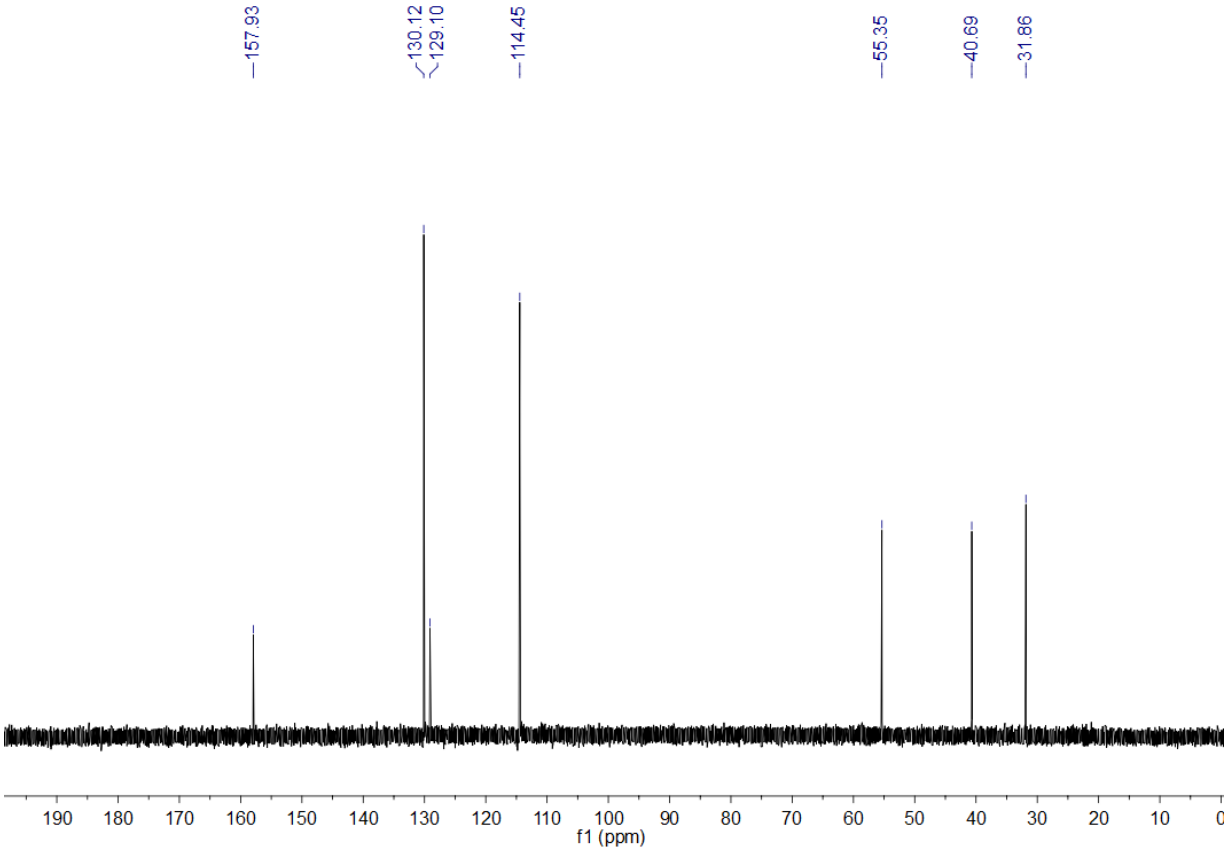


Figure S59. The ^{13}C{^{1}H}-NMR spectrum (in D_2O) of *p*-MeO-C_6H_4-$CH_2CH_2NH_3Cl$ (**15**).

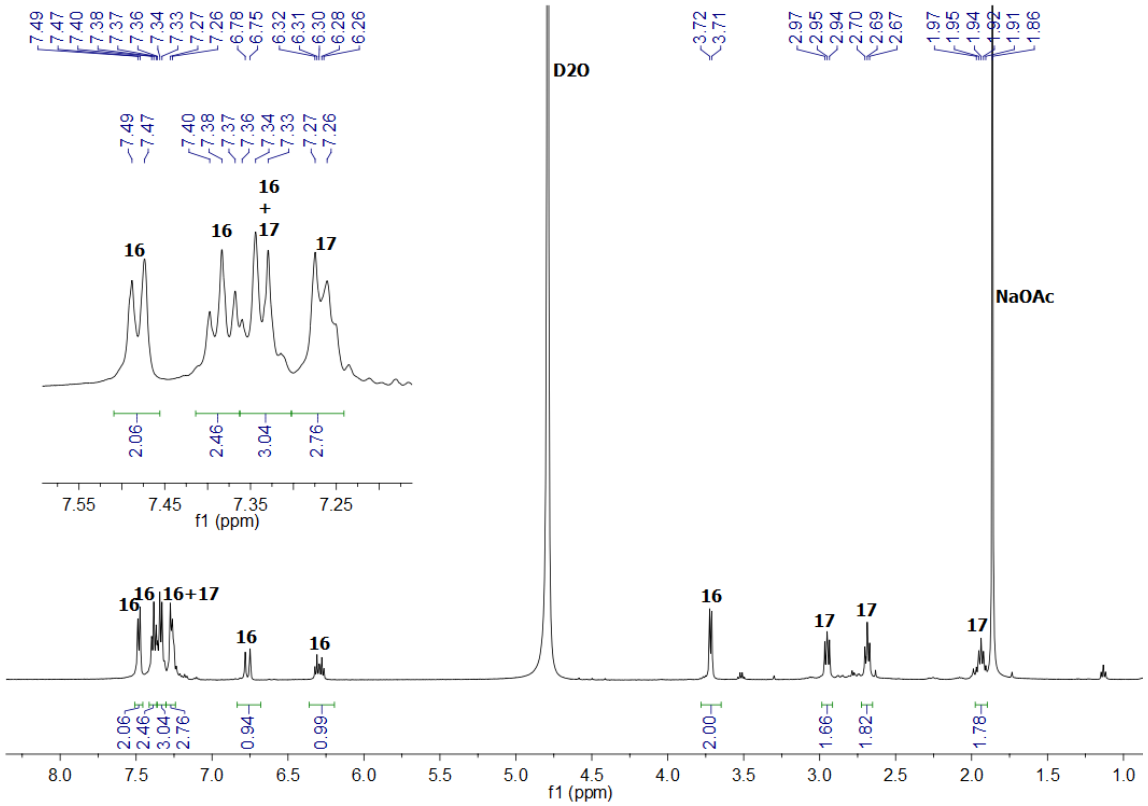


Figure S60. The ^{1}H-NMR spectrum (in D_2O) of the mixture of $PhCH{=}CHCH_2NH_3Cl$ (**16**) and $PhCH_2CH_2CH_2NH_3Cl$ (**17**) obtained by the **1-Fe**-catalyzed reaction of cinnamonitrile with 3 equiv. of AB for 24 h at 60 °C.

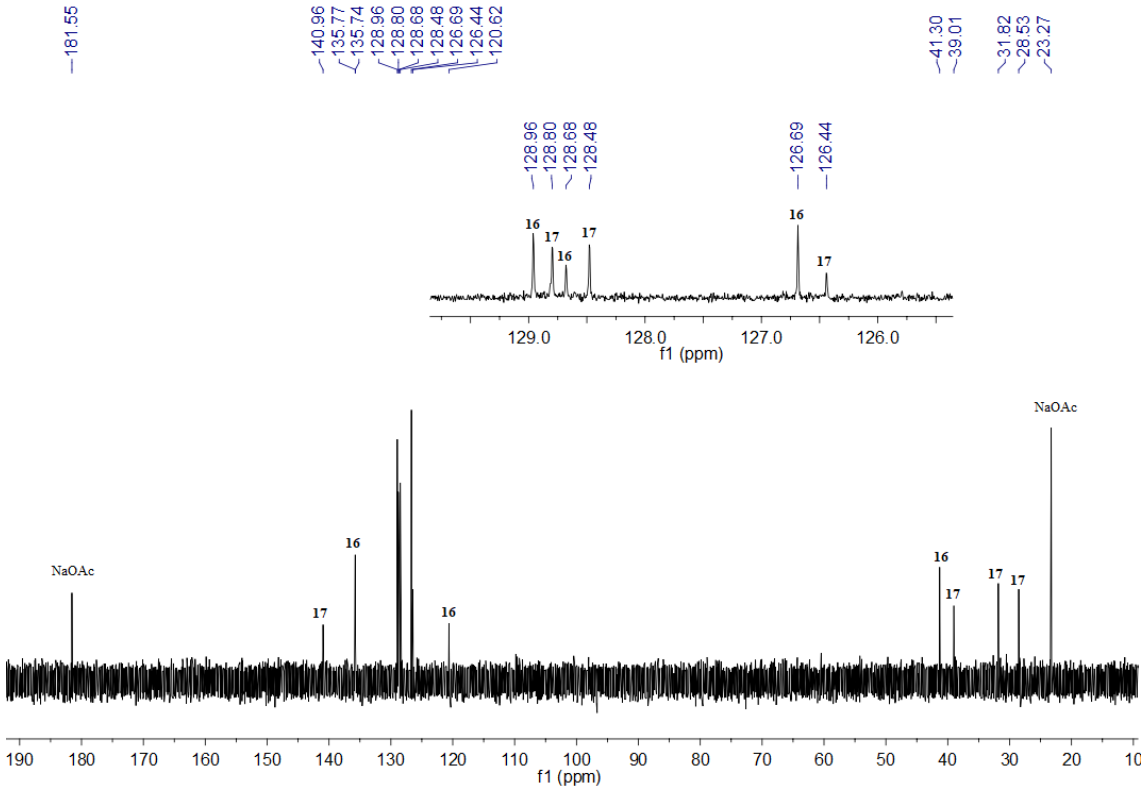


Figure S61. The ^{13}C{^{1}H}-NMR spectrum (in D_2O) of the mixture of $PhCH{=}CHCH_2NH_3Cl$ (**16**) and $PhCH_2CH_2CH_2NH_3Cl$ (**17**) obtained by the **1-Fe**-catalyzed reaction of cinnamonitrile with 3 equiv. of AB for 24 h at 60 °C.

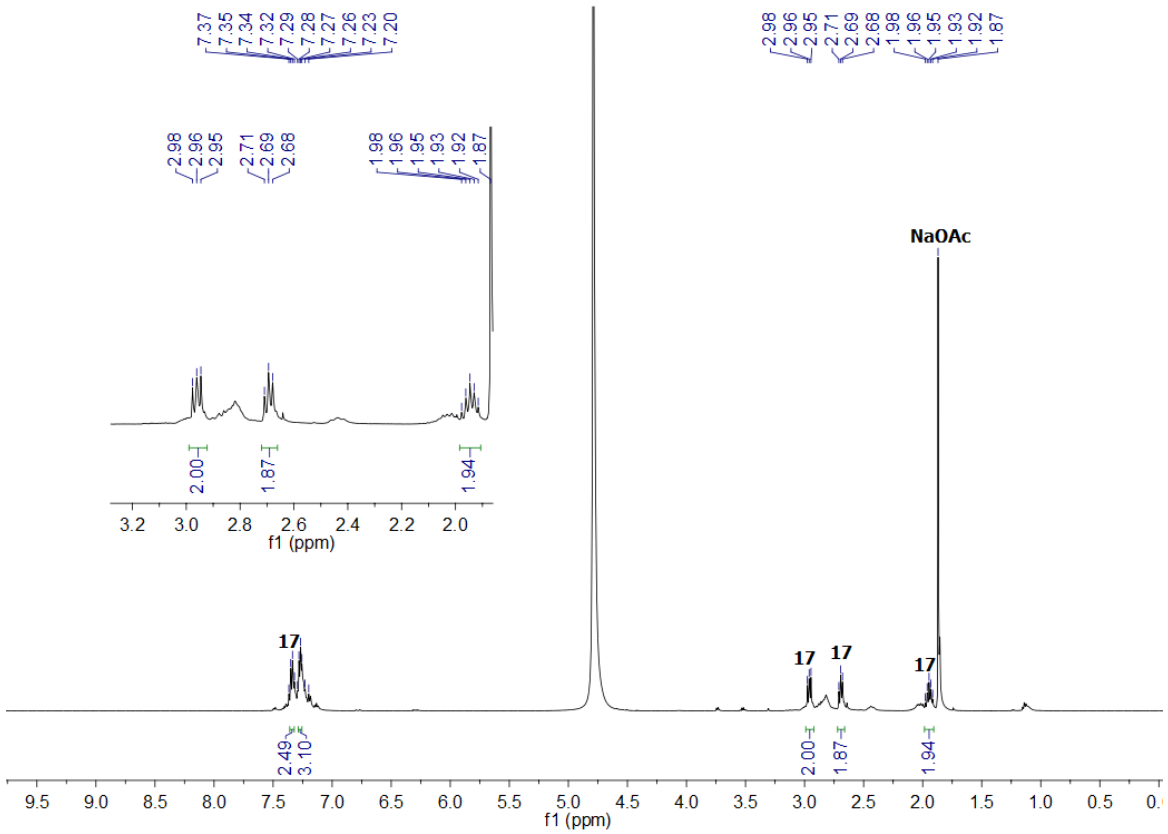
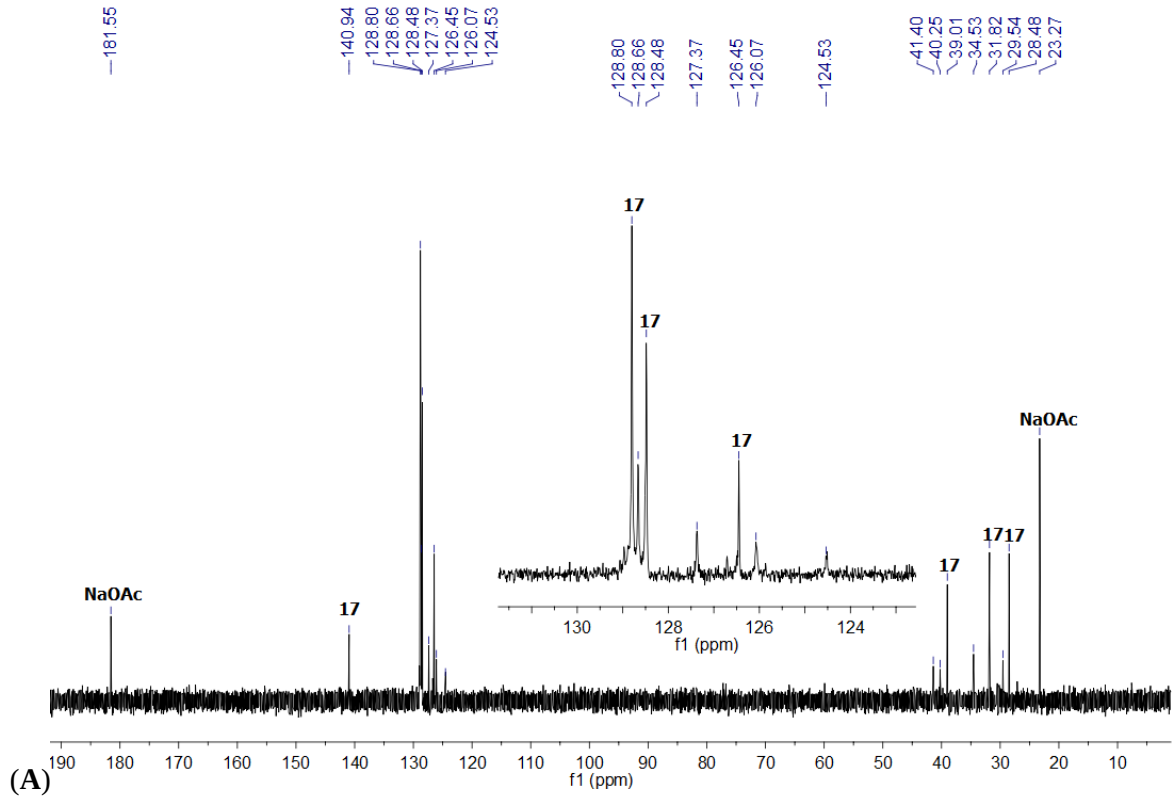
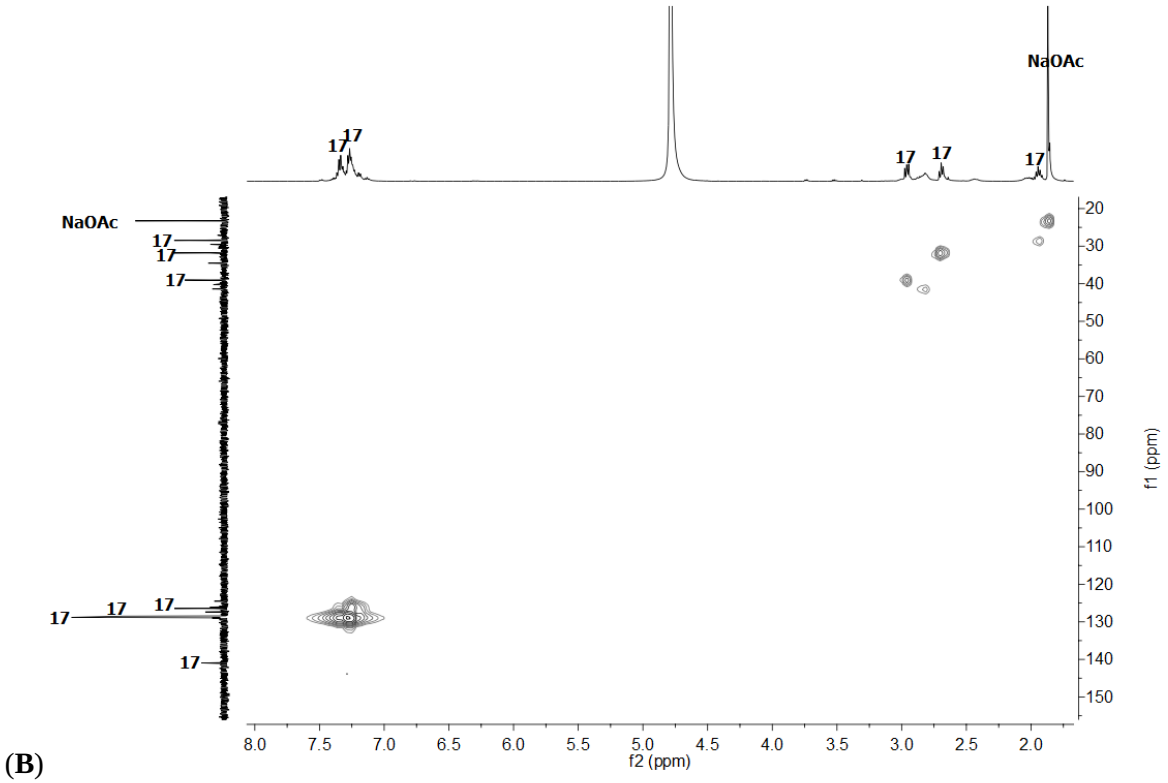


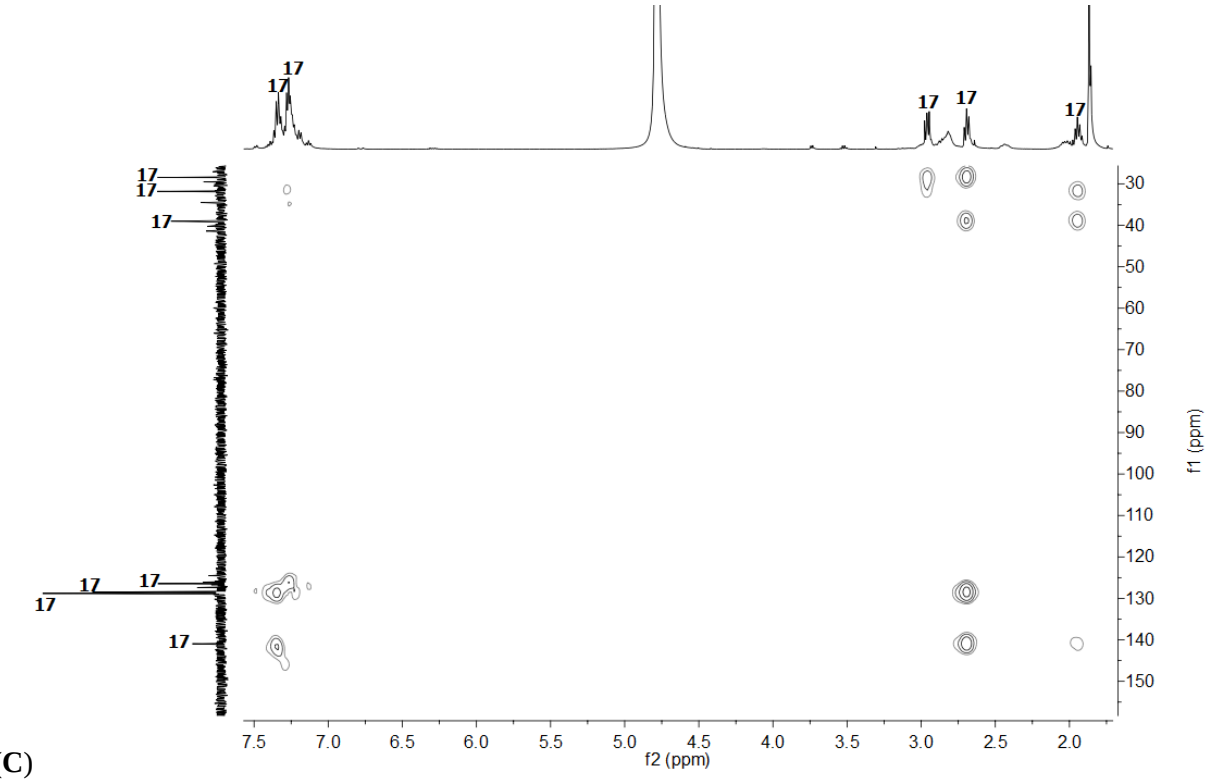
Figure S62. The ^{1}H-NMR spectrum (in D_2O) of $PhCH_2CH_2CH_2NH_3Cl$ (**17**) obtained by the **1-Fe**-catalyzed reaction of cinnamonitrile with 3 equiv. of AB for 24 h at 100 °C.



(**A**)



(**B**)



(**C**)

Figure S63. $^{13}C\{^{1}H\}$-NMR (**A**), ^{1}H-^{13}C HSQC NMR (**B**), and ^{1}H-^{13}C HMBC NMR (**C**) spectra (in D_2O) of $PhCH_2CH_2CH_2NH_3Cl$ (**17**) obtained by the **1-Fe**-catalyzed reduction of cinnamonitrile with 3 equiv. AB at 100 °C for 24 h.

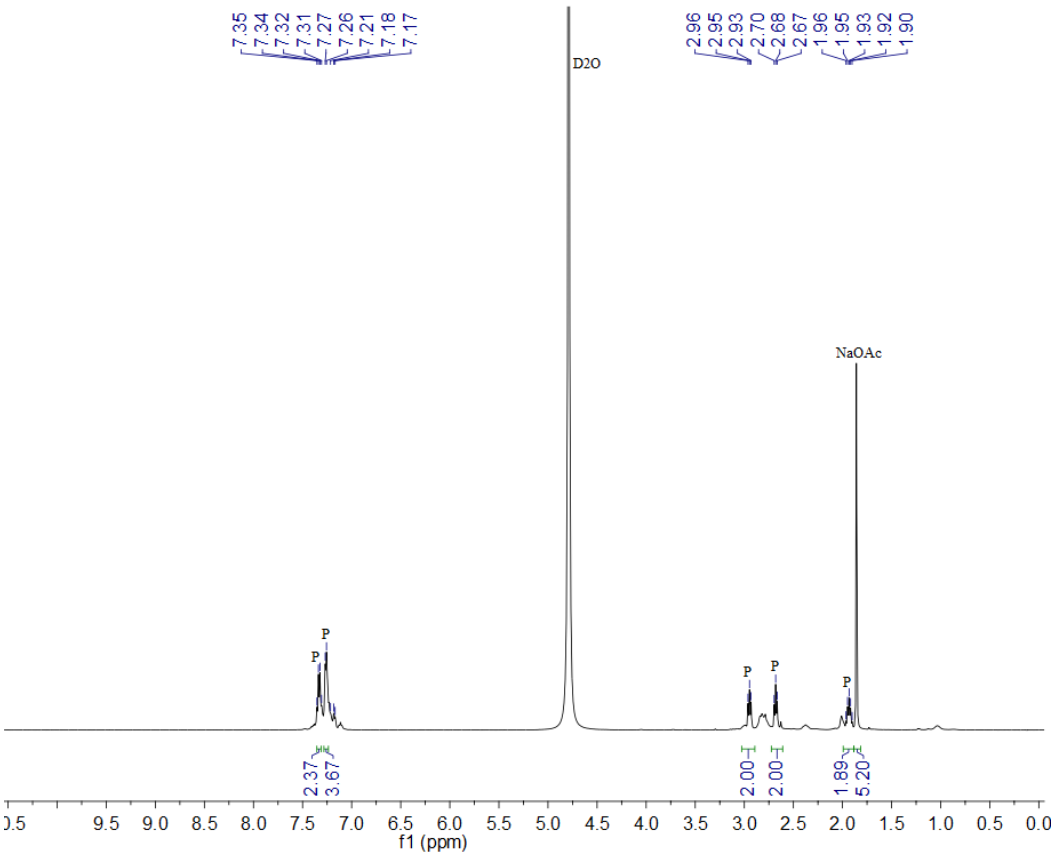


Figure S64. The ^{1}H-NMR spectrum (in D_2O) of $PhCH_2CH_2CH_2NH_3Cl$ (**17**) (marked as P) obtained by the **1-Fe**-catalyzed reduction of cinnamonitrile with 4 equiv. AB at 100 °C for 24 h.

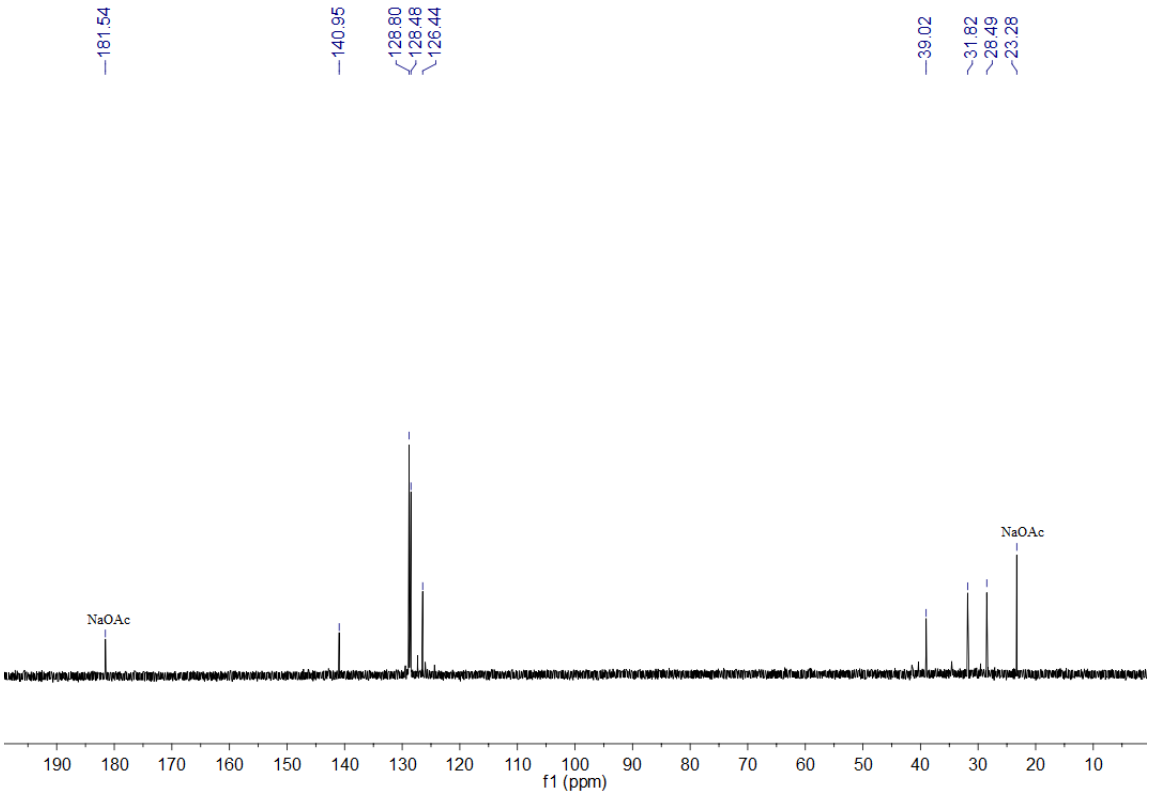


Figure S65. The $^{13}C\{^{1}H\}$-NMR spectrum (in D_2O) of $PhCH_2CH_2CH_2NH_3Cl$ (**17**) obtained by the **1-Fe**-catalyzed reduction of cinnamonitrile with 4 equiv. AB at 100 °C for 24 h.

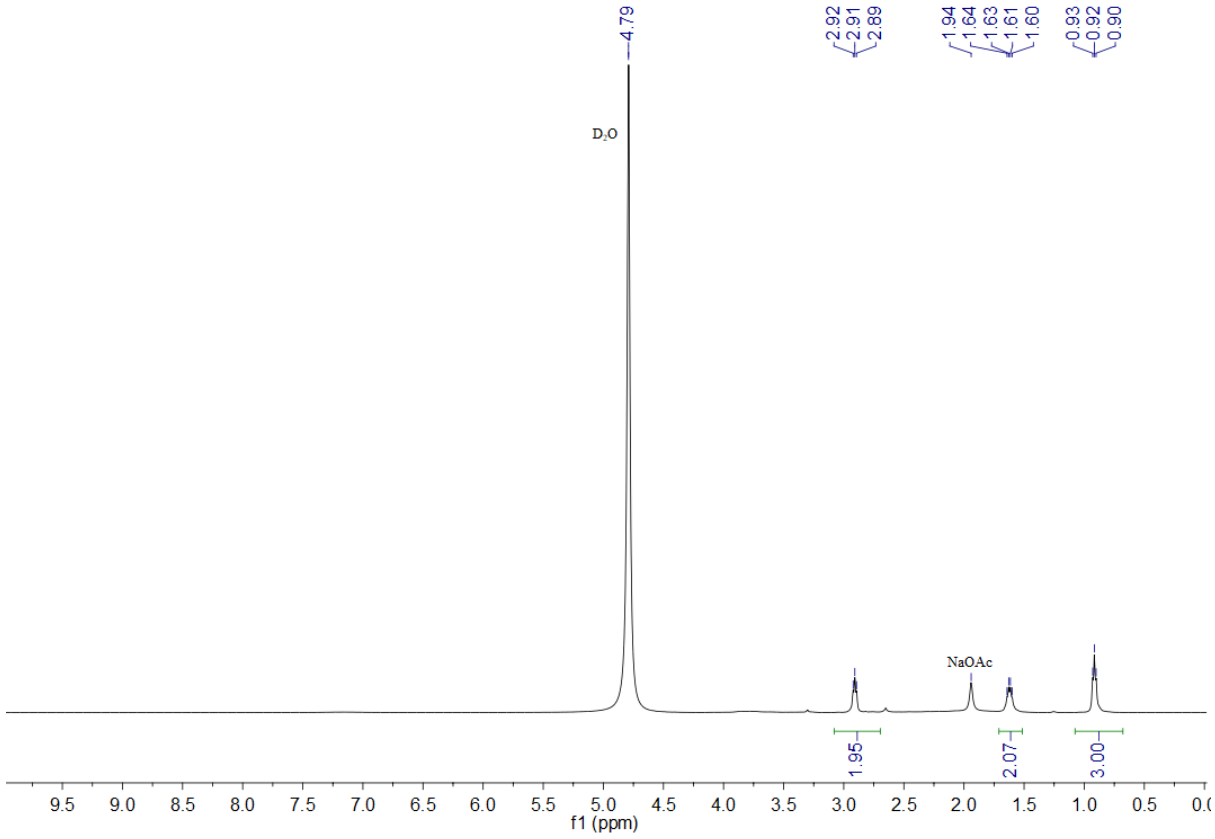


Figure S66. The ^{1}H-NMR spectrum (in D_2O) of $PrNH_3Cl$ (**18**).

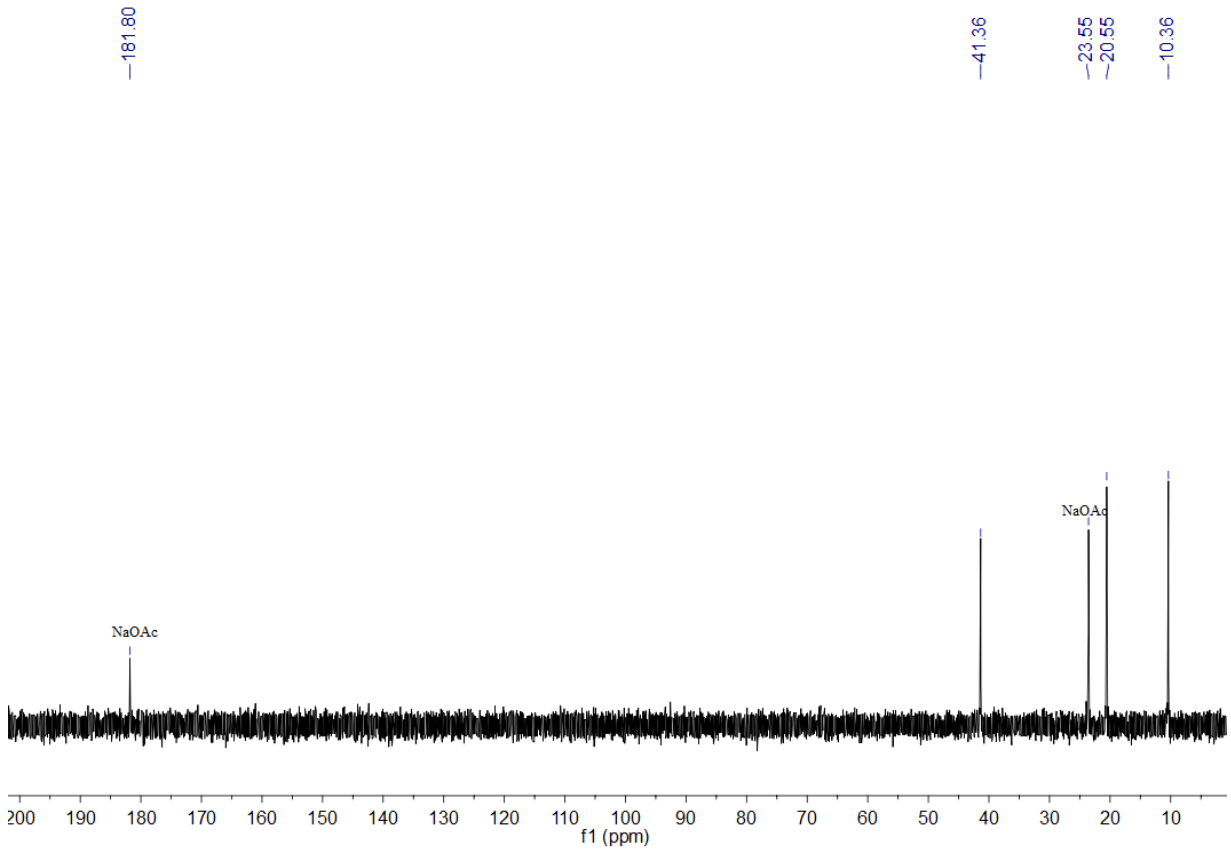


Figure S67. The ^{13}C{^{1}H}-NMR spectrum (in D_2O) of $PrNH_3Cl$ (**18**).

5. X-Ray analysis

The single crystals of **1-Mn**, **1-Fe**, **1-Co**, and **2-Co** suitable for X-Ray diffraction analysis were obtained by appropriate crystallization methods (see Table S1 for details).

Table S1. Crystallization methods for single crystals of **1-Mn**, **1-Fe**, **1-Co**, and **2-Co.**

Complex	Crystallization technique
1-Mn	Crystallized by layering a dichloroethane (DCE) solution of **1-Mn** with hexanes at room temperature
1-Fe	Crystallized by layering a dichloromethane (DCM) solution of **1-Fe** with hexanes at room temperature
1-Co	Crystallized from a dichloromethane (DCM) solution at -28 °C
2-Co	Crystallized from a dichloromethane (DCM) solution at -28 °C

Single crystals of **1-Co** and **2-Co** were investigated on a Bruker D8 QUEST single-crystal X-ray diffractometer equipped with PHOTONII detector, charge-integrating pixel array detector (CPAD), laterally graded multilayer (Goebel) mirror and microfocus Mo-target X-ray tube (λ = 0.73071 Å). Data reduction and integration were performed with the Bruker software package SAINT (Version 8.40B) (SAINT, Version 8.40B; Bruker AXS Inc.: Madison, Wisconsin, USA, 2019).[22] A multi-scan absorption correction was applied within SADABS-2016/2 (Bruker, 2016). Crystal structure solution and refinement were performed using SHELX-2018 package.[23] Structure solution, refinement, and CIF compilation was performed within Olex2SyS software (Dolomanov, 2009).[24] Atomic positions were located using dual methods and refined using a combination of Fourier synthesis and least-square refinement in isotropic and anisotropic approximations. The H atoms were positioned geometrically and refined as riding atoms with relative isotropic displacement parameters.

For **1-Mn** and **1-Fe**, suitable single crystals were mounted on a glass microloop covered with perfluoroether oil (Paratone® N). Crystallographic data were collected on Bruker D8 VENTURE diffractometer equipped with PHOTON III detector and an Oxford Cryosystems low temperature device operating at 170.0(1) K. Generic φ and ω scans (MoKα, λ = 0.71073 Å) were used for the data measurement. The diffraction patterns were indexed, and the unit cells refined with SAINT (Bruker, V.8.34A, after 2013) software.[22] Data reduction, scaling and absorption correction were performed with SAINT and SADABS software (Bruker, 8.34A after 2013). A multi-scan absorption correction was applied within SADABS-2014/4 (Bruker, 2014/4). Space group determination was based upon analysis of systematic absences, E statistics, and successful refinement of all structures. The structures were solved by ShelXT (Sheldrick, 2015) structure solution program with an Intrinsic phasing algorithm and refined with the Least squares method by minimization of $\Sigma w(F_0^2 - F_c^2)^2$. SHELXL weighting scheme was used under the 2018/3

version of ShelXL (Sheldrick, 2015).[23] Structure solution, refinement, and CIF compilation were performed within Olex2SyS software (Dolomanov, 2009).[24] All non-hydrogen atoms were refined anisotropically. The positions of the hydrogen atoms were calculated geometrically and refined using the riding model. Neutral atom scattering factors for all atoms were taken from the International Tables for Crystallography.

The general view of **1-Mn**, **1-Fe**, **1-Co**, and **2-Co** is shown on the Figures S68-S71. Selected structural parameters (bond distances (Å) and bond angles (°)) for complexes **1-Mn**, **1-Fe**, **1-Co**, and **2-Co** are listed in Table S2. Crystal data, data collection, and structure refinement details for **1-Mn**, **1-Fe**, **1-Co**, and **2-Co** are summarized in Table S3. The corresponding CIF files are also provided as separate supporting documents.

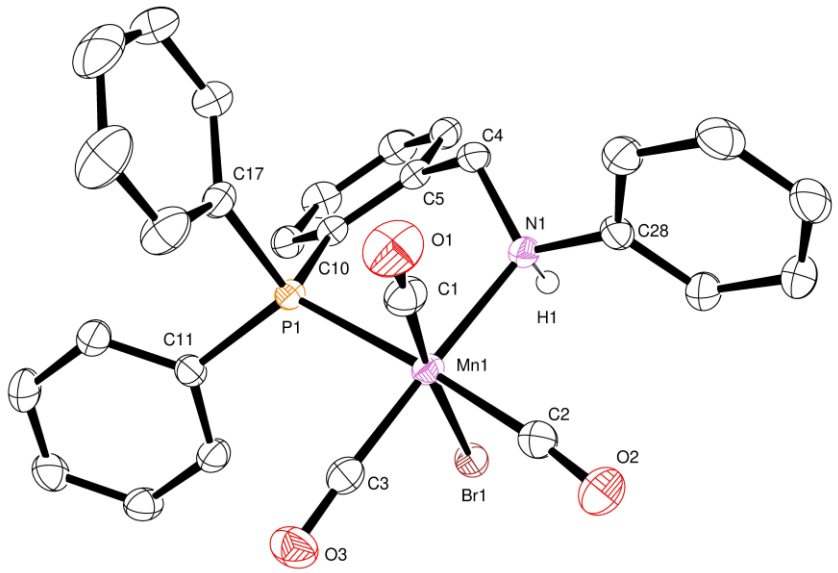


Figure S68. Molecular structure of (PN^{H})$MnBr(CO)_3$ (**1-Mn**), depicted with 50% thermal ellipsoids probability level (hydrogen atoms except for NH are omitted for clarity).

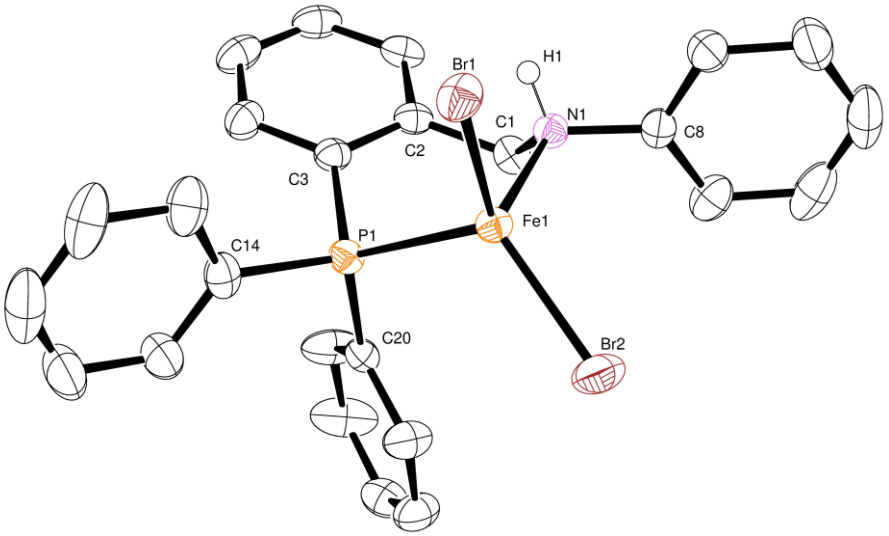


Figure S69. Molecular structure of (PN^{H})$FeBr_2$ (**1-Fe**), depicted with 50% thermal ellipsoids probability level (hydrogen atoms except for NH are omitted for clarity).

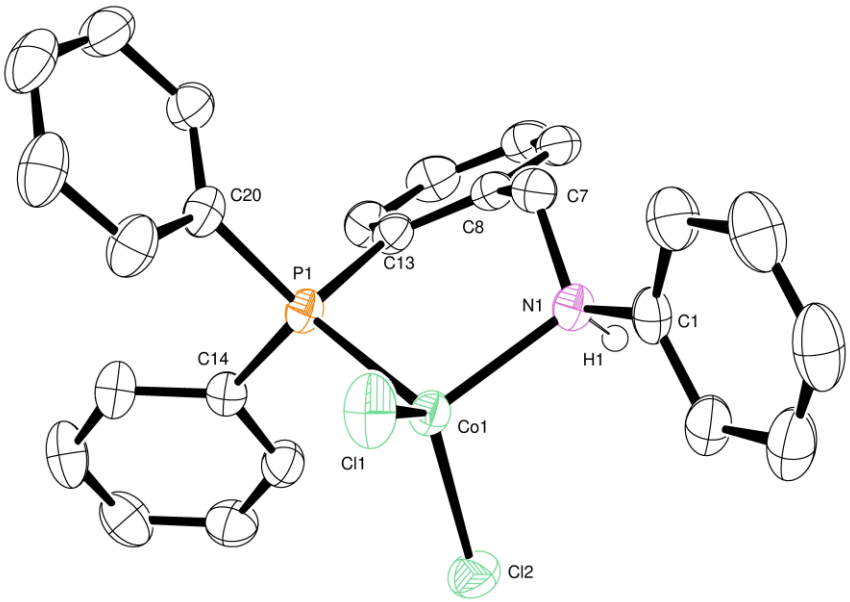


Figure S70. Molecular structure of (PN^{H})$CoCl_2$ (**1-Co**), depicted with 50% thermal ellipsoids probability level (hydrogen atoms except for NH are omitted for clarity).

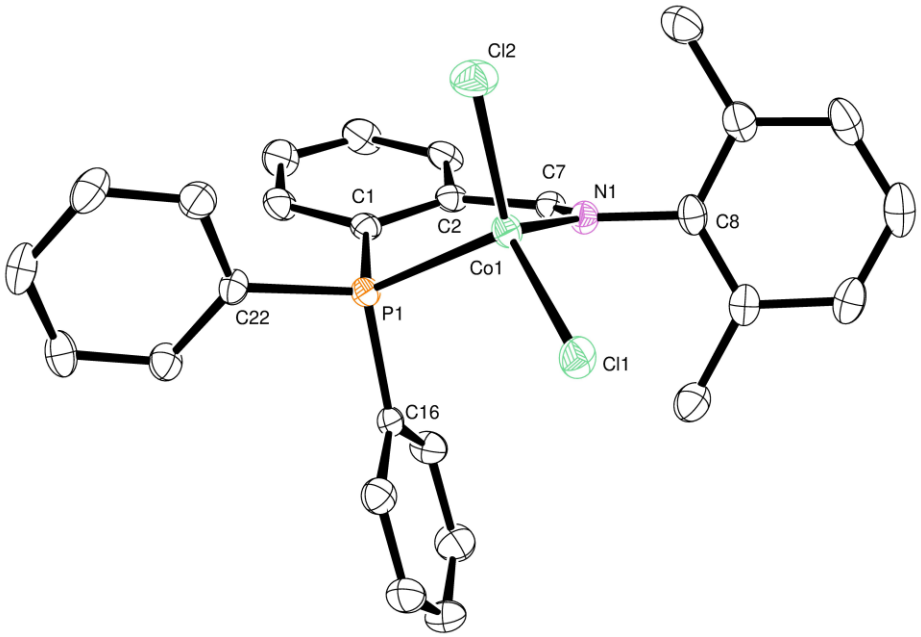


Figure S71. Molecular structure of (PN^{DMP})$CoCl_2$ (**2-Co**), depicted with 50% thermal ellipsoids probability level (hydrogen atoms except for NH are omitted for clarity).

Table S2. Selected bond distances (Å) and angles (°) for **1-Mn**, **1-Fe**, **1-Co**, and **2-Co**

$(PN^{H})MnBr(CO)_3$ (**1-Mn**)			
Mn1–P1	2.3525(4)	P1–Mn1–N1	89.66(3)
Mn1–N1	2.1696(12)	C1–Mn1–Br1	175.06(5)
Mn1–Br1	2.5201(3)	C1–Mn1–N1	92.52(6)
Mn1–C1	1.7972(16)	C1–Mn1–C2	89.15(7)
Mn1–C2	1.8371(16)	C1–Mn1–C3	92.58(7)
Mn1–C3	1.7946(15)	C2–Mn1–C3	87.23(7)
P1–Mn1–C1	92.57(5)	C2–Mn1–N1	93.68(6)
P1–Mn1–C2	176.18(5)	C2–Mn1–Br1	87.00(5)
P1–Mn1–C3	89.28(5)	C3–Mn1–N1	174.83(6)
P1–Mn1–Br1	91.466(11)	C3–Mn1–Br1	90.31(5)
N1–Mn1–Br1	84.66(3)		
$(PN^{H})FeBr_2$ (**1-Fe**)			
Fe1–P1	2.4558(7)	P1–Fe1–Br1	112.50(2)
Fe1–N1	2.171(2)	P1–Fe1–Br2	115.51(2)
Fe1–Br1	2.3812(4)	Br1–Fe1–Br2	117.941(17)
Fe1–Br2	2.3648(4)	Br1–Fe1–N1	102.42(6)
P1–Fe1–N1	89.36(6)	Br2–Fe1–N1	114.81(6)
$(PN^{H})CoCl_2$ (**1-Co**)			
Co1–P1	2.3621(4)	P1–Co1–Cl1	110.288(16)
Co1–N1	2.0805(12)	P1–Co1–Cl2	109.769(17)
Co1–Cl1	2.1927(4)	Cl1–Co1–Cl2	121.003(19)
Co1–Cl2	2.2301(4)	Cl1–Co1–N1	108.42(4)
P1–Co1–N1	98.86(3)	Cl2–Co1–N1	106.11(4)
$(PN^{DMP})CoCl_2$ (**2-Co**)			
Co1–P1	2.3313(6)	P1–Co1–Cl1	110.70(2)
Co1–N1	2.0416(19)	P1–Co1–Cl2	112.12(3)
Co1–Cl1	2.2177(6)	Cl1–Co1–Cl2	113.87(3)
Co1–Cl2	2.2118(7)	Cl1–Co1–N1	111.16(6)
P1–Co1–N1	91.82(5)	Cl2–Co1–N1	115.19(6)

Table S3. X-ray crystallographic data and refinement details for complexes **1-Mn**, **1-Fe**, **1-Co**, and **2-Co**.

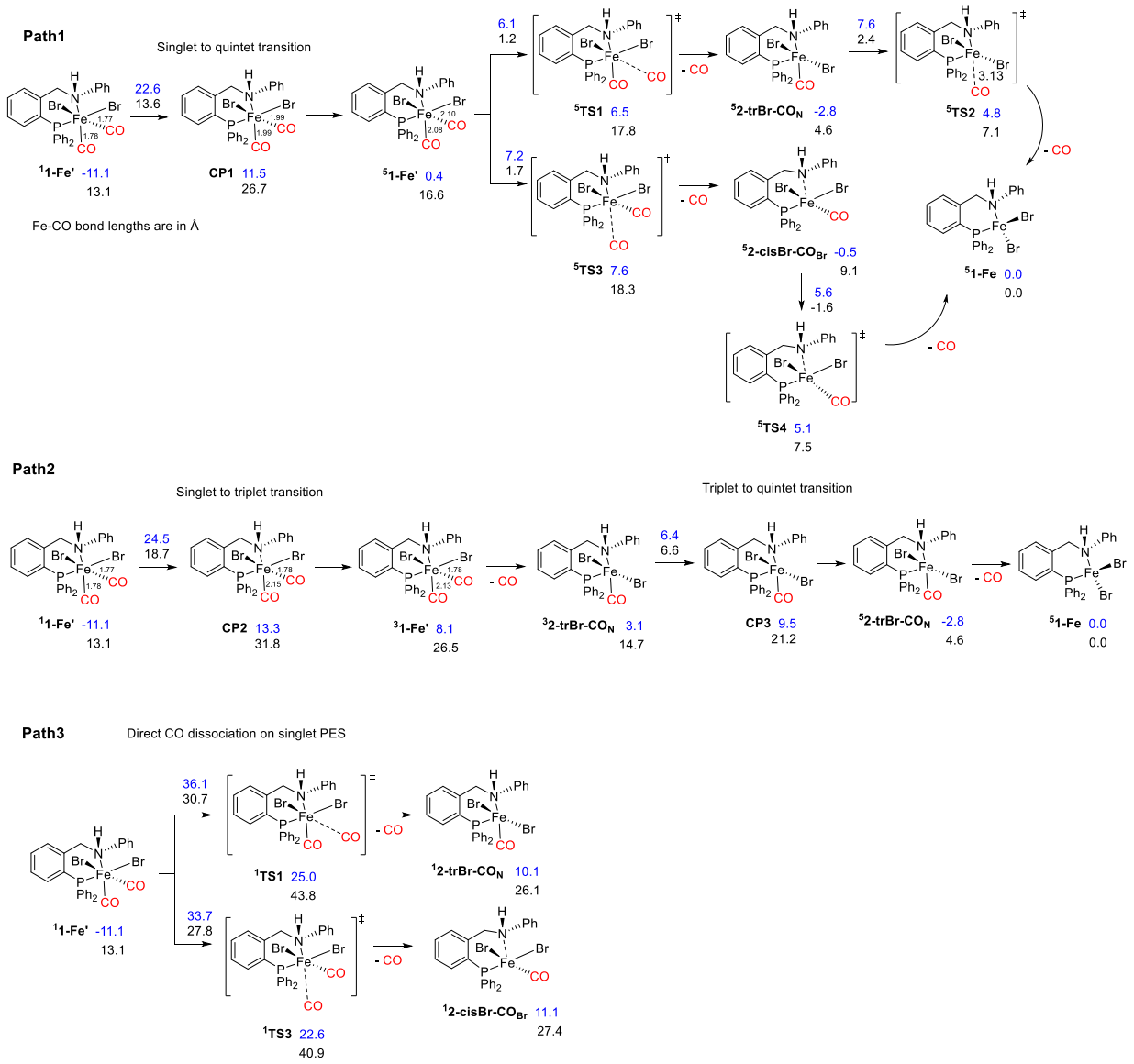
	1-Mn	**1-Fe**	**1-Co**	**2-Co**
Empirical formula	$C_{28}H_{22}BrMnNO_3P$	$C_{25}H_{22}Br_2FeNP$	$C_{25}H_{22}Cl_2CoNP$	$C_{27}H_{24}Cl_2CoNP$
Formula weight (g/mol)	586.28	583.07 g/mol	497.23	523.27
Temperature (K)	170	170	200	120
Crystal system	triclinic	orthorhombic	monoclinic	monoclinic
Space group	P-1	$P2_12_12_1$	$P2_1/n$	$P2_1/c$
Z	2	4	4	4
Unit cell dimensions				
a, Å	7.8512(2)	9.2487(2)	13.6014(6)	9.1513(5)
b, Å	11.7945(2)	15.9203(2)	9.3220(4)	12.9619(7)
c, Å	16.0581(4)	15.9733(3)	18.8813(8)	20.7392(10)
α, °	75.1920(10)	90	90	90
β, °	84.2480(10)	90	107.0510(10)	92.0577(11)
γ, °	84.8350(10)	90	90	90
V, $Å^3$	1427.16(6)	2351.94(7)	2288.77(17)	2458.5(2)
d_{calc}, $g \cdot cm^{-3}$	1.364	1.647	1.443	1.414
μ, cm^{-1}	1.946	4.119	1.006	0.996
F(000)	592	1160	1020	1076
min and max theta, °	2.613, 28.346	2.545, 28.305	2.26, 26.52	2.32, 26.33
Completeness	1.000	0.999	0.994	1.000
Refl. collected	74201	61387	65686	37499

Refl. unique (R_{int})	6813	5855	4661	6556
Refl. with I > 2σ(I)	6332	5454	4247	4713
Parameters				
Final R_1 with I>2σ(I)	0.0229	0.0201	0.0248	0.0394
wR_2 (all data)	0.0566	0.0419	0.0704	0.1034
GOF	1.038	1.044	1.043	1.031
Largest difference in peak / hole (e/Å^3)	0.367, -0.280	0.366, -0.464	0.354, -0.212	0.572, -0.388
CCDC number	2379898	2379897	2380140	2379985

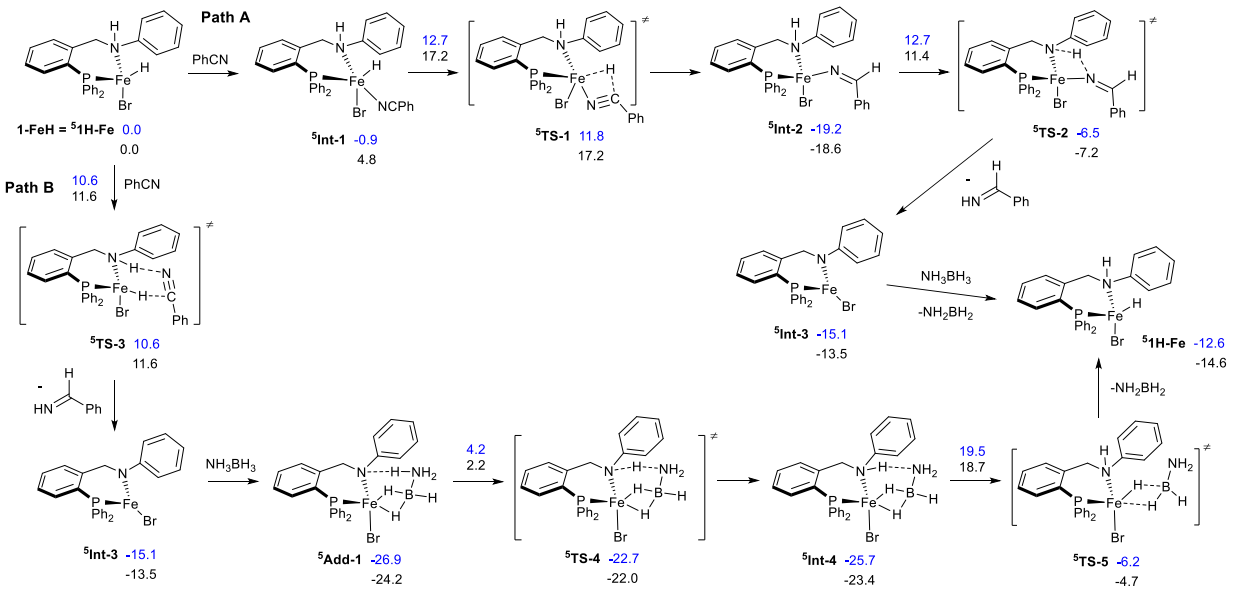
6. Computational details

Quantum chemical calculations were carried out with the Gaussian 16[25] and ORCA 5[26,27] programs. Molecular geometries were optimized at the density functional theory level employing the meta-GGA functional M06-L[28] in conjunction with the split-valence double-zeta def2-SVP[29] basis set. Frequency calculations were performed on the optimized stationary points to characterize minima and transition structures, and to extract thermal contributions to Gibbs energies at 298.15 K. Single-point energy calculations were performed with the hybrid functional PBE0[30,31] in conjunction with the D3 atom-pairwise dispersion correction with Becke-Johnson damping[32] employing the triple-zeta valence polarized def2-TZVPP[29] basis set, abbreviated as PBE0-D3BJ/def2-TZVPP. These functionals, namely M06-L and PBE0, have shown a reasonable accuracy among 250 approximations tested in a recent extensive benchmark study[33] of spin state energy differences and binding energies of Mn(II), Co(II), Fe(II), and Fe(III) porphyrins. The resolution of the identity[34,35] approximation was used with the W06 fitting set of Ahlrichs and coworkers[36] to accelerate DFT calculations for the M06-L functional, while the RIJCOSX method[37] was applied together with def2/J[38] auxiliary basis sets for the exchange part in the PBE0 functional. Minimum energy crossing point (MECP) optimizations and the corresponding numerical frequency calculations performed to confirm a minimum in the 3N−7-dimensional subspace of the crossing hyperline were done as implemented in ORCA 5. Solvation effects were mimicked using the polarized continuum solvation model (PCM)[39], the dielectric constant $\varepsilon = 8.93$ and 2.3741 for dichloromethane and toluene, respectively, was used.

All energies given are relative free energies at 298.15 K and 1 M (ΔG^{298}) in kcal·mol^{-1}.



Scheme S1. DFT calculated pathways for the transformation of **1-Fe'** to **1-Fe** (^{1}Fe, ^{3}Fe and ^{5}Fe denote singlet, triplet and quintet states, respectively). Gibbs free energies are shown in kcal·mol^{-1} relative to **1-Fe**. Fe-CO bond lengths are shown in Å. Geometries were optimized using the M06L/def2-SVP method (values in blue), while additional single point calculations were performed on each optimized geometry with the aid of the PBE0-D3BJ/def2-TZVPP method (values in black). Solvation effects were taken into account employing the PCM model, the dielectric constant ε = 8.93 for dichloromethane was used.



Scheme S2. DFT calculated pathways for **1-FeH**-catalyzed transfer hydrogenation of PhCN with AB. Gibbs free energies are shown in kcal·mol^{-1} relative to **1-FeH** (= ^{5}**1H-Fe**, where 5 denotes the quintet state). Geometries were optimized using the M06L/def2-SVP method (values in blue), while additional single point calculations were performed on each optimized geometry with the aid of the PBE0-D3BJ/def2-TZVPP method (values in black). The corresponding low and intermediate spin complexes ^{1}**1H-Fe**, ^{3}**1H-Fe,** ^{1}**Int1,** ^{3}**Int1,** ^{1}**Int2,** ^{3}**Int2,** ^{1}**Int3,** ^{3}**Int3** were found to be significantly less stable than the high-spin complexes (see Table S5 for details). Solvation effects were taken into account employing the PCM model, the dielectric constant ε = 2.3741 for toluene was used.

Table S4. Electronic energies (E), thermal corrections to Gibbs free energy (G_{corr}) and solvation energies (ΔG°_{solv}) in dichloromethane of all stationary points in the reaction of **1-Fe'** to **1-Fe** transformation calculated using two functionals: M06-L – (1) and PBE0-D3BJ – (2). Imaginary frequencies ($\tilde{\nu}_{imag}$) of the corresponding transition states at the M06-L/def2-SVP theory level.

	E(1), a.u.	E(2), a.u.	G_{corr}(1), a.u.	ΔG°_{solv}(1), kcal·mol^{-1}	$\tilde{\nu}_{imag}$, cm^{-1}
CO	-113.2088608	-113.2311362	-0.01405	-0.5	-
^{1}1-Fe	-7772.18291	-7772.45486	0.342884	-11.9	-
^{3}1-Fe	-7772.20865	-7772.485209	0.338377	-11.5	-
^{5}1-Fe	-7772.24717	-7772.52943	0.337764	-11.3	-
^{1}1-Fe'	-7998.72579	-7999.014029	0.356897	-11.0	-
^{3}1-Fe'	-7998.689204	-7998.986636	0.34965	-10.3	-
^{5}1-Fe'	-7998.697093	-7998.998088	0.34422	-9.6	-
CP1	-7998.690967	-7999.0	0.355802	-9.6	-
CP2	-7998.689109	-7998.98656	0.357997	-10.3	-
CP3	-7885.471224	-7885.757011	0.352718	-9.1	-
^{5}TS3	-7998.683062	-7998.992851	0.343027	-10.4	*i*33
^{5}TS1	-7998.688926	-7998.997705	0.345561	-9.4	*i*45
^{1}TS3	-7998.667312	-7998.964921	0.352771	-11.4	*i*63
^{1}TS1	-7998.667873	-7998.964711	0.353678	-9.2	*i*64
^{1}2-cisBr-CO$_{Br}$	-7885.462856	-7885.741352	0.350951	-11.6	-
^{3}2-cisBr-CO$_{Br}$	-7885.463353	-7885.747706	0.345513	-11.8	-
^{5}2-cisBr-CO$_{Br}$	-7885.476489	-7885.765731	0.341514	-8.7	-
^{1}2-trBr-CO$_{N}$	-7885.466733	-7885.745715	0.350574	-9.9	-
^{3}2-trBr-CO$_{N}$	-7885.475392	-7885.761461	0.346662	-9.1	-
^{5}2-trBr-CO$_{N}$	-7885.478976	-7885.771711	0.34075	-9.0	-
^{5}TS4	-7885.464259	-7885.764869	0.340804	-10.4	*i*18
^{5}TS2	-7885.464549	-7885.765498	0.339875	-9.9	*i*37

Table S5. Electronic energies (E), thermal corrections to Gibbs free energy (G_{corr}) and solvation energies (ΔG°_{solv}) in toluene of all stationary points in the reaction of catalytic transfer hydrogenation of PhCN calculated using two functionals: M06-L – (1) and PBE0 – (2). Imaginary frequencies ($\tilde{\nu}_{imag}$) of the corresponding transition states at the M06-L/def2-SVP theory level.

	E(1), a.u.	E(2), a.u.	G_{corr}(1), a.u.	ΔG°_{solv}(1), kcal·mol^{-1}	$\tilde{\nu}_{imag}$, cm^{-1}
AB (NH_3BH_3)	-83.1412215	-83.141093	0.047546	-5.4	-
NH_2BH_2	-81.9660765	-81.966716	0.026079	-1.1	-
PhCN	-324.214468	-324.229541	0.069671	-2.2	-
PhCH=NH	-325.418554	-325.436070	0.091992	-1.5	-
Path A (Insertion)					
^{5}1H-Fe (= 1-FeH)	-5198.992580	-5199.160285	0.345094	-6.3	-
^{5}Int-1	-5523.231963	-5523.403042	0.435677	-6.6	-
^{5}TS-1	-5523.213661	-5523.385244	0.436247	-5.8	*i*469
^{5}Int-2	-5523.269042	-5523.448407	0.441219	-5.1	
^{5}TS-2	-5523.246291	-5523.427656	0.437505	-4.4	*i*1118
^{5}Int-3	-5197.821129	-5197.983751	0.328120	-5.0	-
Path B (Concerted)					
^{5}TS-3	-5523.212196	-5523.393408	0.435544	-5.9	*i*378
^{5}Int-3	-5197.821129	-5197.983751	0.328120	-5.0	-
^{5}Add-1	-5281.003456	-5281.164185	0.394864	-6.6	-
^{5}TS-4	-5280.995932	-5281.159993	0.391818	-5.2	*i*673
^{5}Int-4	-5281.004509	-5281.165991	0.395094	-4.9	-
^{5}TS-5	-5280.966077	-5281.128862	0.388186	-5.1	*i*53
^{1}1H-Fe	-5198.959827	-5199.110582	0.352430	-5.4	-
^{3}1H-Fe	-5198.967742	-5199.131818	0.346180	-5.1	-
^{1}Int1	-5523.220144	-5523.383822	0.444080	-5.9	-
^{3}Int1	-5523.220086	-5523.389150	0.439456	-5.6	-
^{1}Int2	-5523.225191	-5523.389967	0.450692	-4.4	-
^{3}Int2	-5523.252223	-5523.421856	0.444666	-5.5	-
^{1}Int3	-5197.749339	-5197.900267	0.331820	-4.7	-
^{3}Int3	-5197.803824	-5197.963307	0.330015	-4.7	-

Table S6. Cartesian coordinates (in Å) of all optimized geometries (M06-L/def2-SVP) in the reaction of **1-Fe'** to **1-Fe** transformation.

^{1}1-Fe			
C	-1.999572000	4.529739000	1.112638000
C	-1.897253000	3.592101000	2.137347000
C	4.892096000	1.360473000	0.718582000
C	3.612381000	0.988660000	1.120801000
C	5.644896000	0.531877000	-0.112396000
C	-1.835777000	4.126889000	-0.213886000
C	-1.632026000	2.254306000	1.839809000
C	1.088913000	0.004028000	2.151959000
C	3.080150000	-0.225409000	0.682222000
C	-0.240281000	-1.431630000	3.723655000
C	-1.564213000	2.796013000	-0.513339000
C	-1.460934000	1.843447000	0.512137000
C	5.112308000	-0.684542000	-0.536778000
C	-0.164781000	-0.744141000	2.510233000
C	-1.369819000	-2.178395000	4.057439000
C	3.833980000	-1.068983000	-0.143179000
C	-1.259065000	-0.798639000	1.618933000
C	-2.435399000	-2.252137000	3.165568000
C	-2.378249000	-1.565921000	1.952731000
C	-3.856002000	0.209195000	-0.587821000
C	-2.600920000	-0.316470000	-0.933886000
C	-4.984986000	-0.123230000	-1.331180000
C	-2.493342000	-1.160416000	-2.045300000
C	-4.871195000	-0.971421000	-2.434250000
C	-3.626459000	-1.485445000	-2.790706000
H	-2.208381000	5.576379000	1.345853000
H	5.300760000	2.315895000	1.054223000
H	-2.031207000	3.897852000	3.177645000
H	3.024409000	1.661818000	1.745932000
H	6.645151000	0.834346000	-0.428307000
H	-1.913023000	4.856751000	-1.022771000
H	1.786127000	0.004913000	3.006972000
H	-1.573652000	1.526716000	2.654493000
H	0.881378000	1.058276000	1.901674000
H	0.605979000	-1.385632000	4.415178000
H	-1.408642000	-2.711313000	5.009769000
H	5.694081000	-1.344520000	-1.183539000
H	-1.422310000	2.491018000	-1.553296000
H	1.688876000	-1.637565000	1.077174000
H	3.404342000	-2.017275000	-0.479836000
H	-3.318365000	-2.846308000	3.410770000
H	-3.948514000	0.883729000	0.268901000
H	-3.218199000	-1.630315000	1.256577000
H	-5.958390000	0.286548000	-1.051782000
H	-1.519286000	-1.573613000	-2.319391000
H	-5.757424000	-1.226776000	-3.019999000
H	-3.531315000	-2.144239000	-3.656596000
Br	1.467938000	1.679997000	-1.754526000
Br	0.600845000	-2.763654000	-0.986651000
Fe	0.818400000	-0.368846000	-0.807052000
N	1.731737000	-0.616003000	0.978895000
P	-1.106472000	0.104908000	0.032975000

^{3}1-Fe			
C	-0.808240000	4.942368000	0.043966000
C	-1.644076000	4.274005000	0.939063000
C	4.262597000	1.938936000	0.152071000
C	3.109772000	1.569710000	0.842855000
C	5.128294000	0.974769000	-0.360417000
C	-0.042218000	4.215356000	-0.867037000
C	-1.713419000	2.882126000	0.923992000
C	0.812928000	0.627819000	2.472451000
C	2.817589000	0.211227000	1.019995000
C	-0.899736000	-0.339031000	4.031552000
C	-0.104160000	2.822661000	-0.884490000
C	-0.945501000	2.144842000	0.009254000
C	4.839406000	-0.377169000	-0.173203000
C	-0.550223000	0.049845000	2.738067000
C	-2.147759000	-0.900190000	4.303296000
C	3.691626000	-0.764360000	0.509120000
C	-1.485895000	-0.119270000	1.690937000
C	-3.060427000	-1.082211000	3.269316000
C	-2.728939000	-0.695673000	1.970713000
C	-3.453756000	0.742464000	-1.327496000
C	-2.390699000	-0.134493000	-1.077218000
C	-4.521565000	0.332722000	-2.124198000
C	-2.398037000	-1.416650000	-1.643537000
C	-4.531838000	-0.948473000	-2.675384000
C	-3.470419000	-1.820953000	-2.434705000
H	-0.753025000	6.033429000	0.058904000
H	4.481645000	2.999941000	0.013734000
H	-2.246067000	4.839296000	1.654464000
H	2.442765000	2.342745000	1.227950000
H	6.025629000	1.275500000	-0.904079000
H	0.613785000	4.734827000	-1.569417000
H	1.356321000	0.784595000	3.419961000
H	-2.368237000	2.363869000	1.631561000
H	0.717238000	1.615133000	1.995594000
H	-0.175353000	-0.205828000	4.840341000
H	-2.398811000	-1.203835000	5.321677000
H	5.507763000	-1.143387000	-0.570591000
H	0.504315000	2.249648000	-1.592432000
H	1.652229000	-1.187978000	1.936561000
H	3.448020000	-1.823329000	0.639724000
H	-4.036684000	-1.529436000	3.468411000
H	-3.447800000	1.750578000	-0.903269000
H	-3.450259000	-0.844672000	1.162903000
H	-5.347342000	1.020792000	-2.319250000
H	-1.557345000	-2.094563000	-1.460435000
H	-5.368343000	-1.265304000	-3.302750000
H	-3.470437000	-2.821132000	-2.873126000
Br	1.159854000	-0.219413000	-2.638839000
Br	0.640329000	-3.092140000	0.320478000
Fe	0.840758000	-0.760782000	-0.366778000
N	1.583578000	-0.234339000	1.569645000
P	-0.978198000	0.310126000	-0.018590000

^{5}1-Fe			
C	-1.184678000	4.911222000	0.325852000
C	-1.998778000	4.160318000	1.175484000

^{1}3-cisBr-cisCO-1			
C	-2.552594000	3.854675000	-2.653697000
C	-2.435638000	4.032711000	-1.277057000

C	4.612026000	1.800084000	0.622550000
C	3.329399000	1.434293000	1.030220000
C	5.534680000	0.836808000	0.224517000
C	-0.409594000	4.272183000	-0.640896000
C	-2.038624000	2.772809000	1.058345000
C	0.830522000	0.515994000	2.223969000
C	2.964414000	0.085159000	1.035262000
C	-0.667150000	-0.631118000	3.865700000
C	-0.442610000	2.883221000	-0.761311000
C	-1.262370000	2.124254000	0.085655000
C	5.167052000	-0.509863000	0.236806000
C	-0.479861000	-0.137945000	2.571924000
C	-1.849064000	-1.271316000	4.235679000
C	3.892074000	-0.887825000	0.638384000
C	-1.523331000	-0.285577000	1.627623000
C	-2.867936000	-1.424672000	3.301455000
C	-2.703326000	-0.934453000	2.006579000
C	-3.833071000	0.803007000	-1.187007000
C	-2.795316000	-0.111561000	-0.968685000
C	-4.980783000	0.406425000	-1.872595000
C	-2.914294000	-1.421700000	-1.458021000
C	-5.102169000	-0.901322000	-2.340163000
C	-4.068109000	-1.814736000	-2.130744000
H	-1.152256000	5.998994000	0.422254000
H	4.886656000	2.857242000	0.614871000
H	-2.605076000	4.658421000	1.935672000
H	2.616029000	2.207355000	1.322030000
H	6.535307000	1.131708000	-0.096878000
H	0.233267000	4.855540000	-1.303812000
H	1.388420000	0.750811000	3.148299000
H	-2.674330000	2.186805000	1.729611000
H	0.659521000	1.477406000	1.715030000
H	0.137361000	-0.511767000	4.597238000
H	-1.968123000	-1.652471000	5.252006000
H	5.878671000	-1.276745000	-0.076280000
H	0.183335000	2.380358000	-1.506587000
H	1.636700000	-1.297129000	1.679846000
H	3.591793000	-1.940173000	0.622829000
H	-3.798084000	-1.926806000	3.575955000
H	-3.745136000	1.831243000	-0.825911000
H	-3.509977000	-1.059164000	1.279823000
H	-5.784336000	1.126517000	-2.043318000
H	-2.095980000	-2.134073000	-1.302747000
H	-6.002555000	-1.208136000	-2.877337000
H	-4.154112000	-2.837790000	-2.503290000
Br	1.897660000	0.323282000	-2.502939000
Br	0.524676000	-3.109472000	-0.182402000
Fe	0.810320000	-0.784406000	-0.724598000
N	1.637687000	-0.333369000	1.339213000
P	-1.255041000	0.305634000	-0.089786000
CO			
C	0.000000000	0.000000000	-0.647583000
O	0.000000000	0.000000000	0.485688000

C	4.740174000	2.218585000	-0.420474000
C	3.386013000	1.999220000	-0.176054000
C	5.703874000	1.392038000	0.154321000
C	-2.327031000	2.595467000	-3.212156000
C	-2.095918000	2.956999000	-0.455187000
C	0.830540000	1.898475000	1.244094000
C	2.993478000	0.940240000	0.644557000
C	-0.304314000	2.031174000	3.474089000
C	-1.980567000	1.523766000	-2.396186000
C	-1.861629000	1.692530000	-1.008324000
C	5.305831000	0.338934000	0.977002000
C	-0.324538000	1.584313000	2.150076000
C	-1.341097000	1.723236000	4.353270000
C	3.955893000	0.110033000	1.222505000
C	-1.421342000	0.816591000	1.707512000
C	-2.413180000	0.951544000	3.914589000
C	-2.451452000	0.498440000	2.596977000
C	-4.146327000	-0.209452000	-0.435508000
C	-2.905635000	-0.817070000	-0.180175000
C	-5.303959000	-0.978432000	-0.523546000
C	-2.850333000	-2.207468000	-0.014052000
C	-5.239167000	-2.362124000	-0.362362000
C	-4.012409000	-2.971571000	-0.107621000
H	-2.819381000	4.697755000	-3.294693000
H	5.040794000	3.043827000	-1.069593000
H	-2.614948000	5.014816000	-0.833772000
H	2.638632000	2.646525000	-0.640578000
H	6.763811000	1.566291000	-0.041379000
H	-2.416354000	2.448231000	-4.290482000
H	1.497991000	2.618451000	1.744101000
H	-2.022471000	3.105593000	0.626057000
H	0.495058000	2.384690000	0.312089000
H	0.544986000	2.626732000	3.820344000
H	-1.304172000	2.080170000	5.384607000
H	6.051647000	-0.320523000	1.425629000
H	-1.802833000	0.540032000	-2.844044000
H	1.533682000	0.011567000	1.667666000
H	3.634381000	-0.734538000	1.837629000
H	-3.224802000	0.695703000	4.598872000
H	-4.213381000	0.873896000	-0.565044000
H	-3.291488000	-0.113849000	2.260382000
H	-6.261307000	-0.491422000	-0.722151000
H	-1.898743000	-2.695822000	0.207584000
H	-6.146911000	-2.965341000	-0.437082000
H	-3.952178000	-4.054446000	0.019872000
Br	2.766669000	-1.721278000	-1.271344000
Br	0.403324000	-2.174922000	1.421613000
Fe	0.629070000	-0.642397000	-0.560950000
N	1.604513000	0.679322000	0.891647000
P	-1.403796000	0.219644000	-0.014464000
C	-0.073625000	-1.881067000	-1.621104000
O	-0.540010000	-2.671101000	-2.313332000
C	0.962180000	0.500263000	-1.872189000
O	1.198062000	1.252204000	-2.712304000

^{3}3-cisBr_cisCO-1			
C	-2.673993000	3.616339000	-3.003431000
C	-2.679712000	3.881863000	-1.635468000
C	4.660378000	2.368810000	-0.590269000
C	3.322554000	2.210483000	-0.231500000
C	5.640618000	1.534575000	-0.057860000
C	-2.300901000	2.352814000	-3.463655000

^{5}3-cisBr_cisCO-1			
C	-2.587703000	3.298809000	-3.358314000
C	-2.564197000	3.718542000	-2.029761000
C	4.635785000	2.288885000	-0.354781000
C	3.280627000	2.178818000	-0.045810000
C	5.568621000	1.440811000	0.236932000
C	-2.324274000	1.963471000	-3.667814000

C	-2.316686000	2.889327000	-0.724857000	C	-2.281851000	2.810173000	-1.009035000
C	0.726542000	2.145391000	1.099193000	C	0.588381000	2.163103000	1.065191000
C	2.957252000	1.200586000	0.665405000	C	2.851034000	1.200782000	0.859757000
C	-0.487558000	2.436072000	3.270394000	C	-0.716027000	2.616198000	3.152208000
C	-1.929294000	1.363925000	-2.558471000	C	-2.032151000	1.057753000	-2.653076000
C	-1.934564000	1.620770000	-1.179186000	C	-2.012173000	1.468943000	-1.310017000
C	5.272707000	0.531787000	0.840859000	C	5.137315000	0.475344000	1.148607000
C	-0.448320000	1.865007000	1.995527000	C	-0.632741000	1.959610000	1.920830000
C	-1.530391000	2.163476000	4.154293000	C	-1.799881000	2.418665000	4.005872000
C	3.942215000	0.362304000	1.202677000	C	3.789930000	0.351965000	1.462059000
C	-1.496202000	1.002740000	1.606629000	C	-1.679493000	1.091585000	1.538814000
C	-2.554497000	1.304177000	3.768845000	C	-2.821754000	1.551138000	3.632124000
C	-2.536809000	0.727903000	2.499866000	C	-2.760605000	0.893149000	2.405078000
C	-4.117870000	-0.441263000	-0.701204000	C	-4.221411000	-0.573176000	-0.643521000
C	-2.903530000	-0.859175000	-0.134771000	C	-2.986760000	-0.928736000	-0.079294000
C	-5.212557000	-1.303222000	-0.730560000	C	-5.285575000	-1.472503000	-0.626345000
C	-2.808121000	-2.152858000	0.401191000	C	-2.837065000	-2.198164000	0.500288000
C	-5.110037000	-2.587711000	-0.198633000	C	-5.131198000	-2.731472000	-0.046307000
C	-3.907453000	-3.007862000	0.368047000	C	-3.907414000	-3.090103000	0.517501000
H	-2.958500000	4.395453000	-3.713984000	H	-2.809290000	4.012251000	-4.154990000
H	4.934001000	3.154407000	-1.298252000	H	4.960902000	3.048523000	-1.069217000
H	-2.973431000	4.868263000	-1.269506000	H	-2.773349000	4.761524000	-1.781028000
H	2.562694000	2.860346000	-0.671579000	H	2.559408000	2.844579000	-0.525793000
H	6.686559000	1.661679000	-0.343864000	H	6.627974000	1.529717000	-0.011211000
H	-2.291148000	2.138067000	-4.534266000	H	-2.338182000	1.627148000	-4.706807000
H	1.290561000	3.010242000	1.491790000	H	1.127437000	3.064898000	1.406044000
H	-2.336616000	3.105445000	0.347080000	H	-2.278626000	3.149249000	0.031061000
H	0.392606000	2.438027000	0.086742000	H	0.310510000	2.359232000	0.011987000
H	0.322936000	3.104252000	3.574533000	H	0.092596000	3.291000000	3.447129000
H	-1.536544000	2.619469000	5.146496000	H	-1.840009000	2.939139000	4.965018000
H	6.029937000	-0.134303000	1.260180000	H	5.858627000	-0.197871000	1.616662000
H	-1.632754000	0.376865000	-2.928399000	H	-1.815622000	0.013728000	-2.905872000
H	1.525557000	0.387488000	1.834825000	H	1.335400000	0.461076000	1.981002000
H	3.645270000	-0.444923000	1.877958000	H	3.443678000	-0.425329000	2.149262000
H	-3.373751000	1.078249000	4.454499000	H	-3.673544000	1.383605000	4.294654000
H	-4.216843000	0.562990000	-1.119892000	H	-4.355941000	0.412863000	-1.096071000
H	-3.345210000	0.055390000	2.203229000	H	-3.567830000	0.215125000	2.117501000
H	-6.152048000	-0.965073000	-1.173486000	H	-6.242684000	-1.184973000	-1.067669000
H	-1.871424000	-2.483924000	0.861009000	H	-1.878315000	-2.481843000	0.948365000
H	-5.968980000	-3.262075000	-0.226774000	H	-5.966880000	-3.435049000	-0.036024000
H	-3.818062000	-4.012081000	0.787933000	H	-3.778612000	-4.075056000	0.971526000
Br	2.788430000	-1.880652000	-1.201433000	Br	3.027810000	-1.705271000	-1.411528000
Br	0.577737000	-2.000584000	1.665820000	Br	0.631679000	-2.013270000	1.831074000
Fe	0.741243000	-0.732412000	-0.506600000	Fe	0.997990000	-0.823277000	-0.379493000
N	1.600617000	0.971381000	0.999279000	N	1.474826000	0.995693000	1.120514000
P	-1.455274000	0.256001000	-0.058340000	P	-1.560828000	0.213131000	-0.059418000
C	-0.186626000	-2.431701000	-1.396469000	C	-0.050045000	-2.288461000	-1.423043000
O	-0.469171000	-3.472687000	-1.761247000	O	-0.534721000	-3.193173000	-1.919793000
C	1.024550000	0.350781000	-1.885762000	C	1.120070000	0.609742000	-1.908470000
O	1.238129000	1.080188000	-2.755382000	O	1.287779000	1.246242000	-2.841859000
CP1				**CP2**			
C	-2.599935000	3.341973000	-3.325893000	C	-2.684225000	3.603976000	-3.015488000
C	-2.611486000	3.727714000	-1.986755000	C	-2.685101000	3.878506000	-1.649295000
C	4.623418000	2.364387000	-0.426899000	C	4.678326000	2.361180000	-0.553267000
C	3.270295000	2.166479000	-0.154355000	C	3.338687000	2.216955000	-0.195216000
C	5.594941000	1.618496000	0.236124000	C	5.645690000	1.498620000	-0.042971000
C	-2.292732000	2.023556000	-3.665516000	C	-2.313651000	2.337213000	-3.468845000
C	-2.320238000	2.801201000	-0.985315000	C	-2.320063000	2.891609000	-0.733314000
C	0.609463000	2.103907000	1.026640000	C	0.732772000	2.153818000	1.110840000
C	2.883471000	1.205622000	0.785006000	C	2.958037000	1.192234000	0.678573000
C	-0.631503000	2.511222000	3.159551000	C	-0.498617000	2.458451000	3.268833000

C	-1.993564000	1.099307000	-2.669325000
C	-2.007066000	1.476863000	-1.317233000
C	5.204278000	0.665736000	1.178165000
C	-0.592037000	1.891499000	1.907178000
C	-1.699778000	2.312454000	4.032185000
C	3.858317000	0.456542000	1.453019000
C	-1.667486000	1.059607000	1.527401000
C	-2.752618000	1.483863000	3.655848000
C	-2.735092000	0.861400000	2.409140000
C	-4.249698000	-0.518816000	-0.683006000
C	-3.026718000	-0.917554000	-0.121161000
C	-5.337865000	-1.388903000	-0.686631000
C	-2.915205000	-2.200458000	0.436406000
C	-5.219980000	-2.662598000	-0.131180000
C	-4.008778000	-3.063695000	0.430761000
H	-2.828712000	4.069551000	-4.107803000
H	4.915992000	3.111514000	-1.168238000
H	-2.854891000	4.757527000	-1.715109000
H	2.518994000	2.752311000	-0.689601000
H	6.653224000	1.776319000	0.018626000
H	-2.279614000	1.714585000	-4.713034000
H	1.158662000	2.995742000	1.374909000
H	-2.344186000	3.111110000	0.063630000
H	0.311769000	2.322277000	-0.014813000
H	0.199108000	3.158445000	3.455676000
H	-1.704578000	2.802964000	5.007926000
H	5.955950000	0.069636000	1.700249000
H	-1.748594000	0.067394000	-2.944560000
H	1.403649000	0.416425000	1.912071000
H	3.546727000	-0.314036000	2.163554000
H	-3.593163000	1.317223000	4.332913000
H	-4.357645000	0.477891000	-1.118941000
H	-3.562888000	0.208257000	2.121884000
H	-6.284719000	-1.066619000	-1.126171000
H	-1.971137000	-2.516576000	0.892159000
H	-6.074127000	-3.343801000	-0.137845000
H	-3.908066000	-4.059630000	0.867783000
Br	2.971204000	-1.796804000	-0.977188000
Br	0.401916000	-1.911703000	1.953318000
Fe	0.794030000	-0.814584000	-0.326546000
N	1.509448000	0.934936000	1.035264000
P	-1.581441000	0.200309000	-0.079396000
C	0.011984000	-2.413995000	-1.208242000
O	-0.386090000	-3.391163000	-1.644888000
C	1.085981000	0.327337000	-1.925031000
O	1.320439000	0.925839000	-2.872008000

C	-1.939575000	1.354225000	-2.558475000
C	-1.940710000	1.620093000	-1.181004000
C	5.262642000	0.481273000	0.832722000
C	-0.449472000	1.877164000	1.998818000
C	-1.548906000	2.195070000	4.146517000
C	3.930208000	0.325134000	1.193436000
C	-1.495541000	1.013443000	1.607745000
C	-2.570470000	1.333239000	3.760028000
C	-2.542987000	0.746837000	2.495924000
C	-4.113549000	-0.456483000	-0.688757000
C	-2.893166000	-0.863521000	-0.127291000
C	-5.201226000	-1.327318000	-0.711580000
C	-2.784909000	-2.155128000	0.410923000
C	-5.085952000	-2.609863000	-0.177354000
C	-3.877394000	-3.019032000	0.384607000
H	-2.970137000	4.378817000	-3.730271000
H	4.963557000	3.158754000	-1.243189000
H	-2.976447000	4.867795000	-1.289036000
H	2.590002000	2.890615000	-0.618525000
H	6.693109000	1.614947000	-0.328440000
H	-2.307059000	2.115629000	-4.538179000
H	1.300088000	3.012608000	1.512195000
H	-2.336100000	3.114572000	0.337390000
H	0.407336000	2.456357000	0.098226000
H	0.310276000	3.128200000	3.573965000
H	-1.562826000	2.660013000	5.134586000
H	6.009306000	-0.207251000	1.234627000
H	-1.643056000	0.365007000	-2.922952000
H	1.513312000	0.380558000	1.834698000
H	3.621932000	-0.493605000	1.849661000
H	-3.395747000	1.113853000	4.440688000
H	-4.223182000	0.546178000	-1.108872000
H	-3.350825000	0.073756000	2.198818000
H	-6.145473000	-0.997632000	-1.150977000
H	-1.842381000	-2.478141000	0.865095000
H	-5.939567000	-3.291299000	-0.200129000
H	-3.777894000	-4.021760000	0.806029000
Br	2.772865000	-1.841786000	-1.300406000
Br	0.620128000	-2.025847000	1.612777000
Fe	0.748354000	-0.709518000	-0.529987000
N	1.598416000	0.975261000	1.007774000
P	-1.452472000	0.262314000	-0.055940000
C	-0.210053000	-2.401788000	-1.439326000
O	-0.488276000	-3.443670000	-1.804280000
C	1.010305000	0.408949000	-1.884796000
O	1.209875000	1.161244000	-2.738135000

CP3			
C	-2.340290000	4.634831000	0.126420000
C	-2.233431000	3.973769000	1.348252000
C	5.160522000	1.371598000	0.581335000
C	3.803778000	1.195666000	0.844827000
C	5.957628000	0.292437000	0.205321000
C	-2.141894000	3.933066000	-1.063586000
C	-1.934943000	2.611368000	1.385159000
C	1.168093000	0.624731000	1.903209000
C	3.235338000	-0.076576000	0.735079000
C	0.128486000	-0.413821000	3.926904000
C	-1.830973000	2.577582000	-1.031154000
C	-1.732993000	1.902451000	0.194760000
C	5.385675000	-0.974806000	0.092961000
C	0.005472000	-0.048498000	2.582622000
C	-0.897016000	-1.081453000	4.594008000

^{5}TS3			
C	2.340934000	2.555001000	4.057003000
C	2.527330000	3.221022000	2.846531000
C	-4.797128000	1.959236000	1.234818000
C	-3.494059000	2.107332000	0.758767000
C	-5.660691000	1.027628000	0.664578000
C	1.868499000	1.242212000	4.060953000
C	2.245525000	2.579896000	1.640537000
C	-0.867821000	2.494383000	-0.418336000
C	-3.048417000	1.311499000	-0.302497000
C	0.397903000	3.535572000	-2.304569000
C	1.576774000	0.602243000	2.859170000
C	1.764380000	1.263297000	1.635234000
C	-5.212249000	0.235776000	-0.394576000
C	0.347442000	2.558201000	-1.306547000
C	1.475201000	3.620096000	-3.184809000

C	4.032456000	-1.163848000	0.356601000
C	-1.193559000	-0.357907000	1.901921000
C	-2.069051000	-1.399169000	3.914121000
C	-2.214194000	-1.038031000	2.575713000
C	-4.129025000	0.014718000	-0.354163000
C	-2.895841000	-0.649029000	-0.427018000
C	-5.291638000	-0.618370000	-0.789661000
C	-2.844677000	-1.951272000	-0.945602000
C	-5.235520000	-1.916032000	-1.297560000
C	-4.011902000	-2.580648000	-1.372892000
H	-2.574633000	5.701533000	0.099798000
H	5.593967000	2.370848000	0.663720000
H	-2.388213000	4.518417000	2.282608000
H	3.186306000	2.056206000	1.105245000
H	7.019847000	0.438137000	-0.001598000
H	-2.215669000	4.447561000	-2.024107000
H	1.885709000	0.957230000	2.671907000
H	-1.865518000	2.099569000	2.349450000
H	0.865073000	1.528175000	1.344002000
H	1.053661000	-0.171609000	4.457866000
H	-0.774596000	-1.358232000	5.643368000
H	5.997669000	-1.830836000	-0.200111000
H	-1.654718000	2.038045000	-1.966557000
H	1.706156000	-1.262057000	1.272768000
H	3.578951000	-2.154535000	0.262044000
H	-2.877571000	-1.927472000	4.424130000
H	-4.181856000	1.032031000	0.043937000
H	-3.139166000	-1.285822000	2.048495000
H	-6.247596000	-0.092598000	-0.731617000
H	-1.884968000	-2.474850000	-1.009586000
H	-6.148402000	-2.408718000	-1.640524000
H	-3.960856000	-3.594973000	-1.774847000
Br	1.556638000	1.735761000	-1.634558000
Br	0.853658000	-2.911340000	-0.576243000
Fe	0.792946000	-0.474910000	-0.988632000
N	1.839663000	-0.296077000	0.961855000
P	-1.343887000	0.120645000	0.144667000
C	0.048544000	-0.731812000	-2.680870000
O	-0.451214000	-0.872069000	-3.705040000

C	-3.917473000	0.371805000	-0.879429000
C	1.421297000	1.646471000	-1.191749000
C	2.527082000	2.716895000	-3.071925000
C	2.498485000	1.738999000	-2.079222000
C	3.920230000	-0.715785000	0.680163000
C	2.818287000	-0.708977000	-0.186400000
C	4.967223000	-1.613699000	0.475377000
C	2.784169000	-1.610488000	-1.263292000
C	4.928597000	-2.506191000	-0.594336000
C	3.838748000	-2.496489000	-1.465459000
H	2.562861000	3.060053000	4.999779000
H	-5.134768000	2.582171000	2.066206000
H	2.900396000	4.247785000	2.837953000
H	-2.826156000	2.831492000	1.229699000
H	-6.677313000	0.914074000	1.045519000
H	1.718970000	0.714345000	5.005314000
H	-1.440846000	3.433472000	-0.520762000
H	2.405264000	3.108896000	0.696768000
H	-0.585646000	2.425396000	0.649488000
H	-0.432323000	4.242042000	-2.393871000
H	1.487315000	4.389850000	-3.959215000
H	-5.875528000	-0.504660000	-0.846405000
H	1.205011000	-0.427285000	2.865287000
H	-1.640762000	1.116174000	-1.754323000
H	-3.554517000	-0.264459000	-1.693320000
H	3.377063000	2.770324000	-3.755451000
H	3.964435000	-0.022075000	1.523455000
H	3.329881000	1.034997000	-1.994729000
H	5.818877000	-1.613090000	1.159501000
H	1.920600000	-1.621547000	-1.936978000
H	5.748109000	-3.211825000	-0.748538000
H	3.799468000	-3.194399000	-2.304672000
Br	-2.064595000	-2.792745000	0.659173000
Br	-0.656469000	-1.100849000	-2.529199000
Fe	-0.963478000	-0.755002000	-0.044388000
N	-1.706385000	1.344067000	-0.757912000
P	1.361114000	0.351926000	0.099771000
C	1.106923000	-2.762437000	1.467288000
O	1.511566000	-3.814547000	1.337559000
C	-1.445811000	-0.106687000	1.879115000
O	-1.726945000	0.015283000	2.980543000

^{5}TS1			
C	-1.875388000	4.718459000	-1.307151000
C	-1.832096000	4.439753000	0.057355000
C	4.877673000	1.725304000	0.816346000
C	3.514116000	1.565397000	1.067097000
C	5.718065000	0.619344000	0.733729000
C	-1.836857000	3.671743000	-2.230419000
C	-1.750128000	3.120080000	0.504443000
C	0.822520000	1.150463000	2.019650000
C	2.979540000	0.281910000	1.222125000
C	-0.524409000	0.579130000	4.045809000
C	-1.739646000	2.356469000	-1.788786000
C	-1.699450000	2.066269000	-0.414820000
C	5.184267000	-0.659584000	0.908101000
C	-0.453953000	0.664773000	2.651840000
C	-1.673456000	0.122896000	4.688584000
C	3.827943000	-0.831554000	1.149493000
C	-1.583075000	0.287892000	1.890734000
C	-2.780058000	-0.254372000	3.934367000
C	-2.732348000	-0.172218000	2.544110000
C	-4.170852000	0.264177000	-0.818517000

^{1}TS3			
C	2.747781000	2.102000000	4.049127000
C	2.649817000	2.925397000	2.929728000
C	-4.725106000	1.773020000	1.463419000
C	-3.382812000	1.832265000	1.092799000
C	-5.652266000	1.121148000	0.652984000
C	2.410495000	0.751571000	3.947421000
C	2.218027000	2.404638000	1.708928000
C	-0.822505000	2.453064000	-0.184433000
C	-2.971652000	1.228508000	-0.096822000
C	0.373911000	3.666565000	-2.024385000
C	1.974120000	0.230969000	2.733578000
C	1.873476000	1.051242000	1.599661000
C	-5.232710000	0.522791000	-0.536230000
C	0.340461000	2.597905000	-1.125171000
C	1.408968000	3.793906000	-2.949376000
C	-3.896514000	0.572686000	-0.913932000
C	1.379483000	1.643769000	-1.156193000
C	2.418838000	2.836960000	-2.992020000
C	2.402098000	1.765708000	-2.099673000
C	3.987964000	-0.479907000	-0.028643000

C	-3.020656000	-0.474767000	-0.504690000
C	-5.330376000	-0.385216000	-1.238265000
C	-3.055967000	-1.873436000	-0.612382000
C	-5.357211000	-1.775359000	-1.345091000
C	-4.219758000	-2.516893000	-1.028100000
H	-1.938523000	5.752178000	-1.653729000
H	5.281668000	2.732063000	0.687187000
H	-1.867558000	5.254424000	0.784231000
H	2.872574000	2.446486000	1.132846000
H	6.783838000	0.750113000	0.536795000
H	-1.867835000	3.882596000	-3.301582000
H	1.435378000	1.647416000	2.792960000
H	-1.728395000	2.911161000	1.578200000
H	0.613525000	1.921048000	1.256575000
H	0.347115000	0.874660000	4.636807000
H	-1.699743000	0.059812000	5.778455000
H	5.831597000	-1.537119000	0.846607000
H	-1.686607000	1.541561000	-2.518901000
H	1.421580000	-0.816470000	1.878605000
H	3.403149000	-1.834171000	1.254961000
H	-3.686419000	-0.615356000	4.424980000
H	-4.164581000	1.353937000	-0.732976000
H	-3.604659000	-0.473666000	1.959227000
H	-6.219604000	0.201092000	-1.481026000
H	-2.170137000	-2.462582000	-0.352172000
H	-6.266932000	-2.281197000	-1.676601000
H	-4.232998000	-3.606070000	-1.107261000
Br	2.593105000	-0.561170000	-2.180626000
Br	0.325398000	-2.858079000	0.708507000
Fe	0.695904000	-0.822004000	-0.682224000
N	1.588039000	0.067482000	1.392188000
P	-1.475905000	0.319233000	0.064754000
C	-0.209996000	-1.790595000	-2.279338000
O	-0.547315000	-2.438780000	-3.156194000
C	1.320332000	2.086803000	-1.153957000
O	1.738827000	2.959011000	-1.750360000

C	2.672845000	-0.858081000	-0.342828000
C	5.051552000	-1.333756000	-0.309767000
C	2.441531000	-2.109479000	-0.927164000
C	4.812963000	-2.578904000	-0.892559000
C	3.508977000	-2.964787000	-1.196675000
H	3.086667000	2.511942000	5.003165000
H	-5.044008000	2.238737000	2.398165000
H	2.916575000	3.982383000	3.001101000
H	-2.659409000	2.328435000	1.743341000
H	-6.701759000	1.073975000	0.950152000
H	2.482246000	0.100049000	4.820944000
H	-1.486845000	3.327240000	-0.278024000
H	2.160832000	3.060524000	0.835580000
H	-0.499185000	2.412035000	0.870041000
H	-0.431449000	4.406156000	-2.003127000
H	1.416471000	4.635004000	-3.645684000
H	-5.950556000	0.001568000	-1.172569000
H	1.701010000	-0.826563000	2.660383000
H	-1.539302000	1.053240000	-1.504082000
H	-3.547913000	0.070850000	-1.821146000
H	3.224356000	2.918736000	-3.724848000
H	4.181948000	0.488520000	0.442166000
H	3.192470000	1.012271000	-2.142947000
H	6.071045000	-1.027265000	-0.064988000
H	1.421801000	-2.409900000	-1.180120000
H	5.647230000	-3.251496000	-1.105053000
H	3.314597000	-3.940485000	-1.647177000
Br	-2.385803000	-2.386001000	0.330305000
Br	-0.540072000	-0.994544000	-2.369771000
Fe	-0.794784000	-0.572137000	0.095139000
N	-1.590112000	1.222071000	-0.490625000
P	1.285583000	0.270643000	0.043199000
C	0.674171000	-3.005725000	1.477400000
O	0.713608000	-4.139763000	1.450702000
C	-1.031532000	-0.272427000	1.813090000
O	-1.192867000	-0.061703000	2.937451000

^{1}TS1			
C	-1.710840000	4.684460000	0.768338000
C	-1.640787000	3.867259000	1.895087000
C	5.041679000	0.775263000	1.332884000
C	3.654763000	0.683237000	1.450827000
C	5.773564000	-0.263264000	0.764191000
C	-1.719226000	4.112596000	-0.505163000
C	-1.572718000	2.480447000	1.754794000
C	0.946013000	0.081582000	2.220969000
C	2.992502000	-0.454078000	0.985075000
C	-0.349114000	-1.240311000	3.905100000
C	-1.639803000	2.731180000	-0.649513000
C	-1.565731000	1.901425000	0.481126000
C	5.107624000	-1.402830000	0.310093000
C	-0.312079000	-0.613816000	2.655650000
C	-1.484207000	-1.922410000	4.339005000
C	3.725625000	-1.500275000	0.416429000
C	-1.457211000	-0.672049000	1.832318000
C	-2.603070000	-1.994481000	3.514698000
C	-2.586769000	-1.374606000	2.266620000
C	-4.129680000	0.431258000	-0.281498000
C	-2.981229000	-0.309808000	-0.604412000
C	-5.360338000	0.106515000	-0.845947000
C	-3.089302000	-1.378078000	-1.503802000
C	-5.459242000	-0.957993000	-1.742055000
C	-4.323712000	-1.696557000	-2.068111000

^{1}2-cisBr-CO$_{Br}$			
C	-2.101499000	3.186092000	-3.454552000
C	-1.926624000	3.712177000	-2.176575000
C	5.081457000	1.366437000	-0.976779000
C	3.806043000	1.573352000	-0.455246000
C	5.801514000	0.216770000	-0.657854000
C	-1.964016000	1.812919000	-3.667229000
C	-1.618554000	2.869677000	-1.106937000
C	1.316682000	2.089185000	0.933048000
C	3.241803000	0.615680000	0.393891000
C	0.113273000	2.887254000	2.975663000
C	-1.650521000	0.969899000	-2.606827000
C	-1.477942000	1.493131000	-1.315863000
C	5.236218000	-0.733982000	0.191850000
C	0.101513000	2.104942000	1.817908000
C	-0.969439000	2.894288000	3.853243000
C	3.962208000	-0.543316000	0.717781000
C	-1.036227000	1.318387000	1.532267000
C	-2.078346000	2.098991000	3.583008000
C	-2.108470000	1.315319000	2.430382000
C	-3.818157000	-0.094309000	-0.158231000
C	-2.581148000	-0.702841000	0.111482000
C	-4.998828000	-0.824688000	-0.051803000
C	-2.543515000	-2.053750000	0.475110000
C	-4.955666000	-2.169801000	0.315653000
C	-3.730011000	-2.778862000	0.576605000

H	-1.761714000	5.769574000	0.881278000	H	-2.343671000	3.847340000	-4.289604000
H	5.550536000	1.672305000	1.692871000	H	5.512719000	2.115992000	-1.643693000
H	-1.643602000	4.309756000	2.893846000	H	-2.036236000	4.785512000	-2.005142000
H	3.093908000	1.506334000	1.897593000	H	3.249564000	2.470629000	-0.731005000
H	6.859031000	-0.187023000	0.674543000	H	6.799622000	0.061420000	-1.071695000
H	-1.776481000	4.747208000	-1.392057000	H	-2.094890000	1.396486000	-4.668257000
H	1.661439000	0.072988000	3.059445000	H	2.056021000	2.817565000	1.307912000
H	-1.531211000	1.847325000	2.646034000	H	-1.500363000	3.290340000	-0.103850000
H	0.766350000	1.141308000	1.975953000	H	1.071066000	2.391197000	-0.100773000
H	0.536283000	-1.195661000	4.545375000	H	0.995210000	3.495542000	3.195411000
H	-1.487552000	-2.406637000	5.317807000	H	-0.937125000	3.510910000	4.753872000
H	5.669219000	-2.224242000	-0.140074000	H	5.789924000	-1.638801000	0.450573000
H	-1.637889000	2.291650000	-1.652709000	H	-1.521739000	-0.105433000	-2.777249000
H	1.334865000	-1.569240000	1.069037000	H	1.837427000	0.302239000	1.820406000
H	3.195111000	-2.376331000	0.032415000	H	3.510510000	-1.288478000	1.378526000
H	-3.493988000	-2.536404000	3.838824000	H	-2.926428000	2.082140000	4.270738000
H	-4.062978000	1.269136000	0.418260000	H	-3.861400000	0.958247000	-0.452985000
H	-3.466713000	-1.440651000	1.622549000	H	-2.981231000	0.689875000	2.229873000
H	-6.245634000	0.691450000	-0.586492000	H	-5.955152000	-0.341107000	-0.263628000
H	-2.206865000	-1.969509000	-1.759590000	H	-1.585355000	-2.538747000	0.670686000
H	-6.423901000	-1.208808000	-2.189300000	H	-5.881355000	-2.745283000	0.391647000
H	-4.392780000	-2.528612000	-2.772012000	H	-3.689144000	-3.834066000	0.854930000
Br	2.485090000	0.492631000	-2.068058000	Br	0.205884000	-2.548819000	-1.610118000
Br	0.177867000	-2.694695000	-0.801443000	Br	0.711803000	-1.906590000	1.886538000
Fe	0.524246000	-0.276401000	-0.892608000	Fe	0.880765000	-0.676325000	-0.246653000
N	1.565211000	-0.569947000	1.042651000	N	1.907024000	0.741504000	0.894333000
P	-1.380862000	0.104889000	0.182907000	P	-1.055928000	0.300218000	0.006430000
C	-0.282035000	-0.119725000	-2.434051000	C	1.238025000	0.144705000	-1.757239000
O	-0.829521000	-0.011365000	-3.444404000	O	1.490522000	0.687566000	-2.746464000
C	1.464261000	2.671272000	0.071663000				
O	1.798707000	3.666582000	-0.362758000				
^{3}**2-cisBr-CO$_{Br}$**				^{5}**2-cisBr-CO$_{Br}$**			
C	-2.711923000	3.487535000	-3.052816000	C	-1.376758000	3.479708000	-3.513047000
C	-2.705762000	3.763726000	-1.687260000	C	-1.496362000	3.957606000	-2.208656000
C	4.666646000	2.380404000	-0.623519000	C	5.104983000	1.448527000	-1.029841000
C	3.360102000	2.278216000	-0.145943000	C	3.866860000	1.650679000	-0.419120000
C	5.591295000	1.366903000	-0.384359000	C	5.833680000	0.285560000	-0.799113000
C	-2.312239000	2.230319000	-3.508534000	C	-1.181214000	2.116629000	-3.739954000
C	-2.303626000	2.788077000	-0.774409000	C	-1.425265000	3.076995000	-1.129417000
C	0.760211000	2.120532000	1.138750000	C	1.401506000	2.089147000	0.976650000
C	2.976944000	1.146355000	0.579790000	C	3.335499000	0.671965000	0.433081000
C	-0.532498000	2.365267000	3.266469000	C	0.262281000	2.823541000	3.073790000
C	-1.904817000	1.257005000	-2.602158000	C	-1.097410000	1.234675000	-2.665892000
C	-1.898841000	1.524636000	-1.224560000	C	-1.222950000	1.708648000	-1.350858000
C	5.201189000	0.236545000	0.336276000	C	5.310749000	-0.683869000	0.060782000
C	-0.443745000	1.807364000	1.988354000	C	0.190445000	2.119934000	1.867966000
C	-1.592641000	2.060617000	4.118672000	C	-0.816777000	2.870958000	3.954212000
C	3.902984000	0.120590000	0.817216000	C	4.077590000	-0.499307000	0.672496000
C	-1.463018000	0.927304000	1.560637000	C	-1.010618000	1.451663000	1.538215000
C	-2.581663000	1.177088000	3.698825000	C	-1.994865000	2.206040000	3.630803000
C	-2.514883000	0.614009000	2.425417000	C	-2.088723000	1.502895000	2.431086000
C	-3.999336000	-0.677435000	-0.371035000	C	-3.898908000	0.328189000	-0.541163000
C	-2.652034000	-1.061611000	-0.279674000	C	-2.778808000	-0.273596000	0.045265000
C	-4.990700000	-1.640691000	-0.534008000	C	-5.147715000	-0.285268000	-0.451903000
C	-2.308502000	-2.415774000	-0.384325000	C	-2.920129000	-1.499548000	0.711669000
C	-4.644336000	-2.990181000	-0.624344000	C	-5.285656000	-1.497425000	0.223096000
C	-3.306680000	-3.374030000	-0.555696000	C	-4.171525000	-2.102171000	0.805913000
H	-3.026706000	4.253219000	-3.765252000	H	-1.434061000	4.171857000	-4.356167000
H	4.958509000	3.265480000	-1.193101000	H	5.499510000	2.217949000	-1.697734000
H	-3.020461000	4.744917000	-1.324552000	H	-1.651303000	5.023814000	-2.027747000
H	2.642528000	3.073045000	-0.358487000	H	3.310543000	2.565431000	-0.630477000
H	6.611123000	1.452308000	-0.764288000	H	6.800603000	0.133100000	-1.282145000

H	-2.310738000	2.008084000	-4.577693000	H	-1.086198000	1.737384000	-4.759713000
H	1.311085000	2.968708000	1.582641000	H	2.101617000	2.884168000	1.297850000
H	-2.312675000	3.013405000	0.295948000	H	-1.528757000	3.457048000	-0.108427000
H	0.466427000	2.442219000	0.122936000	H	1.127601000	2.337753000	-0.065886000
H	0.254467000	3.046980000	3.601247000	H	1.191595000	3.342679000	3.324904000
H	-1.636470000	2.506453000	5.114472000	H	-0.732608000	3.424229000	4.891908000
H	5.912436000	-0.571338000	0.519784000	H	5.869956000	-1.601711000	0.256711000
H	-1.584565000	0.276672000	-2.969091000	H	-0.939977000	0.164372000	-2.843210000
H	1.616599000	0.399881000	1.888042000	H	1.948681000	0.288104000	1.869184000
H	3.582911000	-0.776507000	1.356194000	H	3.661561000	-1.267035000	1.331179000
H	-3.408849000	0.917604000	4.362731000	H	-2.849291000	2.232135000	4.310371000
H	-4.271134000	0.381534000	-0.319019000	H	-3.797372000	1.279121000	-1.071802000
H	-3.287344000	-0.089808000	2.106521000	H	-3.019946000	0.986581000	2.187394000
H	-6.037755000	-1.336363000	-0.598517000	H	-6.017108000	0.187218000	-0.914696000
H	-1.259524000	-2.720960000	-0.329568000	H	-2.042956000	-1.983823000	1.154715000
H	-5.423199000	-3.744466000	-0.758223000	H	-6.264884000	-1.977316000	0.288835000
H	-3.031123000	-4.427258000	-0.638648000	H	-4.272838000	-3.056921000	1.326134000
Br	2.118609000	-2.424416000	-1.363665000	Br	-0.513523000	-2.708442000	-1.724938000
Br	0.509333000	-1.914795000	1.762123000	Br	0.881962000	-2.144699000	2.046537000
Fe	0.875696000	-0.643558000	-0.342725000	Fe	0.622746000	-1.274551000	-0.174536000
N	1.638247000	0.949816000	1.023821000	N	2.051117000	0.788458000	0.986470000
P	-1.341163000	0.188640000	-0.104589000	P	-1.119179000	0.475646000	-0.009293000
C	1.154174000	0.287855000	-1.817376000	C	1.747095000	-0.556325000	-1.692010000
O	1.335040000	0.919875000	-2.768691000	O	2.270837000	-0.244611000	-2.658677000
^{1}2-trBr-CO$_N$				**^{3}2-trBr-CO$_N$**			
C	-2.169430000	4.597882000	0.378691000	C	-2.333464000	4.633049000	0.115728000
C	-1.935956000	3.891213000	1.555286000	C	-2.241119000	3.973604000	1.339791000
C	5.196531000	1.164820000	0.496063000	C	5.154736000	1.353569000	0.589289000
C	3.863683000	0.997607000	0.863006000	C	3.793213000	1.184676000	0.830968000
C	5.895005000	0.135841000	-0.133017000	C	5.949669000	0.271203000	0.218319000
C	-2.097720000	3.942395000	-0.852409000	C	-2.123794000	3.929810000	-1.071550000
C	-1.634129000	2.528669000	1.507407000	C	-1.945460000	2.610836000	1.381387000
C	1.275150000	0.425242000	1.991909000	C	1.165627000	0.623716000	1.886181000
C	3.219756000	-0.214501000	0.600844000	C	3.218323000	-0.082691000	0.703008000
C	0.125253000	-0.665098000	3.932114000	C	0.139775000	-0.406335000	3.923702000
C	-1.785887000	2.589244000	-0.904872000	C	-1.815600000	2.573821000	-1.035067000
C	-1.556956000	1.868823000	0.276956000	C	-1.732695000	1.900861000	0.193449000
C	5.249315000	-1.072162000	-0.392410000	C	5.371650000	-0.991393000	0.090267000
C	0.074875000	-0.243819000	2.600474000	C	0.009789000	-0.045680000	2.578859000
C	-0.945272000	-1.338588000	4.518132000	C	-0.884344000	-1.069524000	4.597702000
C	3.917669000	-1.252532000	-0.028355000	C	4.013034000	-1.173061000	0.331935000
C	-1.090972000	-0.502734000	1.847565000	C	-1.193712000	-0.355452000	1.906565000
C	-2.083059000	-1.611986000	3.765382000	C	-2.060472000	-1.388679000	3.925033000
C	-2.153537000	-1.195990000	2.436691000	C	-2.212249000	-1.032932000	2.585964000
C	-3.953900000	0.074052000	-0.273546000	C	-4.121823000	0.001051000	-0.370579000
C	-2.742188000	-0.583938000	-0.541955000	C	-2.885956000	-0.659492000	-0.428889000
C	-5.157392000	-0.449221000	-0.738923000	C	-5.278518000	-0.639183000	-0.810849000
C	-2.760317000	-1.769254000	-1.288220000	C	-2.824989000	-1.964566000	-0.939377000
C	-5.166899000	-1.629893000	-1.481669000	C	-5.213260000	-1.939901000	-1.309951000
C	-3.968377000	-2.286090000	-1.753815000	C	-3.986576000	-2.600238000	-1.372209000
H	-2.406376000	5.663506000	0.417913000	H	-2.565466000	5.700050000	0.085418000
H	5.689522000	2.118273000	0.697684000	H	5.593462000	2.349124000	0.685033000
H	-1.993380000	4.397795000	2.521379000	H	-2.404766000	4.519832000	2.271559000
H	3.321183000	1.823633000	1.323365000	H	3.177127000	2.046535000	1.088895000
H	6.939046000	0.275390000	-0.420541000	H	7.015815000	0.410929000	0.028602000
H	-2.273370000	4.492812000	-1.779019000	H	-2.186127000	4.443556000	-2.033114000
H	2.032288000	0.595500000	2.775583000	H	1.902560000	0.936167000	2.643893000
H	-1.468766000	1.981410000	2.439709000	H	-1.886756000	2.099084000	2.346328000
H	1.034515000	1.412148000	1.556457000	H	0.865474000	1.536561000	1.341589000
H	1.027611000	-0.464823000	4.516588000	H	1.067989000	-0.164568000	4.449223000
H	-0.882278000	-1.659169000	5.560135000	H	-0.757435000	-1.342691000	5.647359000
H	5.784917000	-1.888876000	-0.881164000	H	5.982525000	-1.849834000	-0.197348000

H	-1.712470000	2.087112000	-1.874232000	H	-1.630657000	2.033033000	-1.967973000
H	1.700839000	-1.405487000	1.160997000	H	1.681652000	-1.260286000	1.230881000
H	3.407273000	-2.197867000	-0.231548000	H	3.555740000	-2.160204000	0.226370000
H	-2.922695000	-2.150947000	4.209251000	H	-2.866566000	-1.914009000	4.441633000
H	-3.958911000	1.001752000	0.305017000	H	-4.180950000	1.021076000	0.019283000
H	-3.051292000	-1.412609000	1.852936000	H	-3.139002000	-1.281262000	2.062132000
H	-6.092491000	0.072462000	-0.522914000	H	-6.236719000	-0.116672000	-0.764223000
H	-1.827383000	-2.297631000	-1.499403000	H	-1.862376000	-2.483612000	-0.995931000
H	-6.111190000	-2.035793000	-1.851948000	H	-6.121427000	-2.438056000	-1.657138000
H	-3.967136000	-3.208827000	-2.337923000	H	-3.928487000	-3.616007000	-1.769137000
Br	1.494178000	1.842104000	-1.365706000	Br	1.557493000	1.745214000	-1.613238000
Br	0.620282000	-2.819422000	-0.637607000	Br	0.870337000	-2.863731000	-0.624844000
Fe	0.702882000	-0.390208000	-0.906524000	Fe	0.773082000	-0.443344000	-0.967652000
N	1.836027000	-0.418137000	0.919809000	N	1.813898000	-0.293358000	0.918539000
P	-1.171226000	0.086839000	0.117312000	P	-1.344966000	0.120396000	0.152171000
C	-0.089080000	-0.409611000	-2.468312000	C	-0.005609000	-0.633684000	-2.534387000
O	-0.623910000	-0.395763000	-3.491144000	O	-0.551203000	-0.748305000	-3.544447000
^{5}2-trBr-CO$_{N}$				**^{5}TS4**			
C	-2.231527000	4.705540000	-0.327525000	C	-1.261492000	4.786636000	0.733474000
C	-2.252271000	4.140933000	0.946673000	C	-1.392318000	3.954280000	1.843837000
C	5.123711000	1.522337000	0.514256000	C	4.981654000	0.804604000	1.203281000
C	3.777239000	1.346139000	0.826693000	C	3.643797000	0.557002000	1.516693000
C	5.938758000	0.428036000	0.234191000	C	5.684422000	-0.051792000	0.361859000
C	-1.935398000	3.910896000	-1.435520000	C	-1.183889000	4.231952000	-0.545350000
C	-1.982973000	2.782977000	1.116666000	C	-1.449075000	2.569530000	1.681354000
C	1.140452000	0.854807000	1.910723000	C	0.930503000	-0.075913000	2.256759000
C	3.232655000	0.058320000	0.862026000	C	2.996951000	-0.554657000	0.970287000
C	0.036510000	0.020178000	3.993526000	C	-0.560383000	-1.333827000	3.811228000
C	-1.655006000	2.557807000	-1.269753000	C	-1.224643000	2.851111000	-0.711780000
C	-1.683251000	1.980423000	0.008243000	C	-1.363773000	2.007994000	0.402383000
C	5.392489000	-0.855496000	0.267419000	C	5.039643000	-1.171498000	-0.168510000
C	-0.047348000	0.256348000	2.617762000	C	-0.414686000	-0.667062000	2.590612000
C	-1.011199000	-0.575184000	4.694001000	C	-1.767471000	-1.923126000	4.182499000
C	4.050390000	-1.044700000	0.579994000	C	3.706611000	-1.423735000	0.128426000
C	-1.230345000	-0.112196000	1.937745000	C	-1.532333000	-0.582405000	1.725746000
C	-2.168120000	-0.948676000	4.017040000	C	-2.858413000	-1.851303000	3.323065000
C	-2.274669000	-0.716654000	2.646733000	C	-2.737323000	-1.186622000	2.104000000
C	-4.117062000	0.111117000	-0.435418000	C	-4.053870000	0.745156000	-0.572838000
C	-2.906278000	-0.593108000	-0.377484000	C	-2.937423000	-0.081257000	-0.766398000
C	-5.285353000	-0.537085000	-0.832986000	C	-5.248362000	0.472155000	-1.235333000
C	-2.882658000	-1.951851000	-0.726730000	C	-3.029867000	-1.175379000	-1.637073000
C	-5.257159000	-1.889537000	-1.171438000	C	-5.337987000	-0.624863000	-2.093409000
C	-4.055351000	-2.595421000	-1.115402000	C	-4.229737000	-1.447101000	-2.292255000
H	-2.442228000	5.769438000	-0.457916000	H	-1.217374000	5.870218000	0.863761000
H	5.534796000	2.533890000	0.482369000	H	5.474501000	1.682080000	1.628236000
H	-2.483300000	4.759081000	1.817258000	H	-1.457230000	4.383964000	2.846218000
H	3.146743000	2.217679000	1.009088000	H	3.111707000	1.240797000	2.179090000
H	6.992457000	0.573327000	-0.011954000	H	6.729268000	0.149488000	0.118192000
H	-1.908962000	4.349350000	-2.435311000	H	-1.072332000	4.878468000	-1.418598000
H	1.816279000	1.300101000	2.662231000	H	1.549916000	-0.069364000	3.171571000
H	-2.011071000	2.347272000	2.119563000	H	-1.561956000	1.924140000	2.557808000
H	0.846673000	1.678446000	1.234611000	H	0.841493000	0.974641000	1.932040000
H	0.949118000	0.307889000	4.523274000	H	0.300358000	-1.393982000	4.483528000
H	-0.918161000	-0.750961000	5.767787000	H	-1.849367000	-2.442225000	5.139702000
H	6.017563000	-1.724486000	0.049639000	H	5.577743000	-1.853784000	-0.829860000
H	-1.399368000	1.944948000	-2.138758000	H	-1.126451000	2.418868000	-1.712675000
H	1.719350000	-1.089868000	1.528272000	H	1.462742000	-1.824368000	1.305508000
H	3.619285000	-2.049723000	0.597678000	H	3.193663000	-2.289584000	-0.302930000
H	-2.994348000	-1.420348000	4.553250000	H	-3.809542000	-2.313166000	3.596155000
H	-4.148257000	1.171745000	-0.170807000	H	-3.986932000	1.606706000	0.098271000
H	-3.187612000	-1.008029000	2.121145000	H	-3.598809000	-1.138761000	1.433659000
H	-6.223825000	0.020233000	-0.878464000	H	-6.114021000	1.120731000	-1.082242000

H	-1.939252000	-2.507867000	-0.686825000	H	-2.157237000	-1.817657000	-1.795085000
H	-6.174218000	-2.393801000	-1.484672000	H	-6.275328000	-0.835080000	-2.613798000
H	-4.026210000	-3.653800000	-1.383390000	H	-4.293964000	-2.302497000	-2.968213000
Br	1.655653000	1.383166000	-1.950896000	Br	1.611160000	0.699716000	-2.497984000
Br	0.817860000	-2.972438000	-0.199641000	Br	0.272239000	-3.104012000	-0.855901000
Fe	0.758474000	-0.608684000	-0.933529000	Fe	0.666256000	-0.720786000	-0.866015000
N	1.854250000	-0.161395000	1.124906000	N	1.610563000	-0.818570000	1.187136000
P	-1.341068000	0.191946000	0.137156000	P	-1.351245000	0.213599000	0.084633000
C	-0.053473000	-1.219920000	-2.722375000	C	1.808539000	2.658477000	0.156963000
O	-0.489880000	-1.561226000	-3.720444000	O	2.347229000	3.564628000	-0.265567000
^{5}TS2							
C	-1.899836000	3.877616000	-2.811836000				
C	-2.117639000	4.062636000	-1.446868000				
C	5.019810000	1.664154000	-0.305202000				
C	3.696576000	1.697280000	0.132410000				
C	5.826867000	0.559809000	-0.046083000				
C	-1.493395000	2.631384000	-3.289197000				
C	-1.934477000	3.003820000	-0.558444000				
C	1.095441000	1.844193000	1.379847000				
C	3.172414000	0.610279000	0.836354000				
C	-0.159532000	2.223238000	3.506134000				
C	-1.299452000	1.571841000	-2.406359000				
C	-1.524348000	1.750339000	-1.033004000				
C	5.299509000	-0.522208000	0.660535000				
C	-0.149349000	1.691600000	2.212901000				
C	-1.269653000	2.089837000	4.338434000				
C	3.981680000	-0.502007000	1.101977000				
C	-1.299585000	1.014202000	1.744992000				
C	-2.395005000	1.412888000	3.879365000				
C	-2.406939000	0.880522000	2.591031000				
C	-3.994785000	-0.086330000	-0.699989000				
C	-2.862327000	-0.612297000	-0.066120000				
C	-5.161821000	-0.844649000	-0.789233000				
C	-2.911481000	-1.908147000	0.470553000				
C	-5.208848000	-2.127648000	-0.246310000				
C	-4.082526000	-2.656590000	0.385449000				
H	-2.043874000	4.709056000	-3.505690000				
H	5.417401000	2.514481000	-0.863642000				
H	-2.436407000	5.036939000	-1.069147000				
H	3.071277000	2.558819000	-0.106879000				
H	6.860782000	0.538481000	-0.395779000				
H	-1.314625000	2.483084000	-4.356327000				
H	1.756540000	2.593584000	1.850242000				
H	-2.116567000	3.154541000	0.509766000				
H	0.861292000	2.228289000	0.371321000				
H	0.727745000	2.751987000	3.866107000				
H	-1.250237000	2.512253000	5.345226000				
H	5.919306000	-1.396874000	0.869326000				
H	-0.962311000	0.600270000	-2.779321000				
H	1.700703000	-0.001717000	2.074526000				
H	3.559316000	-1.359090000	1.634684000				
H	-3.271272000	1.298908000	4.521157000				
H	-3.967299000	0.918105000	-1.130919000				
H	-3.297250000	0.355874000	2.235520000				
H	-6.039583000	-0.428100000	-1.288690000				
H	-2.021889000	-2.333364000	0.948127000				
H	-6.123817000	-2.719888000	-0.320590000				
H	-4.110439000	-3.664179000	0.806190000				
Br	1.839227000	-0.384726000	-2.344328000				
Br	0.773481000	-2.694192000	1.290682000				
Fe	0.844129000	-0.857727000	-0.251881000				
N	1.802383000	0.563821000	1.229609000				

P	-1.288996000	0.303995000	0.054667000
C	-1.080239000	-2.279662000	-2.271814000
O	-0.829880000	-3.383966000	-2.354139000

Table S7. Cartesian coordinates (in Å) of all optimized geometries (M06-L/def2-SVP) in the catalytic transfer hydrogenation of PhCN with AB

NH_3BH_3				NH_2BH_2			
B	0.000000000	0.000000000	-0.925125000	B	0.000000000	0.000000000	-0.777281000
H	1.020345000	0.589097000	-1.238535000	H	0.000000000	1.051373000	-1.360934000
H	0.000000000	-1.178193000	-1.238535000	H	0.000000000	-1.051373000	-1.360934000
H	-1.020345000	0.589097000	-1.238535000	N	0.000000000	0.000000000	0.609563000
N	0.000000000	0.000000000	0.720232000	H	0.000000000	-0.842238000	1.170666000
H	0.000000000	0.946195000	1.099867000	H	0.000000000	0.842238000	1.170666000
H	-0.819429000	-0.473098000	1.099867000				
H	0.819429000	-0.473098000	1.099867000				
PhCN				PhCH=NH			
C	0.000000000	0.000000000	-1.966115000	H	-3.779442000	-0.062711000	-0.000273000
N	0.000000000	0.000000000	-3.131647000	H	-2.233146000	1.563328000	0.000439000
C	0.000000000	0.000000000	-0.537025000	C	-1.968357000	0.484787000	0.000140000
C	-1.215780000	0.000000000	0.167586000	N	-2.833836000	-0.451613000	-0.000222000
C	1.215780000	0.000000000	0.167586000	C	-0.523840000	0.219657000	0.000063000
C	-1.208956000	0.000000000	1.558228000	C	0.382988000	1.287862000	0.000009000
C	1.208956000	0.000000000	1.558228000	C	-0.031857000	-1.095326000	0.000148000
C	0.000000000	0.000000000	2.254501000	C	1.756130000	1.052120000	-0.000063000
H	-2.156785000	0.000000000	-0.385080000	C	1.337217000	-1.329797000	0.000020000
H	2.156785000	0.000000000	-0.385080000	C	2.234531000	-0.257309000	-0.000096000
H	-2.155185000	0.000000000	2.103018000	H	0.001148000	2.313491000	0.000055000
H	2.155185000	0.000000000	2.103018000	H	-0.753667000	-1.915258000	0.000227000
H	0.000000000	0.000000000	3.346650000	H	2.455435000	1.891241000	-0.000134000
				H	1.714853000	-2.355083000	0.000028000
				H	3.310799000	-0.445682000	-0.000105000
^{5}1H-Fe				**^{5}Int1**			
C	1.010822000	-0.196338000	4.573255000	C	1.228681000	1.864624000	4.374960000
C	1.821738000	0.744097000	3.936106000	C	0.822674000	2.915146000	3.552683000
C	-4.748350000	0.419987000	1.201232000	C	-5.843806000	-1.818601000	0.298544000
C	-3.457386000	0.881518000	0.946963000	C	-4.804051000	-0.891450000	0.303167000
C	-5.621059000	0.130864000	0.156092000	C	-6.092968000	-2.607720000	-0.822333000
C	0.263385000	-1.098096000	3.816605000	C	1.289209000	0.566495000	3.867363000
C	1.888169000	0.780678000	2.544893000	C	0.487815000	2.673328000	2.220812000
C	-0.925124000	2.173903000	0.306261000	C	-2.914045000	1.299754000	0.060956000
C	-3.031280000	1.052803000	-0.373260000	C	-3.994985000	-0.740599000	-0.830550000
C	0.632663000	3.931311000	-0.556951000	C	-2.834384000	3.585938000	-0.959183000
C	0.321431000	-1.063676000	2.423740000	C	0.946006000	0.317641000	2.540842000
C	1.141445000	-0.126974000	1.777992000	C	0.554919000	1.373181000	1.703376000
C	-5.193485000	0.308525000	-1.160717000	C	-5.280137000	-2.464229000	-1.947917000
C	0.416857000	2.588698000	-0.235020000	C	-2.138900000	2.457255000	-0.511199000
C	1.846845000	4.364814000	-1.087776000	C	-2.172147000	4.666888000	-1.537637000
C	-3.909548000	0.766579000	-1.427635000	C	-4.240506000	-1.541241000	-1.957036000
C	1.462414000	1.657767000	-0.442925000	C	-0.733041000	2.430101000	-0.651912000
C	2.867894000	3.445222000	-1.304781000	C	-0.788086000	4.630371000	-1.685803000
C	2.674095000	2.101939000	-0.984050000	C	-0.076498000	3.516629000	-1.245086000
C	3.759440000	-1.214192000	0.358057000	C	2.982956000	1.518886000	-0.230353000
C	2.708719000	-0.947708000	-0.528221000	C	1.813135000	1.090190000	-0.869256000
C	4.910785000	-1.856078000	-0.096877000	C	4.200473000	1.511582000	-0.913450000
C	2.818354000	-1.346096000	-1.869033000	C	1.884357000	0.639260000	-2.198054000
C	5.022620000	-2.231814000	-1.435137000	C	4.259736000	1.082269000	-2.237218000
C	3.975304000	-1.975214000	-2.320971000	C	3.097672000	0.648116000	-2.879314000
H	0.958378000	-0.221542000	5.664283000	H	1.487826000	2.056623000	5.418808000
H	-5.069151000	0.281877000	2.236136000	H	-6.460562000	-1.929090000	1.193632000
H	2.405657000	1.454349000	4.526361000	H	0.765185000	3.931417000	3.949513000
H	-2.784291000	1.083632000	1.782018000	H	-4.598848000	-0.313219000	1.205235000
H	-6.628283000	-0.234847000	0.363893000	H	-6.908464000	-3.333766000	-0.817848000
H	-0.378174000	-1.830735000	4.311429000	H	1.585495000	-0.262804000	4.513746000
H	-1.487463000	3.065218000	0.639648000	H	-3.947435000	1.633513000	0.265019000

H	2.522846000	1.522325000	2.049449000	H	0.174345000	3.503317000	1.580892000
H	-0.801121000	1.536351000	1.195534000	H	-2.499617000	0.971038000	1.033957000
H	-0.173475000	4.651194000	-0.387090000	H	-3.922542000	3.609971000	-0.852957000
H	1.990033000	5.419135000	-1.333617000	H	-2.740911000	5.534728000	-1.878757000
H	-5.864633000	0.081772000	-1.991830000	H	-5.455830000	-3.079103000	-2.833960000
H	-0.285442000	-1.755125000	1.828470000	H	0.949593000	-0.705982000	2.153998000
H	-1.657018000	1.889356000	-1.593627000	H	-2.673980000	0.423729000	-1.806482000
H	-3.565724000	0.882114000	-2.460138000	H	-3.592687000	-1.441908000	-2.832087000
H	3.823381000	3.769802000	-1.722714000	H	-0.258229000	5.469626000	-2.141834000
H	3.678077000	-0.924597000	1.409425000	H	2.946636000	1.856321000	0.809705000
H	3.483809000	1.387611000	-1.154267000	H	1.011184000	3.492308000	-1.357345000
H	5.725129000	-2.065472000	0.600657000	H	5.108724000	1.841064000	-0.402903000
H	1.981949000	-1.157027000	-2.552132000	H	0.980824000	0.256888000	-2.687432000
H	5.925880000	-2.735376000	-1.787387000	H	5.215120000	1.073083000	-2.767502000
H	4.053938000	-2.278412000	-3.367377000	H	3.140174000	0.298185000	-3.913777000
Br	-1.927545000	-2.470494000	-0.396024000	Br	-1.739220000	-1.907318000	1.646274000
H	-0.511322000	-0.098393000	-2.911870000	H	-1.024437000	-1.468499000	-2.167033000
Fe	-0.821824000	-0.586884000	-1.354075000	Fe	-0.846399000	-1.274341000	-0.513356000
N	-1.693482000	1.418495000	-0.689511000	N	-2.914717000	0.159957000	-0.854381000
P	1.160159000	-0.112102000	-0.050595000	P	0.190536000	0.972440000	-0.038481000
				C	2.250859000	-2.129350000	-0.320866000
				N	1.081607000	-2.079762000	-0.306078000
				C	3.665210000	-2.111383000	-0.330084000
				C	4.373330000	-2.343111000	-1.527099000
				C	4.372747000	-1.826064000	0.856961000
				C	5.760805000	-2.286230000	-1.528426000
				C	5.759757000	-1.774792000	0.836558000
				C	6.458418000	-2.002290000	-0.352177000
				H	3.820918000	-2.559205000	-2.443387000
				H	3.820251000	-1.639524000	1.780221000
				H	6.305658000	-2.466720000	-2.457616000
				H	6.303582000	-1.553241000	1.757240000
				H	7.549618000	-1.961308000	-0.360536000
^{5}TS1				**^{5}Int2**			
C	1.642765000	-4.908154000	-2.126623000	C	0.761124000	4.048960000	3.451288000
C	1.709360000	-4.948468000	-0.733839000	C	0.480152000	4.562173000	2.185846000
C	-5.527533000	1.175307000	0.056390000	C	-5.508833000	-1.616488000	0.411363000
C	-4.385911000	0.415523000	0.303376000	C	-4.505334000	-0.698925000	0.104800000
C	-5.548669000	2.542465000	0.324842000	C	-5.497595000	-2.895413000	-0.139505000
C	1.295416000	-3.722811000	-2.773388000	C	0.936328000	2.675458000	3.621848000
C	1.436897000	-3.803926000	0.012802000	C	0.381833000	3.707281000	1.088725000
C	-2.174900000	-1.124686000	1.423624000	C	-2.599527000	1.256900000	-0.857073000
C	-3.242258000	1.027707000	0.828789000	C	-3.473732000	-1.064912000	-0.764912000
C	-1.395281000	-1.963064000	3.649942000	C	-2.207884000	2.821972000	-2.765011000
C	1.009721000	-2.577204000	-2.033316000	C	0.826029000	1.816160000	2.531979000
C	1.091726000	-2.609283000	-0.632858000	C	0.560215000	2.327418000	1.252483000
C	-4.406872000	3.152525000	0.845184000	C	-4.459482000	-3.260213000	-0.998440000
C	-1.071844000	-1.559356000	2.348236000	C	-1.667180000	2.076867000	-1.710290000
C	-0.411591000	-2.354507000	4.554153000	C	-1.400471000	3.582603000	-3.607878000
C	-3.262414000	2.403495000	1.096026000	C	-3.450460000	-2.356202000	-1.310077000
C	0.284850000	-1.551386000	1.957746000	C	-0.268859000	2.107037000	-1.505340000
C	0.927813000	-2.335280000	4.170850000	C	-0.022423000	3.604127000	-3.408333000
C	1.268767000	-1.932245000	2.882730000	C	0.534696000	2.868906000	-2.364682000
C	3.449894000	-0.525448000	-0.353673000	C	3.288760000	1.318265000	0.104150000
C	2.363104000	-0.253043000	0.484628000	C	2.192485000	0.878271000	-0.648217000
C	4.641780000	0.185490000	-0.211124000	C	4.583966000	0.959616000	-0.268449000
C	2.484716000	0.758248000	1.450699000	C	2.417411000	0.088081000	-1.786721000
C	4.760865000	1.173931000	0.764132000	C	4.798650000	0.163580000	-1.391929000
C	3.677479000	1.460272000	1.595366000	C	3.711739000	-0.263517000	-2.155698000
H	1.854633000	-5.807878000	-2.709210000	H	0.836134000	4.720768000	4.309539000
H	-6.410101000	0.685864000	-0.361475000	H	-6.304870000	-1.323382000	1.099462000
H	1.972330000	-5.877923000	-0.223450000	H	0.336565000	5.636481000	2.048928000

H	-4.371914000	-0.645393000	0.049942000	H	-4.510647000	0.285008000	0.575647000
H	-6.446812000	3.130596000	0.126579000	H	-6.286452000	-3.608928000	0.106523000
H	1.230381000	-3.688978000	-3.863009000	H	1.143014000	2.266300000	4.613096000
H	-3.145254000	-1.299943000	1.918040000	H	-3.639523000	1.538566000	-1.098416000
H	1.486251000	-3.847736000	1.104120000	H	0.165289000	4.120096000	0.099597000
H	-2.184070000	-1.727508000	0.496547000	H	-2.461889000	1.466609000	0.220130000
H	-2.445072000	-1.965472000	3.955807000	H	-3.289570000	2.800426000	-2.925458000
H	-0.692144000	-2.666274000	5.562640000	H	-1.849810000	4.153882000	-4.423073000
H	-4.405245000	4.223349000	1.061251000	H	-4.429285000	-4.264043000	-1.428213000
H	0.718674000	-1.650969000	-2.537969000	H	0.929333000	0.736189000	2.674169000
H	-1.460813000	0.791335000	1.720822000	H	-2.050376000	-0.369436000	-2.008213000
H	-2.367545000	2.884204000	1.502432000	H	-2.612598000	-2.649097000	-1.948775000
H	1.708860000	-2.633914000	4.873482000	H	0.621837000	4.195880000	-4.062429000
H	3.364587000	-1.295751000	-1.124932000	H	3.132287000	1.938090000	0.991230000
H	2.321034000	-1.912191000	2.584419000	H	1.616804000	2.889781000	-2.206872000
H	5.484230000	-0.039599000	-0.869356000	H	5.431402000	1.303290000	0.329556000
H	1.635344000	0.999827000	2.099480000	H	1.568050000	-0.275095000	-2.374019000
H	5.695146000	1.730066000	0.871546000	H	5.813276000	-0.129008000	-1.671658000
H	3.755838000	2.245593000	2.350999000	H	3.871650000	-0.892839000	-3.034519000
Br	-2.308485000	-0.982749000	-2.246576000	Br	-1.692157000	-0.740322000	2.406426000
H	-0.866984000	2.133538000	-0.831464000	H	1.032256000	-3.691766000	-2.022487000
Fe	-0.805599000	0.482725000	-1.086896000	Fe	-0.713535000	-0.960199000	0.235810000
N	-2.051044000	0.296764000	1.053603000	N	-2.398197000	-0.184224000	-1.067942000
P	0.736985000	-1.053823000	0.252809000	P	0.464503000	1.139228000	-0.127516000
C	0.759943000	1.813193000	-1.477825000	C	1.042524000	-2.991772000	-1.147141000
N	0.887155000	0.904607000	-2.284939000	N	0.038502000	-2.275259000	-0.879510000
C	1.491193000	2.954697000	-0.945427000	C	2.338312000	-3.020093000	-0.426615000
C	0.967988000	3.788592000	0.048808000	C	3.383375000	-3.817042000	-0.912863000
C	2.795176000	3.175903000	-1.418474000	C	2.565138000	-2.234602000	0.713458000
C	1.735126000	4.826700000	0.568801000	C	4.627715000	-3.824821000	-0.286121000
C	3.557426000	4.215015000	-0.897381000	C	3.804647000	-2.237738000	1.339905000
C	3.031710000	5.040653000	0.098533000	C	4.841439000	-3.032598000	0.841531000
H	-0.052673000	3.605133000	0.397740000	H	3.207703000	-4.432463000	-1.801614000
H	3.193112000	2.512335000	-2.189809000	H	1.748634000	-1.606863000	1.091219000
H	1.320125000	5.475861000	1.343302000	H	5.434243000	-4.450463000	-0.676526000
H	4.571537000	4.382837000	-1.268218000	H	3.969937000	-1.614905000	2.223151000
H	3.632900000	5.857014000	0.506018000	H	5.815775000	-3.034711000	1.336481000
^{5}TS2				**^{5}Int3**			
C	3.257662000	4.009596000	-0.986811000	C	-2.072642000	-4.010025000	-1.124021000
C	2.263753000	4.396888000	-0.085699000	C	-1.062175000	-4.160338000	-0.172543000
C	5.495760000	-1.065237000	0.578987000	C	-4.878286000	-0.542410000	-0.258186000
C	4.301755000	-0.517591000	1.048755000	C	-3.767837000	-0.490325000	0.580048000
C	5.519648000	-2.309756000	-0.044963000	C	-5.073044000	0.401034000	-1.267468000
C	3.159927000	2.789126000	-1.653264000	C	-2.213785000	-2.803475000	-1.807184000
C	1.174415000	3.562453000	0.151991000	C	-0.191613000	-3.105884000	0.093489000
C	1.851376000	0.512949000	2.073251000	C	-1.343970000	-0.380654000	2.137287000
C	3.086875000	-1.214375000	0.899073000	C	-2.797039000	0.527117000	0.427301000
C	0.181985000	0.912873000	3.895965000	C	0.463493000	-0.482282000	3.869815000
C	2.070687000	1.951081000	-1.418825000	C	-1.346410000	-1.745554000	-1.541112000
C	1.068741000	2.334324000	-0.517432000	C	-0.323102000	-1.890799000	-0.595404000
C	4.320611000	-3.013308000	-0.193409000	C	-4.144988000	1.437444000	-1.406335000
C	0.468429000	0.912146000	2.527467000	C	0.112334000	-0.469715000	2.515767000
C	-1.079842000	1.249459000	4.384011000	C	1.784823000	-0.628020000	4.285065000
C	3.126766000	-2.481037000	0.271277000	C	-3.045612000	1.512746000	-0.563914000
C	-0.562269000	1.280563000	1.627398000	C	1.143523000	-0.611702000	1.551254000
C	-2.089790000	1.600112000	3.493761000	C	2.793171000	-0.766866000	3.335406000
C	-1.828430000	1.615542000	2.124552000	C	2.471223000	-0.756219000	1.980680000
C	-1.886780000	3.149700000	-1.390873000	C	2.726576000	-1.994551000	-1.584478000
C	-1.769655000	1.821535000	-0.962207000	C	2.324420000	-0.744591000	-1.096614000
C	-3.068882000	3.592236000	-1.983072000	C	3.953588000	-2.128922000	-2.232653000
C	-2.844954000	0.941646000	-1.154572000	C	3.157573000	0.369802000	-1.280396000
C	-4.141452000	2.717131000	-2.151324000	C	4.786125000	-1.021912000	-2.395572000

C	-4.027765000	1.390191000	-1.735777000
H	4.116359000	4.661446000	-1.163704000
H	6.423887000	-0.501169000	0.705092000
H	2.343796000	5.350353000	0.441666000
H	4.317847000	0.464686000	1.524677000
H	6.458151000	-2.729964000	-0.411703000
H	3.940734000	2.478546000	-2.350722000
H	2.492490000	0.404250000	2.969688000
H	0.408298000	3.854918000	0.877395000
H	2.306732000	1.343203000	1.496673000
H	0.974720000	0.630087000	4.594490000
H	-1.270962000	1.233142000	5.459378000
H	4.315364000	-3.992794000	-0.677638000
H	2.003696000	0.982326000	-1.927614000
H	0.908689000	-1.564513000	1.673781000
H	2.199107000	-3.054789000	0.159997000
H	-3.084161000	1.866726000	3.859072000
H	-1.050010000	3.842546000	-1.269443000
H	-2.627528000	1.891332000	1.431447000
H	-3.150237000	4.628961000	-2.317661000
H	-2.749031000	-0.104804000	-0.848058000
H	-5.065148000	3.068043000	-2.617252000
H	-4.858295000	0.694347000	-1.875654000
Br	0.604078000	-1.696015000	-2.694264000
H	-1.439357000	-2.360914000	2.925049000
Fe	0.457341000	-1.132463000	-0.406795000
N	1.848034000	-0.716518000	1.303614000
P	-0.271772000	1.145475000	-0.176175000
C	-1.343018000	-2.274709000	1.819834000
N	-0.218765000	-2.063374000	1.269700000
C	-2.609594000	-2.379545000	1.074311000
C	-3.833019000	-2.150456000	1.719670000
C	-2.606387000	-2.659873000	-0.302455000
C	-5.026085000	-2.169398000	1.000933000
C	-3.799352000	-2.697729000	-1.016145000
C	-5.011030000	-2.445541000	-0.367262000
H	-3.837515000	-1.936068000	2.792951000
H	-1.654314000	-2.863186000	-0.804576000
H	-5.973300000	-1.973817000	1.508981000
H	-3.784382000	-2.924858000	-2.084823000
H	-5.948049000	-2.472324000	-0.929042000

C	4.386894000	0.227219000	-1.918770000
H	-2.759136000	-4.835695000	-1.325289000
H	-5.607669000	-1.345343000	-0.118858000
H	-0.955311000	-5.102858000	0.369510000
H	-3.646955000	-1.255619000	1.348755000
H	-5.947842000	0.347811000	-1.918280000
H	-3.016436000	-2.672775000	-2.536372000
H	-1.941613000	-0.199576000	3.052207000
H	0.591316000	-3.220016000	0.850367000
H	-1.654538000	-1.390920000	1.790905000
H	-0.329580000	-0.370618000	4.614570000
H	2.025001000	-0.627529000	5.350519000
H	-4.293700000	2.211358000	-2.163410000
H	-1.481485000	-0.788721000	-2.054953000
H	-2.369912000	2.378940000	-0.636271000
H	3.834260000	-0.882255000	3.644537000
H	2.077878000	-2.866320000	-1.460282000
H	3.269236000	-0.865168000	1.241881000
H	4.260666000	-3.105909000	-2.612975000
H	2.830860000	1.354093000	-0.926237000
H	5.746594000	-1.131321000	-2.904420000
H	5.030031000	1.099330000	-2.055357000
Br	0.709640000	3.662383000	-0.544549000
Fe	-0.286495000	1.665255000	0.154331000
N	-1.615051000	0.608982000	1.127409000
P	0.746382000	-0.461367000	-0.238970000

^{5}TS3			
C	2.392773000	4.966595000	0.398858000
C	1.293786000	4.806056000	1.244217000
C	5.210600000	-1.313025000	0.454388000
C	4.003128000	-0.793109000	0.917986000
C	5.295063000	-2.630016000	0.009253000
C	2.666677000	4.010433000	-0.578550000
C	0.466787000	3.692885000	1.110547000
C	1.502139000	0.061319000	2.175856000
C	2.860219000	-1.600654000	0.930241000
C	-0.364810000	0.024444000	3.841526000
C	1.844978000	2.892064000	-0.714712000
C	0.733506000	2.731019000	0.124832000
C	4.155717000	-3.436447000	0.033815000
C	0.071945000	0.342423000	2.554540000
C	-1.694463000	0.197634000	4.220066000
C	2.944989000	-2.931496000	0.491681000
C	-0.859757000	0.863403000	1.627338000
C	-2.612554000	0.695641000	3.301094000
C	-2.195891000	1.025976000	2.012341000
C	-2.182194000	3.121000000	-1.089614000

^{5}Add1			
C	-0.205523000	-2.373424000	4.112029000
C	-1.039385000	-2.985896000	3.174993000
C	4.860683000	-1.323416000	1.177680000
C	3.609013000	-1.523598000	0.595468000
C	5.547861000	-0.123169000	1.018600000
C	0.296060000	-1.094728000	3.871469000
C	-1.372287000	-2.320501000	1.997191000
C	1.159526000	-1.958130000	-0.692553000
C	2.997231000	-0.509851000	-0.176469000
C	-0.202291000	-2.999174000	-2.525000000
C	-0.033444000	-0.425162000	2.694421000
C	-0.876489000	-1.031658000	1.752621000
C	4.956621000	0.889994000	0.257611000
C	-0.138578000	-2.111378000	-1.445358000
C	-1.377256000	-3.188508000	-3.253234000
C	3.714496000	0.701936000	-0.329667000
C	-1.315108000	-1.407478000	-1.086967000
C	-2.525292000	-2.484606000	-2.901149000
C	-2.490479000	-1.599820000	-1.824491000
C	-3.880630000	-0.002095000	1.109901000

C	-1.804260000	1.781241000	-0.942132000	C	-2.860378000	0.589871000	0.352991000
C	-3.375998000	3.440614000	-1.736090000	C	-5.143676000	0.583464000	1.161042000
C	-2.624862000	0.771488000	-1.464965000	C	-3.116213000	1.786207000	-0.331830000
C	-4.199843000	2.430413000	-2.231783000	C	-5.397003000	1.764102000	0.461460000
C	-3.823232000	1.093489000	-2.095097000	C	-4.382554000	2.365649000	-0.282295000
H	3.041944000	5.838552000	0.507944000	H	0.061022000	-2.900813000	5.030939000
H	6.095753000	-0.673109000	0.439429000	H	5.301599000	-2.128357000	1.772392000
H	1.081437000	5.551143000	2.014546000	H	-1.425371000	-3.991223000	3.359581000
H	3.953591000	0.245913000	1.249905000	H	3.101404000	-2.474868000	0.761772000
H	6.243678000	-3.027921000	-0.355977000	H	6.526252000	0.025316000	1.479782000
H	3.530551000	4.129067000	-1.236375000	H	0.958515000	-0.618594000	4.597460000
H	2.100952000	-0.120436000	3.086053000	H	1.865067000	-2.724379000	-1.072675000
H	-0.390117000	3.565490000	1.779686000	H	-2.006388000	-2.811628000	1.251769000
H	1.954192000	0.935533000	1.678209000	H	0.989199000	-2.246547000	0.367337000
H	0.352733000	-0.391843000	4.553578000	H	0.698942000	-3.559192000	-2.795268000
H	-2.012309000	-0.069010000	5.230178000	H	-1.393663000	-3.888072000	-4.092200000
H	4.209092000	-4.472096000	-0.308842000	H	5.471592000	1.843877000	0.118209000
H	2.071044000	2.128440000	-1.467933000	H	0.376858000	0.570502000	2.491814000
H	0.945879000	-1.850818000	1.634835000	H	3.270725000	1.510540000	-0.921028000
H	2.046568000	-3.556090000	0.511218000	H	-3.452877000	-2.622733000	-3.461067000
H	-3.659699000	0.829227000	3.582157000	H	-3.685617000	-0.923495000	1.666334000
H	-1.543549000	3.919085000	-0.701127000	H	-3.394009000	-1.046430000	-1.554312000
H	-2.924774000	1.415698000	1.296944000	H	-5.934194000	0.117260000	1.753676000
H	-3.664264000	4.487952000	-1.851985000	H	-2.309529000	2.270833000	-0.891122000
H	-2.313497000	-0.274260000	-1.368084000	H	-6.387602000	2.222664000	0.506017000
H	-5.135177000	2.686675000	-2.734702000	H	-4.572302000	3.298835000	-0.816993000
H	-4.457852000	0.296027000	-2.488570000	Br	0.727679000	3.133631000	0.525028000
Br	2.114600000	-0.561148000	-2.673599000	Fe	0.673383000	1.105839000	-0.714544000
H	-0.384115000	-2.046864000	-0.382799000	N	1.754285000	-0.634848000	-0.794275000
Fe	0.777819000	-0.807464000	-0.743161000	P	-1.191770000	-0.120207000	0.206053000
N	1.579358000	-1.097294000	1.276490000	B	0.889291000	1.438805000	-3.123449000
P	-0.296511000	1.235339000	-0.078770000	H	-0.114535000	1.047647000	-2.488181000
C	-1.207490000	-2.582729000	0.833958000	N	1.681044000	0.111915000	-3.540044000
N	-0.628918000	-2.750463000	1.869301000	H	1.124002000	-0.523516000	-4.110577000
C	-2.525269000	-2.666691000	0.205334000	H	2.540398000	0.310869000	-4.050061000
C	-2.694053000	-2.826111000	-1.175028000	H	1.917510000	-0.372666000	-2.636431000
C	-3.657259000	-2.584407000	1.032192000	H	0.509358000	2.047626000	-4.095467000
C	-3.971733000	-2.910831000	-1.722063000	H	1.660270000	2.095443000	-2.433613000
C	-4.932328000	-2.644049000	0.478137000				
C	-5.093780000	-2.810862000	-0.898518000				
H	-1.806109000	-2.874165000	-1.812122000				
H	-3.513073000	-2.462834000	2.108145000				
H	-4.092702000	-3.049192000	-2.799226000				
H	-5.808649000	-2.563924000	1.125767000				
H	-6.096417000	-2.863998000	-1.329579000				
^{5}TS4				**^{5}Int4**			
C	0.389509000	0.937540000	4.662516000	C	0.852339000	-2.262230000	4.157614000
C	1.206762000	1.802106000	3.932486000	C	1.357417000	-0.962459000	4.134405000
C	-4.684700000	0.756288000	1.683898000	C	-3.949750000	-1.231531000	1.560684000
C	-3.470779000	1.175241000	1.138211000	C	-2.835425000	-0.411092000	1.408054000
C	-5.456938000	-0.216161000	1.055606000	C	-5.115521000	-0.987290000	0.836768000
C	-0.161649000	-0.187182000	4.049314000	C	0.441091000	-2.870422000	2.970609000
C	1.474431000	1.542407000	2.590182000	C	1.456591000	-0.270834000	2.927535000
C	-1.101142000	2.122323000	-0.052366000	C	-0.937988000	1.904594000	1.415172000
C	-2.992245000	0.616047000	-0.062058000	C	-2.878406000	0.674458000	0.520701000
C	0.303191000	3.681529000	-1.433368000	C	0.597649000	3.874824000	1.202406000
C	0.100113000	-0.450359000	2.705773000	C	0.527082000	-2.180901000	1.763595000
C	0.926300000	0.410459000	1.969342000	C	1.041461000	-0.874903000	1.733011000
C	-4.994832000	-0.773399000	-0.139147000	C	-5.160273000	0.094140000	-0.043766000
C	0.203301000	2.486899000	-0.713972000	C	0.384366000	2.506294000	1.020378000
C	1.492556000	4.064040000	-2.053403000	C	1.802787000	4.477074000	0.843585000
C	-3.786960000	-0.367441000	-0.689219000	C	-4.055470000	0.924794000	-0.199916000

C	1.353107000	1.667136000	-0.607073000	C	1.427567000	1.721187000	0.472904000
C	2.614933000	3.246724000	-1.955127000	C	2.820346000	3.705089000	0.290914000
C	2.542293000	2.054308000	-1.236472000	C	2.630765000	2.336329000	0.106010000
C	3.849181000	-0.511135000	0.970896000	C	3.763583000	-0.986560000	0.085781000
C	2.802417000	-0.759029000	0.072940000	C	2.616275000	-0.683246000	-0.661230000
C	5.081027000	-1.139149000	0.799783000	C	4.907589000	-1.460661000	-0.550970000
C	3.000399000	-1.658577000	-0.983764000	C	2.624750000	-0.879683000	-2.048150000
C	5.276668000	-2.019626000	-0.264931000	C	4.913429000	-1.641365000	-1.935274000
C	4.235511000	-2.279888000	-1.155158000	C	3.772420000	-1.352952000	-2.682137000
H	0.176000000	1.146851000	5.713307000	H	0.775487000	-2.801721000	5.104376000
H	-5.027207000	1.204977000	2.620083000	H	-3.896859000	-2.080577000	2.246046000
H	1.633295000	2.687124000	4.410518000	H	1.679701000	-0.482931000	5.061685000
H	-2.895986000	1.938507000	1.664393000	H	-1.919134000	-0.637508000	1.960163000
H	-6.405102000	-0.539731000	1.489474000	H	-5.983749000	-1.638638000	0.953923000
H	-0.809898000	-0.859493000	4.615495000	H	0.040267000	-3.886487000	2.984770000
H	-1.765822000	3.007917000	-0.068618000	H	-1.518439000	2.643729000	1.995655000
H	2.100098000	2.231610000	2.013695000	H	1.854497000	0.749024000	2.914456000
H	-0.911838000	1.926134000	1.019726000	H	-0.771555000	1.054398000	2.094070000
H	-0.579347000	4.324507000	-1.507932000	H	-0.207756000	4.480540000	1.627627000
H	1.539522000	5.000934000	-2.613048000	H	1.941618000	5.550277000	0.991113000
H	-5.580878000	-1.541232000	-0.649820000	H	-6.067221000	0.295596000	-0.618282000
H	-0.350026000	-1.320377000	2.214791000	H	0.175850000	-2.646048000	0.835677000
H	-3.433839000	-0.824942000	-1.617577000	H	-4.083562000	1.766779000	-0.895944000
H	3.552057000	3.534130000	-2.436864000	H	3.767314000	4.165086000	0.000204000
H	3.699526000	0.172644000	1.811546000	H	3.758874000	-0.850868000	1.171807000
H	3.425402000	1.413473000	-1.165719000	H	3.432958000	1.737163000	-0.332452000
H	5.892357000	-0.942571000	1.504408000	H	5.798783000	-1.694562000	0.035965000
H	2.172787000	-1.880647000	-1.665349000	H	1.720624000	-0.673730000	-2.630026000
H	6.242686000	-2.513062000	-0.394497000	H	5.810653000	-2.017804000	-2.432101000
H	4.379580000	-2.980264000	-1.980585000	H	3.769303000	-1.506228000	-3.763342000
Br	-0.873802000	-3.068110000	-0.334393000	Br	-1.232460000	-2.208258000	-1.811090000
Fe	-0.675972000	-0.834401000	-1.095852000	Fe	-0.875799000	0.083449000	-1.314621000
N	-1.772611000	0.979179000	-0.667275000	N	-1.717322000	1.447975000	0.259457000
P	1.171084000	0.036748000	0.201363000	P	1.096293000	-0.039728000	0.109365000
B	-0.979360000	-0.218458000	-3.362706000	B	-1.281160000	1.843376000	-2.733107000
H	0.087481000	-0.083689000	-2.699459000	H	-0.129732000	1.462610000	-2.322952000
N	-1.759777000	1.128823000	-3.244144000	N	-1.645290000	3.134537000	-1.991540000
H	-1.244650000	1.919655000	-3.627448000	H	-0.891920000	3.818596000	-2.046785000
H	-2.654140000	1.102958000	-3.730692000	H	-2.438332000	3.590731000	-2.439558000
H	-1.888894000	1.197191000	-1.950560000	H	-1.891512000	2.252344000	-0.395890000
H	-0.665159000	-0.572687000	-4.477259000	H	-1.212447000	1.832787000	-3.950227000
H	-1.687113000	-1.093179000	-2.832406000	H	-2.135178000	0.962329000	-2.404164000
^{5}TS5							
C	1.995242000	2.495473000	3.788933000				
C	2.469421000	2.976948000	2.568524000				
C	-4.047750000	1.211545000	1.814734000				
C	-2.854360000	1.165818000	1.101127000				
C	-5.273255000	1.230678000	1.148104000				
C	1.331294000	1.269656000	3.841179000				
C	2.286248000	2.233806000	1.403335000				
C	-0.721430000	2.170872000	-0.812274000				
C	-2.880893000	1.144327000	-0.297215000				
C	0.626975000	2.938056000	-2.772171000				
C	1.136245000	0.526604000	2.678227000				
C	1.618588000	1.000751000	1.448155000				
C	-5.298471000	1.205368000	-0.245522000				
C	0.504869000	2.076493000	-1.678605000				
C	1.733292000	2.883740000	-3.619030000				
C	-4.107478000	1.170607000	-0.967548000				
C	1.535804000	1.142196000	-1.423641000				
C	2.739402000	1.954645000	-3.373409000				
C	2.638461000	1.090938000	-2.283073000				

C	3.964024000	-0.885043000	0.588209000
C	2.778611000	-1.123756000	-0.119349000
C	5.037135000	-1.767471000	0.472548000
C	2.677260000	-2.263031000	-0.931715000
C	4.936526000	-2.890194000	-0.348820000
C	3.756079000	-3.135676000	-1.051036000
H	2.141047000	3.079295000	4.700857000
H	-4.017415000	1.212061000	2.906211000
H	2.990513000	3.936376000	2.523145000
H	-1.898305000	1.099868000	1.627805000
H	-6.206318000	1.259064000	1.714292000
H	0.953837000	0.890331000	4.793633000
H	-1.237158000	3.127827000	-1.008245000
H	2.667729000	2.614464000	0.450775000
H	-0.451695000	2.180750000	0.255030000
H	-0.165653000	3.668475000	-2.961294000
H	1.805101000	3.565650000	-4.469045000
H	-6.252453000	1.221586000	-0.778113000
H	0.593326000	-0.424713000	2.713503000
H	-4.123380000	1.149523000	-2.061768000
H	3.611004000	1.899236000	-4.029460000
H	4.049293000	-0.007341000	1.235356000
H	3.433719000	0.364437000	-2.096352000
H	5.957544000	-1.576903000	1.029635000
H	1.741054000	-2.452447000	-1.469328000
H	5.778854000	-3.580674000	-0.435676000
H	3.669483000	-4.019249000	-1.687543000
Br	-1.360053000	-2.153483000	1.463591000
Fe	-0.835633000	-1.054943000	-0.624152000
N	-1.656976000	1.043178000	-1.026044000
P	1.320289000	-0.031847000	-0.032911000
B	-3.250297000	-2.534070000	-1.635315000
H	-0.421719000	-1.429254000	-2.199952000
N	-4.486434000	-2.668376000	-2.250375000
H	-4.822381000	-3.539451000	-2.640288000
H	-5.163083000	-1.919274000	-2.317930000
H	-1.858169000	0.973444000	-2.024306000
H	-2.504240000	-3.468147000	-1.553796000
H	-2.982238000	-1.440190000	-1.187732000

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