Supporting Information

for

Catalytic reduction of N_2 to NH_3 by an Fe-N_2 complex featuring a C-atom anchor.

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Synthesis of *o*-nitrotriphenylmethane: (*Note:* The synthesis of this species, a precursor to *o*-iodotriphenylmethane, has been previously reported;[1] here we report the synthesis again in order to detail slight modifications to the workup and purification procedures that facilitate its synthesis. The syntheses of *o*-aminotriphenylmethane and *o*-iodotriphenylmethane have not been substantially modified from the previously reported procedures.) Aluminum chloride (30.36 g, 0.228 mol) was suspended in 100 mL of benzene and *o*-nitrobenzaldehyde (15 g, 0.099 mol) was added as a solid in portions over 15 minutes while stirring at room temperature. The reaction mixture was heated to reflux for 6 hours, then cooled to room temperature and poured over ice (300 mL). The mixture was diluted with another 100 mL of benzene and 100 mL of water. The aqueous layer was removed and washed twice with benzene (100 mL); the dark brown organic washings were then combined and washed repeatedly with concentrated H_2SO_4 until the color was light yellow-orange. The organic layer was then washed with water (100 mL) and brine (2 x 50 mL), dried over magnesium sulfate, filtered, and concentrated. The off-white oily residue was recrystallized from methanol to give a white crystalline solid which was collected atop a glass frit and washed with cold methanol (15.6 g, 54%). ^{1}H NMR ($CDCl_3$, 300 MHz, 298 K, δ): 7.89 (d, J = 8 Hz, 1H), 7.49 (t, J = 8 Hz, 1H), 7.39 (t, J = 8 Hz, 1H), 7.34-7.23 (m, 6H), 7.14-7.08 (m, 4H) ppm. ^{13}C NMR ($CDCl_3$, 75.4 MHz, 298 K, δ): 149.77 (s), 141.95 (s), 138.13 (s), 132.41 (s), 132.04 (s), 129.51 (s), 128.54 (s), 127.49 (s), 126.85 (s), 124.76 (s) ppm.

[1] Kliegl, A. *Ber. Deutsch. Chem. Ges.* **1908**, *40*, 4937-42.

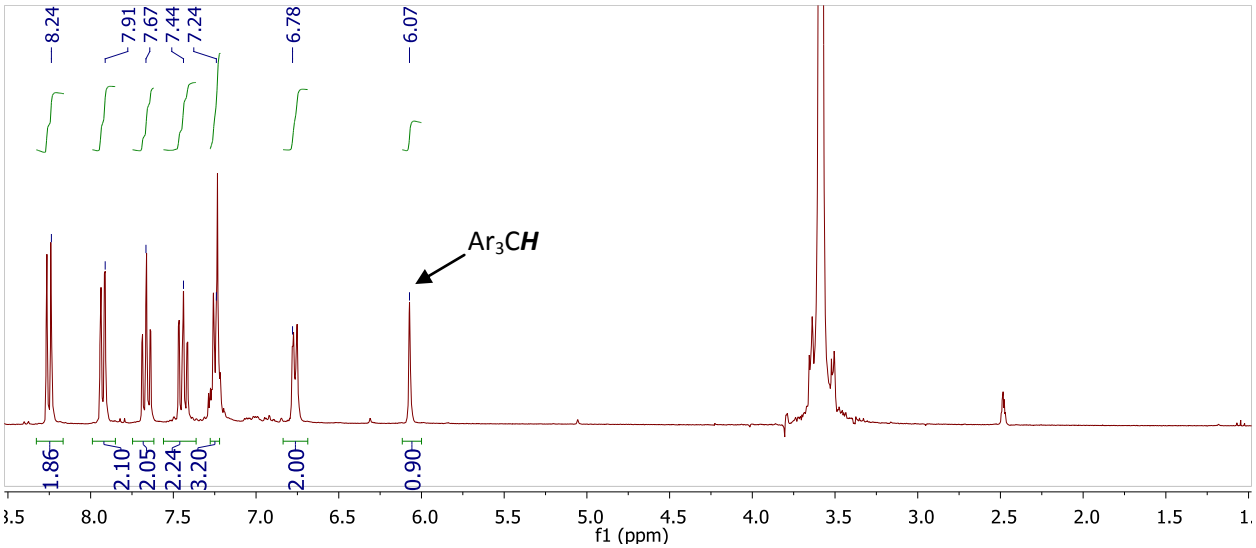

Figure S1. ^{1}H NMR of **2** (DMSO-d_6, 300 MHz)

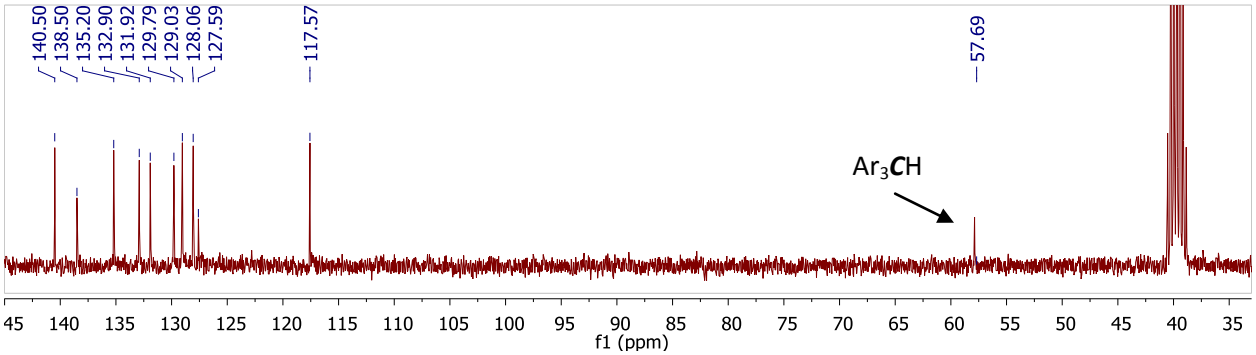

Figure S2. ^{13}C NMR of **2** (DMSO-d_6, 75 MHz)

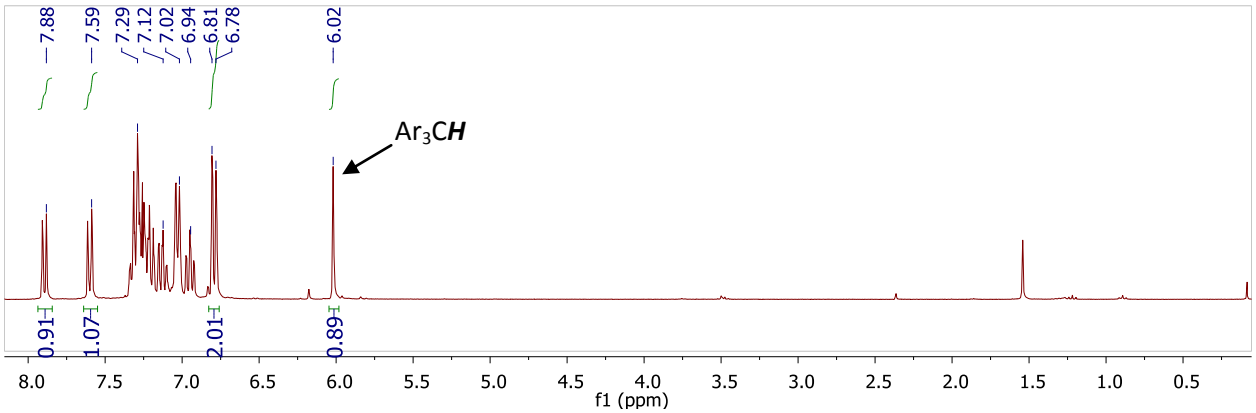

Figure S3. ^{1}H NMR of **3** ($CDCl_3$, 300 MHz)

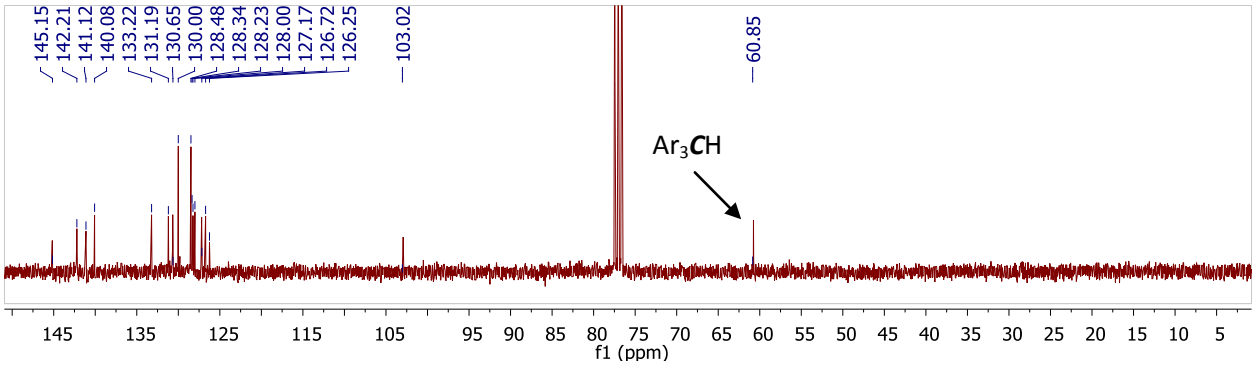

Figure S4. ^{13}C NMR of **3** ($CDCl_3$, 75 MHz)

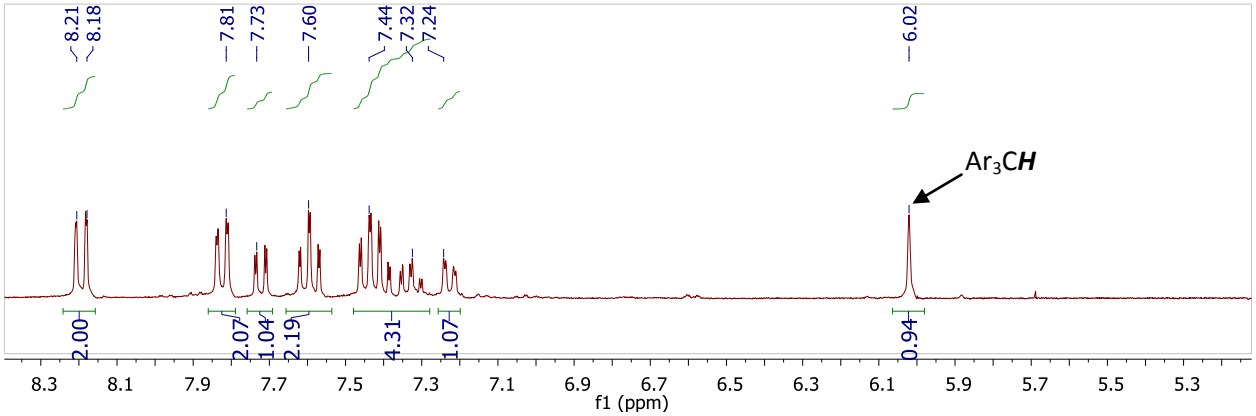

Figure S5. ^{1}H NMR of **4** (aromatic region) in DMSO-d_6 (300 MHz)

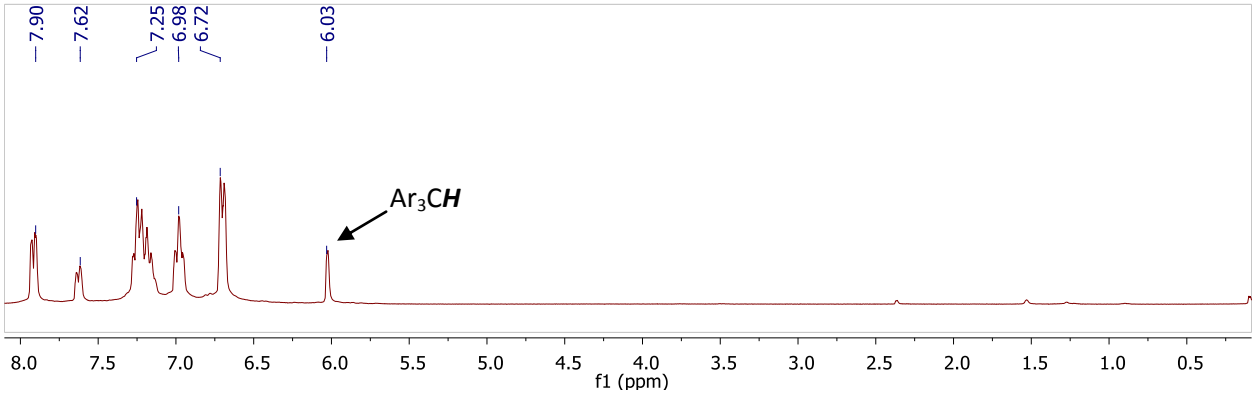

Figure S6. ^{1}H NMR of **5** ($CDCl_3$, 300 MHz)

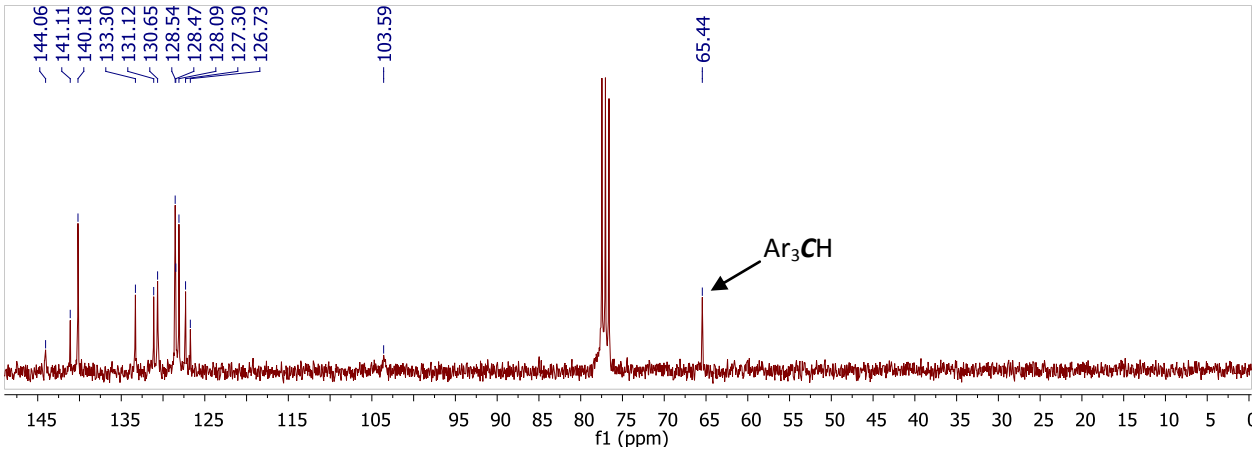

Figure S7. ^{13}C NMR of **5** ($CDCl_3$, 75 MHz)

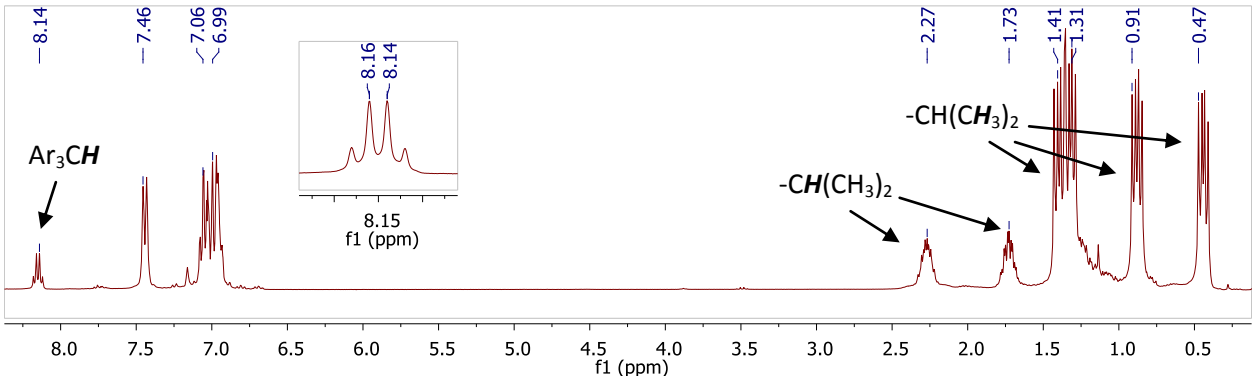

Figure S8. ^{1}H NMR of **1** (C_6D_6, 300 MHz) with inset showing coupling to central methine proton.

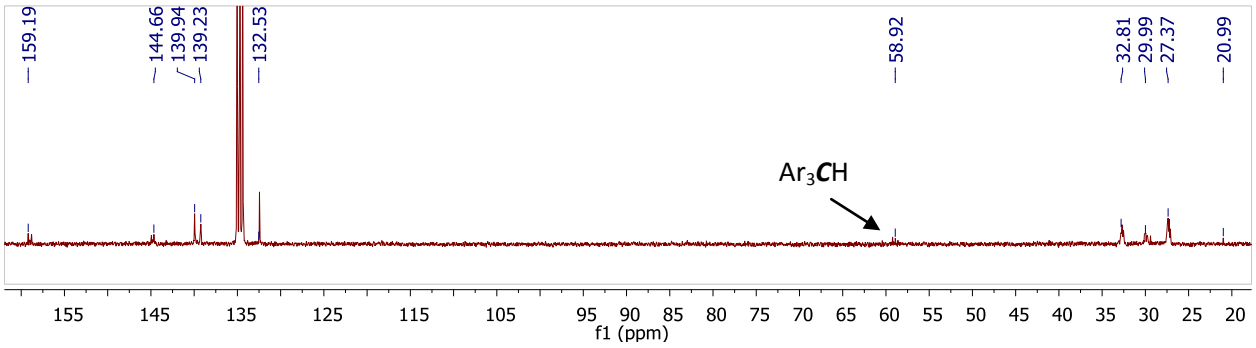

Figure S9. ^{13}C NMR of **1** (C_6D_6, 75 MHz)

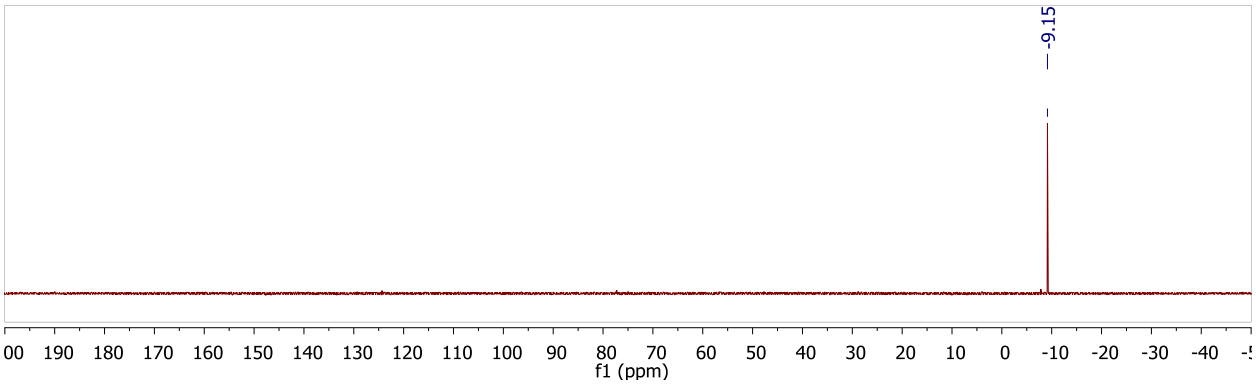

Figure S10. ^{31}P NMR of **1** (C_6D_6, 300 MHz)

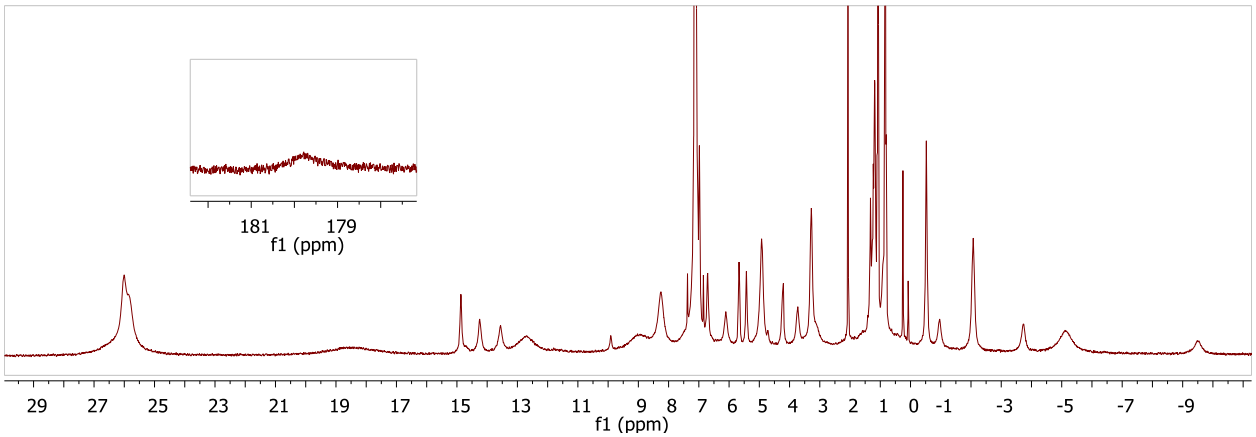

Figure S11. ^{1}H NMR of **6** (C_6D_6) with inset showing peak at 180 ppm. No other peaks appear outside the range depicted.

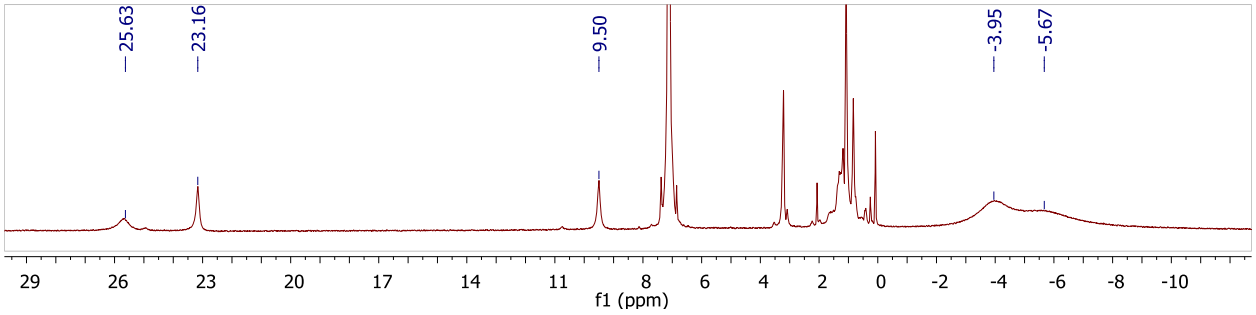

Figure S12. ^{1}H NMR of **7** (C_6D_6, 300 MHz), unpurified, generated by reduction of **6** with sodium amalgam in benzene.

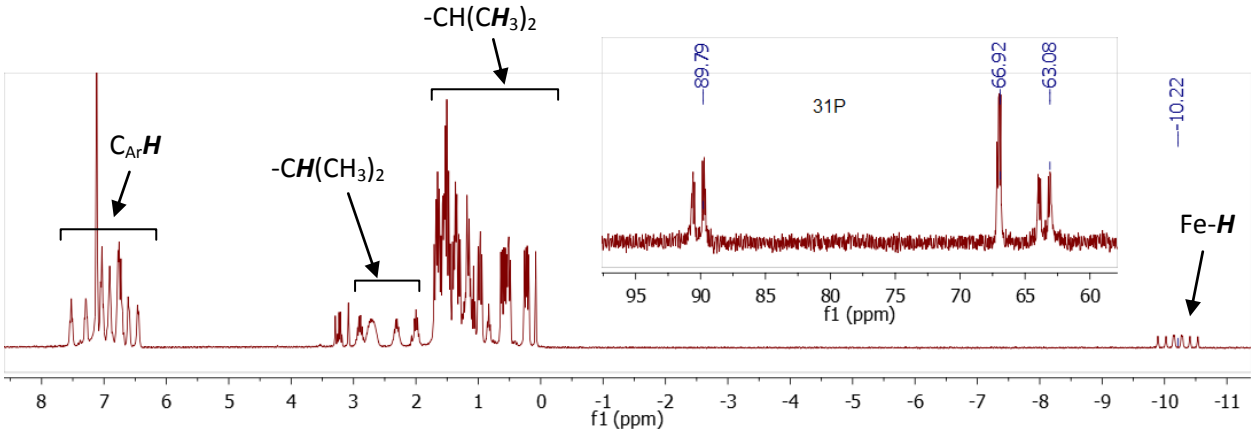

Figure S13. ^{1}H NMR of **9** (C_6D_6, 300 MHz) with inset showing ^{31}P NMR.

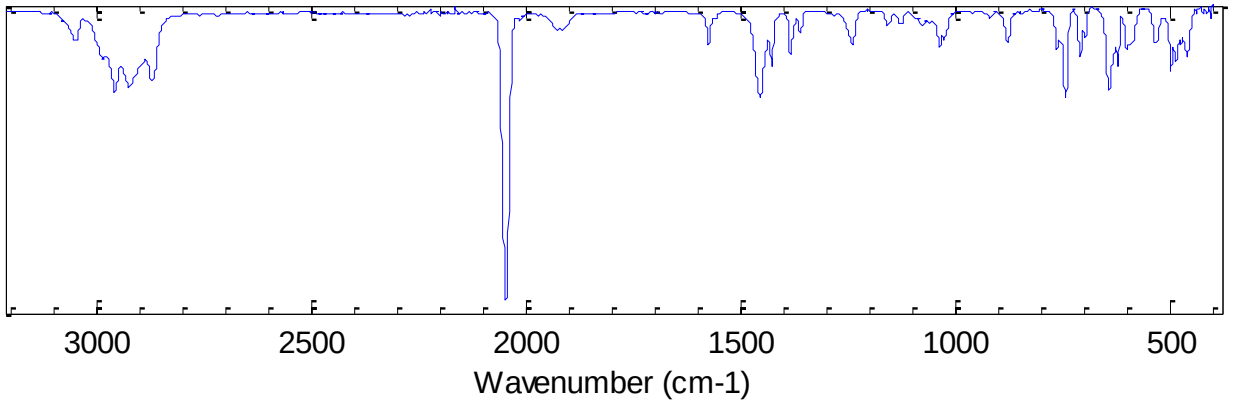

Figure S14. IR (thin film deposited from benzene) of **9**; ν(NN) = 2046 cm^{-1}; ν(FeH) = 1920 cm^{-1}

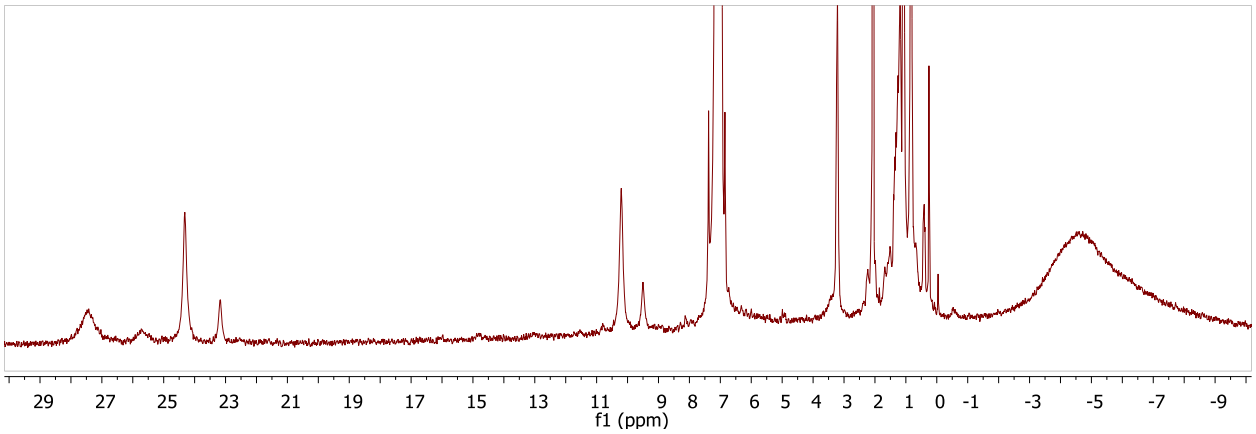

Figure S15. ^{1}H NMR of **8** (C_6D_6, 300 MHz), unpurified, generated by reduction of CP3HFeBr2 with isopropyl magnesium chloride in toluene. For unknown reasons the reaction appears to yield a mixture of two closely related paramagnetic species.

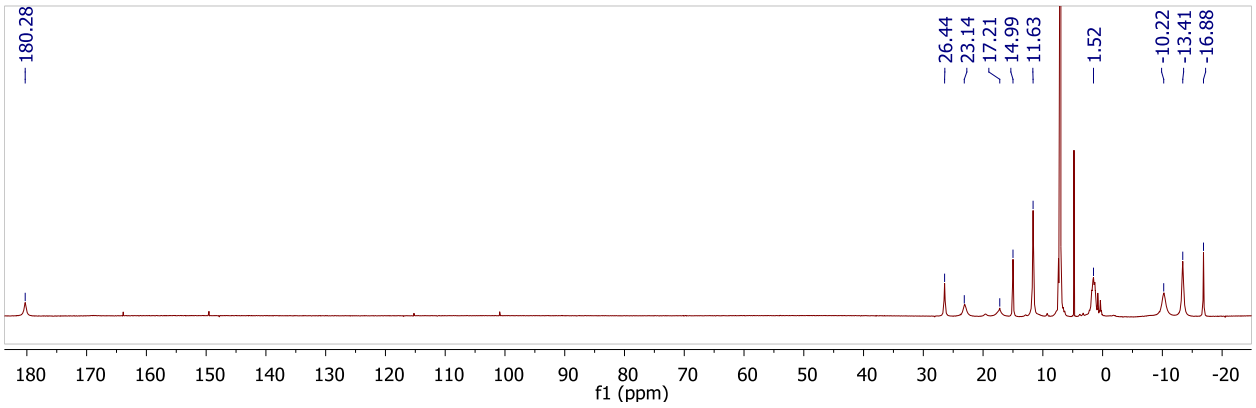

Figure S16. ^{1}H NMR of **10** (C_6D_6, 300 MHz)

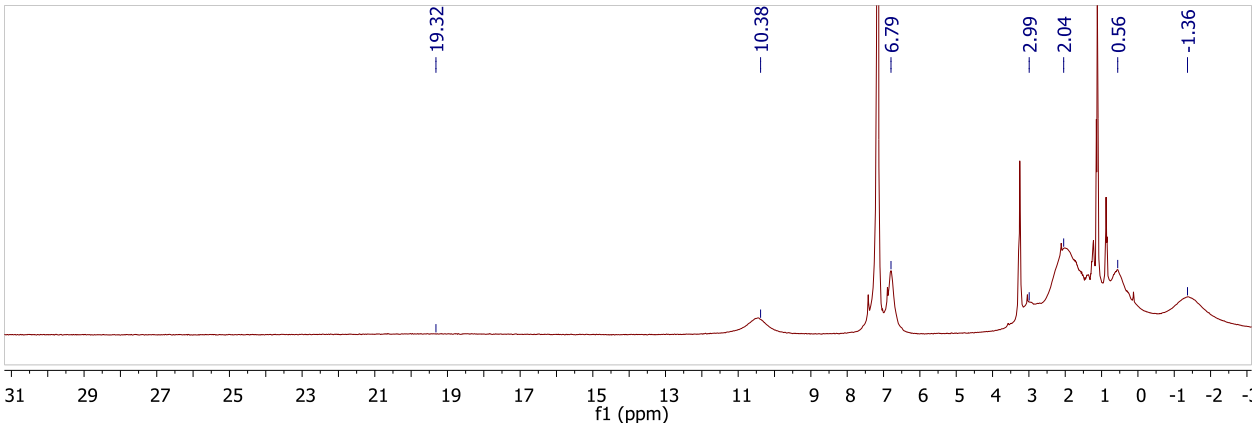

Figure S17. ^{1}H NMR of **11** (C_6D_6, 300 MHz).

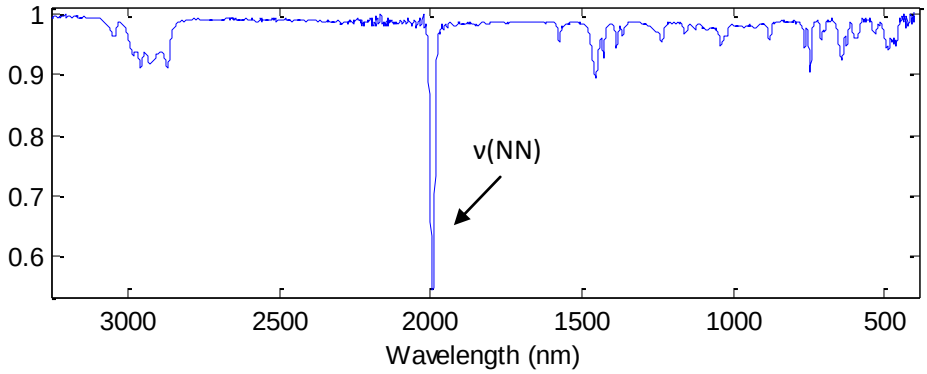

Figure S18. IR (thin film deposited from benzene) of **11**. ν(NN) = 1992 cm^{-1}.

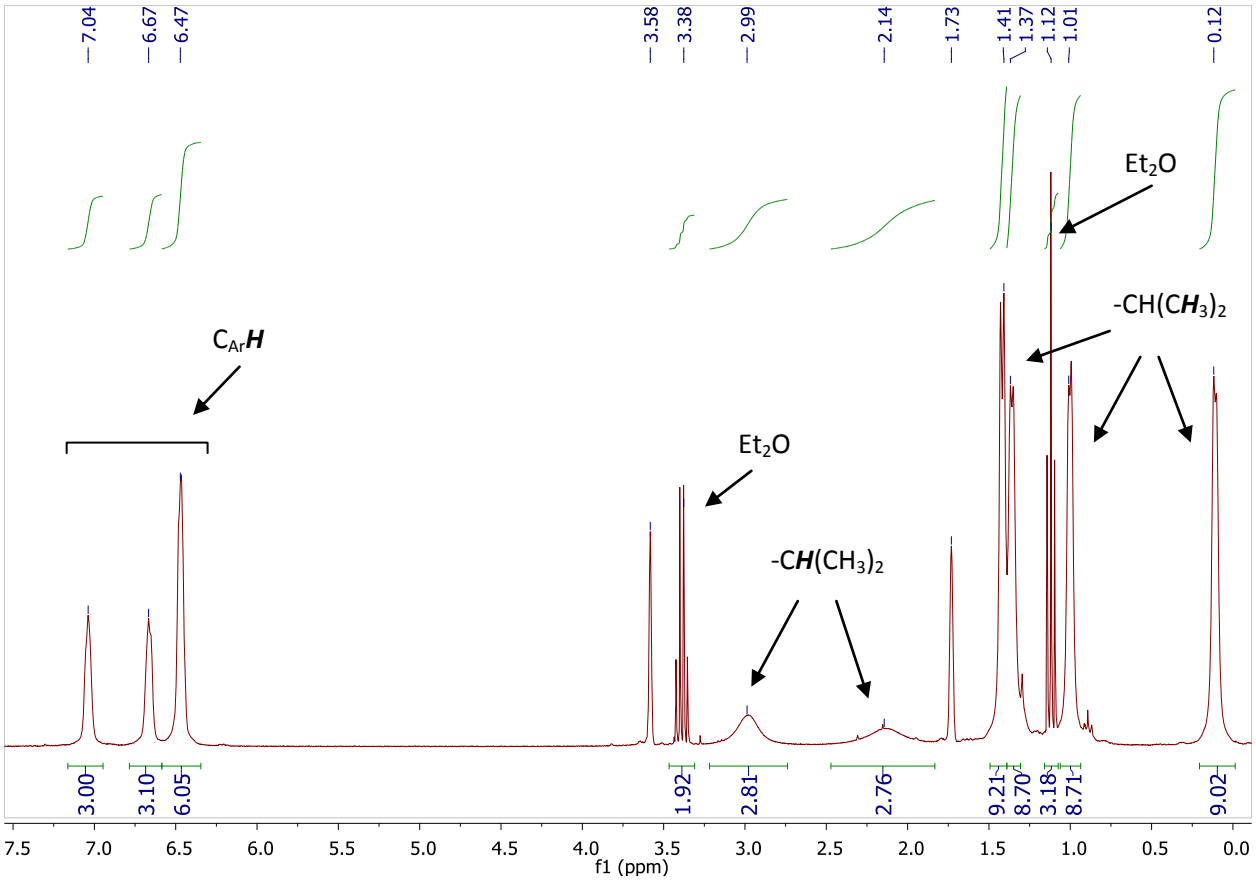

Figure S19. ^{1}H NMR of **12** (d^{8}-THF, 300 MHz).

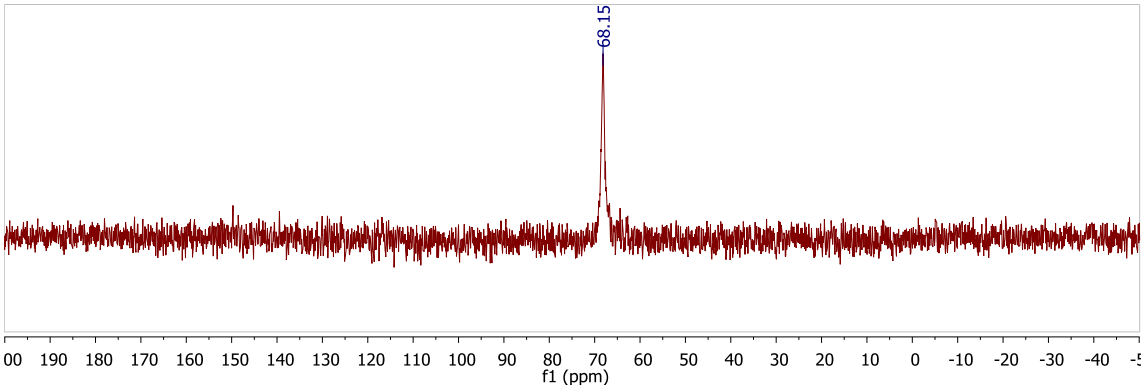

Figure S20. ^{31}P NMR of **12**.

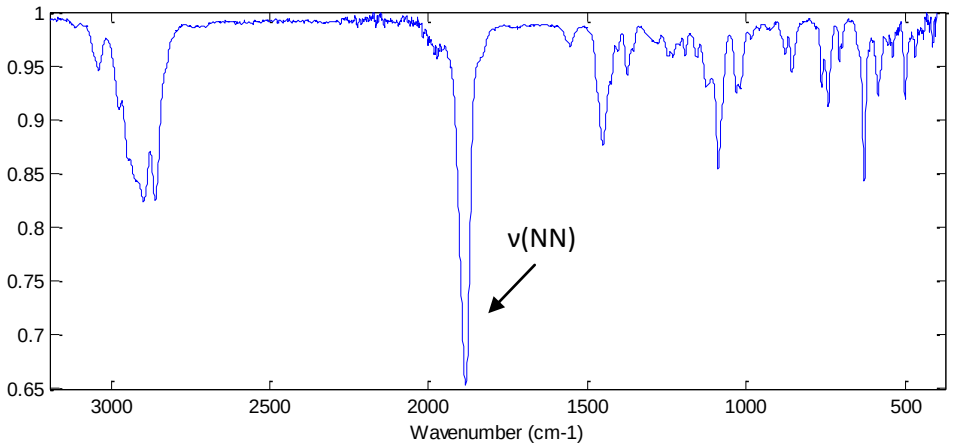

Figure S21. IR spectrum of **12** as a thin film deposited from dimethoxyethane.

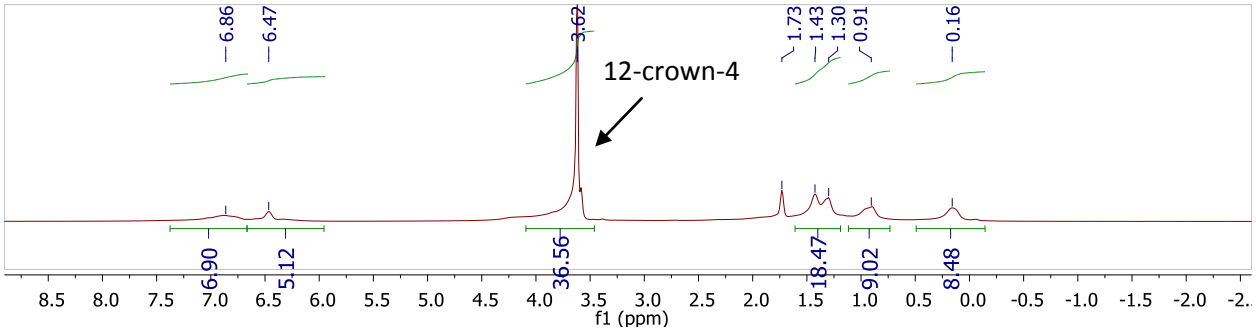

Figure S22. ^{1}H NMR of **12**[K(12-crown-4)$_2$] in d_8-THF.

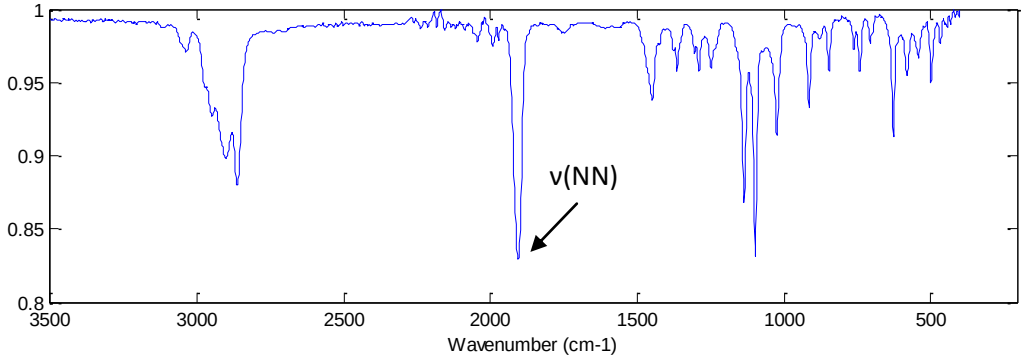

Figure S23. IR spectrum of **12**[K(12-crown-4)$_2$] (thin film from THF).

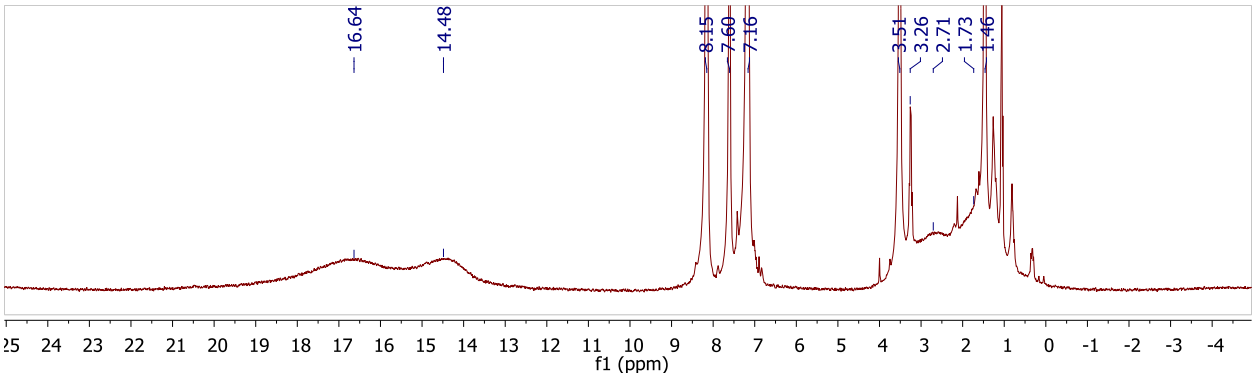

Figure S24. ^{1}H NMR (4:1 C_6D_6/THF-d_8 under N_2, 300 MHz, 298 K) of **13**

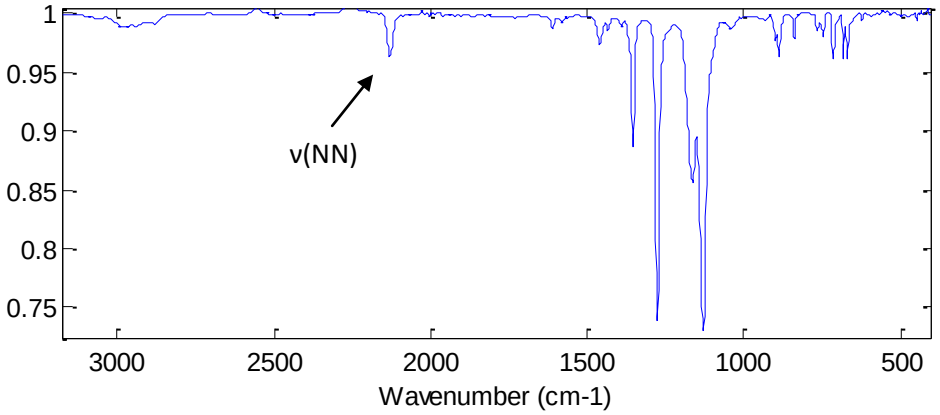

Figure S25. IR of **13** as a thin film deposited from THF.

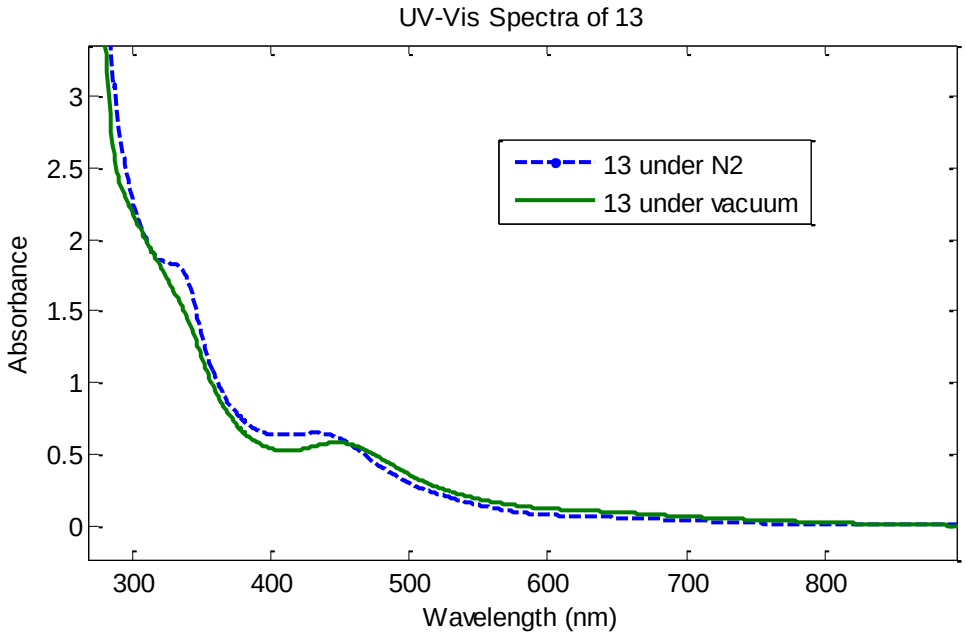

Figure S26. UV-Vis spectra of **13** under N_2 and under static vacuum (after three freeze-pump-thaw cycles). **13** is in a solution of 3:1 Et_2O:THF at a concentration of 0.54 mM.

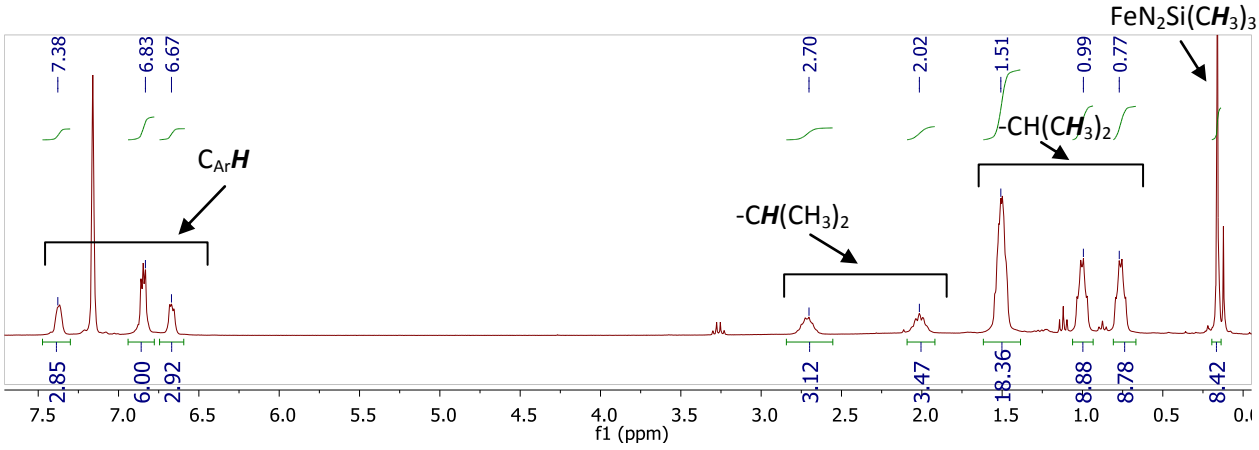

Figure S27. ^{1}H NMR of **14**, C_6D_6.

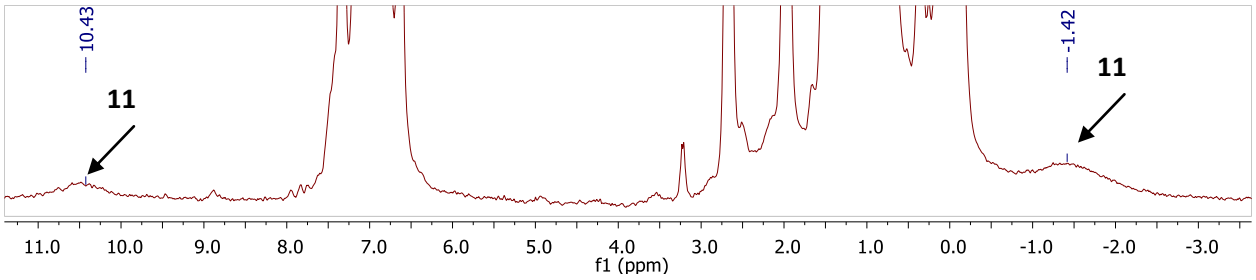

Figure S28. ^{1}H NMR of **14**, showing paramagnetic regions magnified to show minor contamination with $CP^{iPr}_{3}FeN_2$ (**11**).

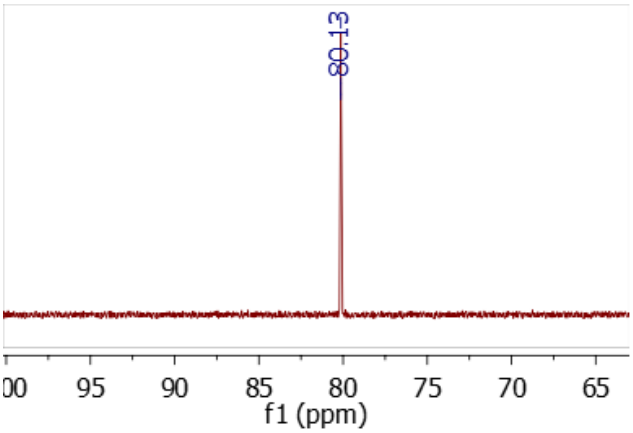

Figure S29. ^{31}P NMR of **14** (C_6D_6).

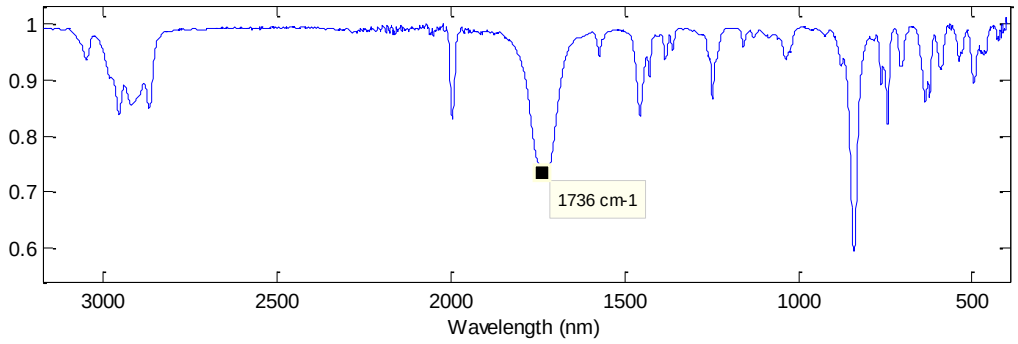

Figure S30. IR (thin-film from C_6D_6) of **14**. Peak at 1992 cm^{-1} is contamination by $CP^{iPr}_{3}FeN_2$.

Catalytic production of NH_3 using $[(CP^{iPr}_3)FeN_2][K(Et_2O)_{0.5}]$

Standard catalytic procedure with $[(CP^{iPr}_3)FeN_2][K(Et_2O)_{0.5}]$ (12): $[(CP^{iPr}_3)FeN_2][K(Et_2O)_{0.5}]$ (1.9 mg, 0.0025 mmol) was suspended in Et_2O (0.5 mL) in a small Schlenk tube equipped with a stir bar. This solution was cooled to -78 °C in a cold well inside of the glove box. A suspension of KC_8 (14 mg, 0.100 mmol) in Et_2O (0.75 mL) was cooled to -78 ^{o}C and added to the reaction mixture with stirring. After five minutes, a similarly cooled solution of $HBAr^F_4 \cdot 2\ Et_2O$ (93 mg, 0.092 mmol) in Et_2O (1.0 mL) was added to the suspension in one portion with rapid stirring. Any remaining acid was dissolved in cold Et_2O (0.25 mL) and added subsequently, and the Schlenk tube was sealed. The reaction was allowed to stir for 60 minutes at -78 °C before being warmed to room temperature and stirred for 15 minutes.

Results of Individual Runs

Run	Absorbance	Eq. NH_3/Fe	% Yield based on H+
A[1]	0.446	3.6	28
B	0.466	4.3	34
C	0.655	6.0	47
D	0.476	4.4	35
E	0.491	4.5	36
F	0.451	4.2	33
G	0.472	4.3	34
H	0.587	5.4	43
Avg	0.514 ± 0.08	4.6 ± 0.8	36 ± 6

[1]Used 2.2 mg (.0029 mmol) of catalyst; omitted from average absorbance.

Hydrazine was not detected in the catalytic runs using a standard UV-Vis quantification method[2].

Modified "acid-first" catalytic procedure with [(CP$^{iPr}_3$)FeN$_2$][K(Et$_2$O)$_{0.5}$] (12): [(CP$^{iPr}_3$)FeN$_2$][K(Et$_2$O)$_{0.5}$] (1.9 mg, 0.0025 mmol) was dissolved in Et$_2$O (0.5 mL) in a 20 mL scintillation vial equipped with a stir bar. This dark brown solution was vigorously stirred and cooled to -78 °C in a cold well inside of the glove box. A similarly cooled solution of HBAr$^F_4$ · 2 Et$_2$O (93 mg, 0.092 mmol) in Et$_2$O (1.5 mL) was added to the solution in one portion with rapid stirring. Any remaining acid was dissolved in cold Et$_2$O (0.25 mL) and added subsequently. The reaction mixture turned light orange upon addition of acid and the resulting solution was allowed to stir for 5 minutes before being transferred into a pre-cooled Schlenk tube equipped with a stirbar. The original reaction vial was washed with cold Et$_2$O (0.25 mL) which was subsequently transferred to the Schlenk tube. Solid KC$_8$ (14 mg, 0.100 mmol) was suspended in cold Et$_2$O (0.75 mL) and added dropwise to the rapidly stirred solution in the Schlenk tube which was then tightly sealed. The reaction was allowed to stir for 60 minutes at -78 °C before being warmed to room temperature and stirred for 15 minutes.

Results of individual runs

Run	Absorbance	Eq. NH_3/Fe	% Yield based on H_2
I[1]	0.375	3.0	24
J	0.483	4.3	34
K	0.484	4.4	35
M	0.407	3.8	30
Avg.	0.458 ± 0.04	3.8 ± 0.6	30 ± 5

[1]Used 2.2 mg (.0029 mmol) of catalyst; omitted from average absorbance.

[2] Watt, G.W.; Chrisp, J.D. *Anal. Chem.* **1952**, *24*, 2006.

Standard catalytic procedure with [(TPB)FeN$_2$][Na(12-c-4)$_2$]: [(TPB)FeN$_2$][Na(12-c-4)$_2$] (2.0 mg, 0.002 mmol) was suspended in Et$_2$O (0.5 mL) in a small Schlenk tube equipped with a stir bar. This solution was cooled to -78 °C in a cold well inside of the glove box. A suspension of KC$_8$ (14 mg, 0.100 mmol) in Et$_2$O (0.75 mL) was cooled to -78 ^{o}C and added to the reaction mixture with stirring. After five minutes, a similarly cooled solution of HBAr$^{F}_{4}$ · 2 Et$_2$O (93 mg, 0.092 mmol) in Et$_2$O (1.0 mL) was added to the suspension in one portion with rapid stirring. Any remaining acid was dissolved in cold Et$_2$O (0.25 mL) and added subsequently, and the Schlenk tube was sealed. The reaction was allowed to stir for 60 minutes at -78 °C before being warmed to room temperature and stirred for 15 minutes.

Results of Individual Runs

Run	Absorbance	Eq. NH_3/Fe	% Yield based on H+
N	0.528	6.1	38
O	0.422	3.9	24
Avg.	0.475 ± 0.05	5.0 ± 1.1	31 ± 7

Standard catalytic procedure with [(CP$^{iPr}_3$)FeN$_2$][K(12-c-4)$_2$] (12[K(12-crown-4)$_2$]): [(CP$^{iPr}_3$)FeN$_2$][K(12-c-4)$_2$] (2.0 mg, 0.002 mmol) was suspended in Et$_2$O (0.5 mL) in a small Schlenk tube equipped with a stir bar. This solution was cooled to -78 °C in a cold well inside of the glove box. A suspension of KC$_8$ (14 mg, 0.100 mmol) in Et$_2$O (0.75 mL) was cooled to -78 ^{o}C and added to the reaction mixture with stirring. After five minutes, a similarly cooled solution of HBAr$^{F}_{4}$ · 2 Et$_2$O (93 mg, 0.092 mmol) in Et$_2$O (1.0 mL) was added to the suspension in one portion with rapid stirring. Any remaining acid was dissolved in cold Et$_2$O (0.25 mL) and added subsequently, and the Schlenk tube was sealed. The reaction was allowed to stir for 60 minutes at -78 °C before being warmed to room temperature and stirred for 15 minutes.

Results of Individual Runs

Run	Absorbance	Eq. NH_3/Fe	% Yield based on H+
P	0.327	3.7	23
Q	0.328	3.7	23
R[1]	0.344	3.1	24
Avg.	0.328 ± 0.001	3.5 ± 0.3	23 ± 0.3

[1] Used 2.5 mg (.0025 mmol) of catalyst; omitted from average absorbance.

Standard catalytic procedure with [(SiP$^{iPr}_3$)FeN$_2$][Na(12-c-4)$_2$]: [(SiP$^{iPr}_3$)FeN$_2$][Na(12-c-4)$_2$] (2.0 mg, 0.002 mmol) was suspended in Et_2O (0.5 mL) in a small Schlenk tube equipped with a stir bar. This solution was cooled to -78 °C in a cold well inside of the glove box. A suspension of KC_8 (14 mg, 0.100 mmol) in Et_2O (0.75 mL) was cooled to -78 °C and added to the reaction mixture with stirring. After five minutes, a similarly cooled solution of $HBAr^F_4 \cdot 2\ Et_2O$ (93 mg, 0.092 mmol) in Et_2O (1.0 mL) was added to the suspension in one portion with rapid stirring. Any remaining acid was dissolved in cold Et_2O (0.25 mL) and added subsequently, and the Schlenk tube was sealed. The reaction was allowed to stir for 60 minutes at -78 °C before being warmed to room temperature and stirred for 15 minutes.

Results of Individual Runs

Run	Absorbance	Eq. NH_3/Fe	% Yield based on H+
S	0.109	1.2	8
T	0.040	0.4	3
Avg.	0.075 ± 0.03	0.8 ± 0.4	5 ± 3

Identification of H_2 in a standard catalytic run. A catalytic run was performed with 0.0025 mmol of **12** according to the standard procedure. Prior to the vacuum transfer of volatiles, the solutions inside of

the Schlenk tubes were frozen. The ground glass joint of the Schlenk tube was then sealed with a rubber septum and the head space between the Teflon stopcock of the Schlenk tube and the septum was evacuated. This head space was left under static vacuum and the Teflon stopcock of the reaction vessel was opened after which a 10 mL aliquot of the headspace was sampled through the septum *via* a gas-tight syringe. This sample was then analyzed for hydrogen with an Agilent 7890A gas chromatograph using a thermal conductivity detector. 45% yield of H_2 relative to H^+ was quantified.

IR spectral analysis of addition of 12 equiv. of KC_8, followed by 10 equiv of $HBAr^F_4 \cdot 2\ Et_2O$ to $[(CP^{iPr}_3)FeN_2][K(Et_2O)_{0.5}]$. A 20 mL scintillation vial was charged with a stir bar and $[(CP^{iPr}_3)FeN_2][K(Et_2O)_{0.5}]$ (7.6 mg, 0.0101 mmol). In a separate vial, $HBAr^F_4 \cdot 2\ Et_2O$ (75 mg, 0.074 mmol) was dissolved in Et_2O (1 mL). Finally, a third vial was prepared containing a suspension of potassium graphite (12 mg, 0.090 mmol) in Et_2O (1 mL). All three vials were chilled in the cold well to -78 ^oC for 10 minutes. The suspension of KC_8 was quickly added to the stirring suspension of $[(CP^{iPr}_3)FeN_2][K(Et_2O)_{0.5}]$. After stirring for 5 minutes, $HBAr^F_4 \cdot 2\ Et_2O$ was added rapidly to the stirring reaction mixture. This solution was capped and stirred at -78 ^oC for 60 minutes and then brought to r.t. and stirred for 15 minutes. The resulting reaction mixture was concentrated to dryness, taken up in C_6D_6, and filtered through Celite, giving an orange solution which was analyzed by IR and NMR. By IR, the major species appeared to be $(CP^{iPr}_3)FeN_2$ (**11**), and the presence of a smaller amount of $(CP^{iPr}_3)Fe(N_2)(H)$ (**9**) was also apparent. By NMR, **11**, **9**, and $(CP^{iPr}_3)FeCl$ (**10**) were detected as well as an additional unidentified diamagnetic species present in small amounts. No uncoordinated $(CP^{iPr}_3)H$ ligand could be detected.

IR spectral analysis of addition of 40 equiv. of KC_8, followed by 38 equiv of $HBAr^F_4 \cdot 2\ Et_2O$ to $[(CP^{iPr}_3)FeN_2][K(Et_2O)_{0.5}]$. A 20 mL scintillation vial was charged with a stir bar and $[(CP^{iPr}_3)FeN_2][K(Et_2O)_{0.5}]$ (8.0 mg, 0.0106 mmol). In a separate vial, $HBAr^F_4 \cdot 2\ Et_2O$ (392 mg, 0.403 mmol) was dissolved in Et_2O (1 mL). Finally, a third vial was prepared containing a suspension of potassium

graphite (59 mg, 0.424 mmol) in Et_2O (1 mL). All three vials were chilled in the cold well to -78 °C for 10 minutes. The suspension of KC_8 was quickly added to the stirring suspension of $[(CP^{iPr}_3)FeN_2][K(Et_2O)_{0.5}]$. After stirring for 5 minutes, $HBAr^F_4 \cdot 2\ Et_2O$ was added rapidly to the stirring reaction mixture. This solution was capped and stirred at -78 °C for 60 minutes and then brought to r.t. and stirred for 15 minutes. The resulting reaction mixture was concentrated to dryness, taken up in C_6D_6, and filtered through Celite, giving an orange solution which was analyzed by IR and NMR. By IR and NMR, the major species appeared to be $(CP^{iPr}_3)Fe(N_2)(H)$ (**9**), and some $(CP^{iPr}_3)FeN_2$ (**11**) was also present. No uncoordinated $(CP^{iPr}_3)H$ ligand could be detected.

In a separate experiment, the reaction was carried out as above, but after being allowed to stir at room temperature for 15 minutes the reaction mixture was filtered and to the filtrate was added an aliquot of a standard solution of 1,3,5-trimethoxybenzene (0.0106 mmol). The combined solution was concentrated to dryness, taken up in C_6D_6, filtered through Celite, and analyzed by IR and NMR. NMR integration (d1 = 10 sec) of the diamagnetic peaks shows approximately 70% yield of **9** relative to the starting catalyst (Figure S31).

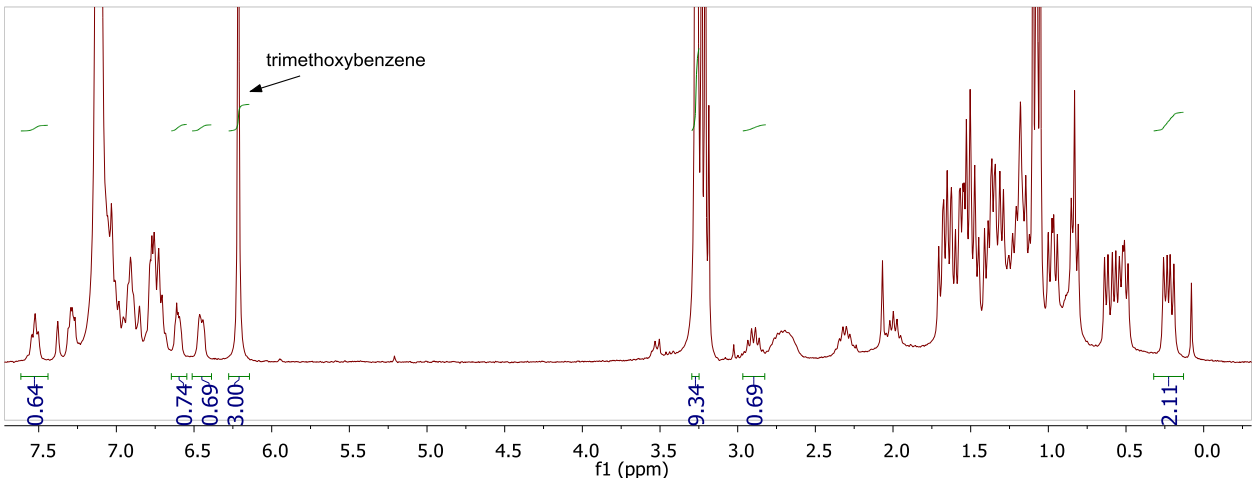

Figure S31. NMR of reaction mixture after catalysis with internal standard (1,3,5-trimethoxybenzene).

Calibration Curves for NH_3 and N_2H_4 Quantification

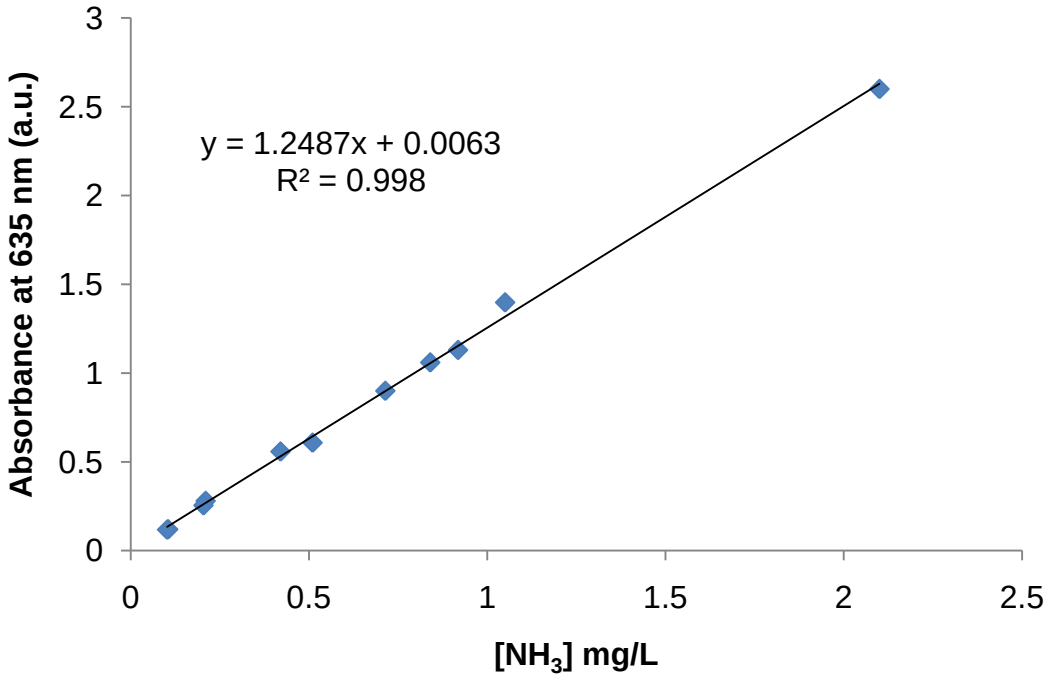

Figure S32. Calibration curve for NH_3 quantification *via* indophenol method.

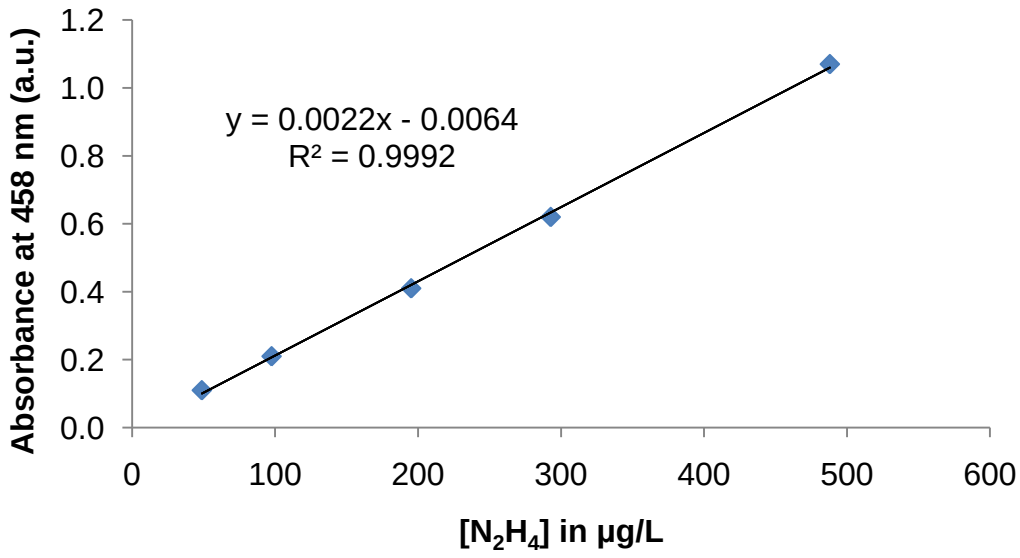

Figure S33. Calibration curve for UV-Vis quantification of hydrazine.

Curves were generated by creating solutions of $[NH_4][Cl]$ and $[N_2H_5][HSO_4]$ of known concentrations and then analyzing by the appropriate UV-Vis methodology (*vide supra)*

Quantification of ammonia formed without added reductant. A sample of **12**$[K(Et_2O)_{0.5}]$ was dissolved in Et_2O (1 mL) and cooled to -78^0 C in a Schlenk tube. $HBAr^F_4 \cdot 2\ Et_2O$ (10 equiv.) was dissolved in cold Et_2O (1 mL) and added in one portion with rapid stirring. The reaction mixture was stirred at -78^{o}C for 1 hour and then at room temperature for 20 minutes, and then subjected to the standard ammonia quantification procedure. One run using 0.0025 mmol of **12**$[K(Et_2O)_{0.5}]$ gave <0.05 equiv. of NH_3 (below detection limits) while a second run using 0.005 mmol of **12**$[K(Et_2O)_{0.5}]$ gave 0.06 equiv. of NH_3/Fe.

Attempted catalysis with 9. $(CP_3^{iPr})Fe(N_2)(H)$ (1.7 mg, 0.002 mmol) was suspended in Et_2O (0.5 mL) in a small Schlenk tube equipped with a stir bar. This solution was cooled to -78 °C in a cold well inside of the glove box. A suspension of KC_8 (14 mg, 0.100 mmol) in Et_2O (0.75 mL) was cooled to -78 ^{o}C and added to the reaction mixture with stirring. After five minutes, a similarly cooled solution of $HBAr^F_4 \cdot 2\ Et_2O$ (93 mg, 0.092 mmol) in Et_2O (1.0 mL) was added to the suspension in one portion with rapid stirring. Any remaining acid was dissolved in cold Et_2O (0.25 mL) and added subsequently, and the Schlenk tube was sealed. The reaction was allowed to stir for 60 minutes at -78 °C before being warmed to room temperature and stirred for 15 minutes. The reaction was subjected to the standard workup and ammonia detection procedure; no ammonia was detected.

Attempted catalysis with $[(C^{Si}P^{Ph}_3)FeN_2][K(benzo\text{-}15\text{-}crown\text{-}5)_2]$: $[(C^{Si}P^{Ph}_3)FeN_2][K(benzo\text{-}15\text{-}crown\text{-}5)_2]$ (2.0 mg, 0.0020 mmol) was dissolved in Et_2O (0.5 mL) in a 20 mL scintillation vial equipped with a stir bar. This dark brown solution was vigorously stirred and cooled to -78 °C in a cold well inside of the glove box. A similarly cooled solution of $HBAr^F_4 \cdot 2\ Et_2O$ (93 mg, 0.092 mmol) in Et_2O (1.5 mL) was added to the solution in one portion with rapid stirring. Any remaining acid was dissolved in cold Et_2O (0.25 mL) and added subsequently. The reaction mixture was allowed to stir for 5 minutes before being

transferred into a pre-cooled Schlenk tube equipped with a stirbar. The original reaction vial was washed with cold Et_2O (0.25 mL) which was subsequently transferred to the Schlenk tube. Solid KC_8 (14 mg, 0.100 mmol) was suspended in cold Et_2O (0.75 mL) and added dropwise to the rapidly stirred solution in the Schlenk tube which was then tightly sealed. The reaction was allowed to stir for 60 minutes at -78 °C before being warmed to room temperature and stirred for 15 minutes. Ammonia was quantified via the standard method. Two trials were performed, giving 0.40 and 0.14 equiv. NH_3/Fe.

Crystal Structure Tables and Refinement Information

*Crystal data and structure refinement for [(CP$^{iPr}{}_3$)H]FeI$_2$ (**6**)*

Empirical formula	C40.50 H59 Fe I2 P3	
Formula weight	948.44	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 39.338(2) Å	α= 90°.
	b = 12.1860(7) Å	β= 111.327(2)°.
	c = 18.6670(11) Å	γ = 90°.
Volume	8335.6(8) Å^3	
Z	8	
Density (calculated)	1.512 Mg/m^3	
Absorption coefficient	1.985 mm^{-1}	
F(000)	3832	
Theta range for data collection	1.76 to 26.37°.	
Index ranges	-49<=h<=49, -15<=k<=15, -23<=l<=23	
Reflections collected	117932	
Independent reflections	8536 [R(int) = 0.0714]	
Completeness to theta = 26.37°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	.7460 and .6679	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8536 / 464 / 433	
Goodness-of-fit on F^2	1.037	
Final R indices [I>2sigma(I)]	R1 = 0.0256, wR2 = 0.0462	
R indices (all data)	R1 = 0.0397, wR2 = 0.0501	
Largest diff. peak and hole	0.491 and -0.498 e.Å^{-3}	

One solvent molecule is present in the structure of **6**, a toluene molecule which was modeled as disordered over a two-fold special position. Additionally, one isopropyl group on the ligand was refined as a disorder over two positions in a 76:24 ratio.

*Crystal data and structure refinement for [(CP$^{iPr}{}_3$)H]FeBr (**8**)*

Empirical formula	C43 H61 Br Fe P3	
Formula weight	814.48	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 12.5154(8) Å	α= 90°.
	b = 15.3220(10) Å	β= 92.849(3)°.
	c = 20.9097(10) Å	γ = 90°.
Volume	4004.7(4) Å^3	
Z	4	
Density (calculated)	1.351 Mg/m^3	
Absorption coefficient	1.525 mm^{-1}	
F(000)	1684	
Crystal size	0.30 x 0.06 x 0.02 mm^3	
Theta range for data collection	1.63 to 27.89°.	
Index ranges	-16<=h<=16, -19<=k<=19, -27<=l<=26	
Reflections collected	61095	
Independent reflections	9120 [R(int) = 0.1687]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9701 and 0.6576	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9120 / 0 / 427	
Goodness-of-fit on F^2	0.970	
Final R indices [I>2sigma(I)]	R1 = 0.0618, wR2 = 0.1127	
R indices (all data)	R1 = 0.1742, wR2 = 0.1545	
Largest diff. peak and hole	1.110 and -0.862 e.Å^{-3}	

The structure of **8** includes one benzene molecule per asymmetric unit.

*Crystal data and structure refinement for (CP^{iPr}_3)Fe(N_2)(H) (**9**)*

Empirical formula	C37 H55 Fe N2 P3	
Formula weight	676.59	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 10.8051(3) Å	α= 90°.
	b = 15.4905(5) Å	β= 90°.
	c = 20.7380(7) Å	γ = 90°.
Volume	3471.05(19) $Å^3$	
Z	4	
Density (calculated)	1.295 Mg/m^3	
Absorption coefficient	0.601 mm^{-1}	
F(000)	1448	
Crystal size	0.50 x 0.49 x 0.38 mm^3	
Theta range for data collection	1.96 to 25.00°.	
Index ranges	-12<=h<=12, -18<=k<=18, -24<=l<=24	
Reflections collected	65697	
Independent reflections	6113 [R(int) = 0.0393]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8037 and 0.7530	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6113 / 341 / 398	
Goodness-of-fit on F^2	1.059	
Final R indices [I>2sigma(I)]	R1 = 0.0304, wR2 = 0.0776	
R indices (all data)	R1 = 0.0306, wR2 = 0.0777	
Absolute structure parameter	0.099(12)	
Largest diff. peak and hole	1.783 and -0.639 e.$Å^{-3}$	

*Crystal data and structure refinement for (CP^{iPr}_3)FeN_2 (**11**)*

Empirical formula	C37 H54 Fe N2 P3	
Formula weight	675.58	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Trigonal	
Space group	R-3	
Unit cell dimensions	a = 19.4069(5) Å	α= 90°.
	b = 19.4069(5) Å	β= 90°.
	c = 47.9751(17) Å	γ = 120°.
Volume	15648.0(8) $Å^3$	
Z	18	
Density (calculated)	1.290 Mg/m^3	
Absorption coefficient	0.600 mm^{-1}	
F(000)	6498	
Theta range for data collection	1.27 to 25.03°.	
Index ranges	-23<=h<=11, -23<=k<=23, -57<=l<=57	
Reflections collected	12326	
Independent reflections	12326 [R(int) = 0.0000]	
Completeness to theta = 25.03°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12326 / 335 / 389	
Goodness-of-fit on F^2	1.106	
Final R indices [I>2sigma(I)]	R1 = 0.0624, wR2 = 0.1624	
R indices (all data)	R1 = 0.0655, wR2 = 0.1672	
Largest diff. peak and hole	2.593 and -0.891 e.$Å^{-3}$	

The refinement of the crystal structure of **11** used SHELX HKLF 5 refinement to treat the presence of a non-merohedral twin accounting for 20% of the observed reflections.

Crystal data and structure refinement for [(CP^{iPr}_3)FeN_2][$K(Et_2O)_3$] (**12**)

Empirical formula	C49 H84 Fe K N2 O3 P3	
Formula weight	937.04	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	Cc	
Unit cell dimensions	a = 10.9229(4) Å	α= 90°.
	b = 26.9376(10) Å	β= 94.663(2)°.
	c = 17.6054(7) Å	γ = 90°.
Volume	5163.0(3) $Å^3$	
Z	4	
Absorption coefficient	0.505 mm^{-1}	
F(000)	2024	
Theta range for data collection	1.91 to 35.46°.	
Index ranges	-17<=h<=17, -38<=k<=43, -28<=l<=28	
Reflections collected	77464	
Independent reflections	21119 [R(int) = 0.0624]	
Completeness to theta = 35.46°	94.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9701 and 0.6576	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	21119 / 2 / 544	
Goodness-of-fit on F^2	1.008	
Final R indices [I>2sigma(I)]	R1 = 0.0438, wR2 = 0.0843	
R indices (all data)	R1 = 0.0755, wR2 = 0.0949	
Absolute structure parameter	0.130(8)	
Largest diff. peak and hole	0.902 and -0.524 e.$Å^{-3}$	

*Crystal data and structure refinement for [(CP^{iPr}_3)FeN_2][BAr_4^F] (**13**)*

Empirical formula	C69 H66 B Cl0.12 F24 Fe N1.77 P3	
Formula weight	1539.84	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 19.7846(11) Å	α= 90°.
	b = 25.8800(14) Å	β= 90°.
	c = 26.6463(13) Å	γ = 90°.
Volume	13643.6(13) $Å^3$	
Z	8	
Density (calculated)	1.499 Mg/m^3	
Absorption coefficient	0.405 mm^{-1}	
F(000)	6291	
Theta range for data collection	1.50 to 30.53°.	
Index ranges	-28<=h<=28, -36<=k<=36, -38<=l<=36	
Reflections collected	224578	
Independent reflections	20858 [R(int) = 0.1311]	
Completeness to theta = 30.53°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9701 and 0.6576	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	20858 / 1048 / 946	
Goodness-of-fit on F^2	1.118	
Final R indices [I>2sigma(I)]	R1 = 0.0845, wR2 = 0.2235	
R indices (all data)	R1 = 0.1320, wR2 = 0.2520	
Largest diff. peak and hole	1.915 and -1.004 $e.Å^{-3}$	

This crystal structure was modeled with a 12% occupancy of the chloride complex, CP_3FeCl.

Additionally, one isopropyl group of the CP_3 ligand was modeled as disordered over two positions in a 49:51 ratio, and one trifluoromethyl group of the BArF anion was modeled as disordered over two positions in a 48:52 ratio.

Tables of Selected Bond Lengths and Angles

Selected bond lengths [Å] and angles [°] for [(CP$^{iPr}_3$)H]FeI$_2$ (**6**):

I(2)-Fe(1)	2.5884(4)
I(1)-Fe(1)	2.6062(4)
Fe(1)-P(2)	2.4587(7)
Fe(1)-P(1)	2.5134(7)
P(2)-Fe(1)-P(1)	113.21(2)
P(2)-Fe(1)-I(2)	109.349(19)
P(1)-Fe(1)-I(2)	116.625(19)
P(2)-Fe(1)-I(1)	102.335(19)
P(1)-Fe(1)-I(1)	99.721(18)
I(2)-Fe(1)-I(1)	114.490(14)

Selected bond lengths [Å] and angles [°] for [(CP$^{iPr}_3$)H]FeBr (**8**)

Br(1)-Fe(1)	2.4647(7)
Fe(1)-P(1)	2.3759(15)
Fe(1)-P(2)	2.3940(15)
Fe(1)-P(3)	2.3968(15)
P(1)-Fe(1)-P(2)	110.58(5)
P(1)-Fe(1)-P(3)	109.39(5)
P(2)-Fe(1)-P(3)	110.12(5)
P(1)-Fe(1)-Br(1)	109.39(4)
P(2)-Fe(1)-Br(1)	107.70(4)
P(3)-Fe(1)-Br(1)	109.63(4)

Selected bond lengths [Å] and angles [°] for $(CP^{iPr}_3)Fe(N_2)(H)$ (**9**).

Fe(1)-N(1)	1.8144(19)
Fe(1)-C(0)	2.155(2)
Fe(1)-P(2)	2.1857(7)
Fe(1)-P(3)	2.2502(7)
Fe(1)-P(1)	2.2779(7)
Fe(1)-H(01)	1.45(3)
N(1)-N(2)	1.106(3)
N(1)-Fe(1)-C(0)	177.27(9)
N(1)-Fe(1)-P(2)	95.87(7)
C(0)-Fe(1)-P(2)	86.48(6)
N(1)-Fe(1)-P(3)	94.18(7)
C(0)-Fe(1)-P(3)	83.11(6)
P(2)-Fe(1)-P(3)	141.23(3)
N(1)-Fe(1)-P(1)	97.38(7)
C(0)-Fe(1)-P(1)	83.41(6)
P(2)-Fe(1)-P(1)	103.08(3)
P(3)-Fe(1)-P(1)	112.60(2)
N(1)-Fe(1)-H(01)	95.5(13)
C(0)-Fe(1)-H(01)	83.9(13)
P(2)-Fe(1)-H(01)	72.5(13)
P(3)-Fe(1)-H(01)	69.3(13)
P(1)-Fe(1)-H(01)	166.8(13)

Selected bond lengths [Å] and angles [°] for $(CP^{iPr}_3)FeN_2$ (**11**)

Fe(1)-N(1)	1.797(2)
Fe(1)-C(01)	2.152(3)
Fe(1)-P(1)	2.2349(8)
Fe(1)-P(3)	2.2602(8)
Fe(1)-P(2)	2.2660(8)
N(1)-N(2)	1.134(4)
N(1)-Fe(1)-C(01)	174.80(11)
N(1)-Fe(1)-P(1)	96.71(8)
C(01)-Fe(1)-P(1)	82.62(6)
N(1)-Fe(1)-P(3)	103.51(9)
C(01)-Fe(1)-P(3)	81.50(7)
P(1)-Fe(1)-P(3)	110.81(3)
N(1)-Fe(1)-P(2)	94.67(9)
C(01)-Fe(1)-P(2)	82.11(6)
P(1)-Fe(1)-P(2)	132.54(3)
P(3)-Fe(1)-P(2)	110.90(3)

Selected bond lengths [Å] and angles [°] for $[(CP^{iPr}_3)FeN_2][K(Et_2O)_3]$

Fe(1)-N(1)	1.7397(16)
Fe(1)-C(01)	2.1646(17)
Fe(1)-P(3)	2.1947(5)
Fe(1)-P(2)	2.2045(5)
Fe(1)-P(1)	2.2047(5)
K(1)-N(2)	2.6560(18)
N(1)-N(2)	1.153(2)
N(1)-Fe(1)-C(01)	179.68(7)
N(1)-Fe(1)-P(3)	96.27(5)
C(01)-Fe(1)-P(3)	83.81(5)

N(1)-Fe(1)-P(2)	96.29(5)
C(01)-Fe(1)-P(2)	83.93(5)
P(3)-Fe(1)-P(2)	120.051(19)
N(1)-Fe(1)-P(1)	96.07(5)
C(01)-Fe(1)-P(1)	83.62(5)
P(3)-Fe(1)-P(1)	118.686(19)
P(2)-Fe(1)-P(1)	117.797(19)
N(2)-N(1)-Fe(1)	179.86(19)
N(1)-N(2)-K(1)	155.77(15)

Selected bond lengths [Å] and angles [°] for $[(CP^{iPr}_3)FeN_2][BAr_4^F]$ (**13**)

Fe(1)-N(1)	1.864(7)
Fe(1)-C(01)	2.081(3)
Fe(1)-P(1)	2.3248(9)
Fe(1)-P(3)	2.3604(9)
Fe(1)-P(2)	2.3885(10)

N(1)-Fe(1)-C(01)	177.7(2)
N(1)-Fe(1)-P(1)	93.62(18)
C(01)-Fe(1)-P(1)	84.31(8)
N(1)-Fe(1)-P(3)	96.5(2)
C(01)-Fe(1)-P(3)	85.20(8)
P(1)-Fe(1)-P(3)	117.04(3)
N(1)-Fe(1)-P(2)	95.8(2)
C(01)-Fe(1)-P(2)	84.67(8)
P(1)-Fe(1)-P(2)	124.77(4)
P(3)-Fe(1)-P(2)	115.66(3)
N(2)-N(1)-Fe(1)	178.4(6)

Computational Results:

*Coordinates for NBO analysis of **12**[K(Et$_2$O)$_3$] (from crystallographic structure):*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-1.103223	-0.012183	0.135795
2	19	0	4.315234	-0.139004	-0.090250
3	15	0	-1.675324	-1.173876	1.915082
4	15	0	-1.065123	-1.018414	-1.816226
5	15	0	-1.284994	2.184405	0.235987
6	8	0	4.528660	2.280807	-1.344490
7	8	0	5.911867	0.348888	1.940111
8	7	0	0.612427	-0.071693	0.411598
9	7	0	1.748732	-0.115596	0.595993
10	8	0	4.713206	-2.836955	-0.525656
11	6	0	-3.683547	-1.101439	-1.107075
12	6	0	-2.848212	2.944956	2.477923
13	1	0	-2.902445	3.411133	3.314657
14	1	0	-2.943217	2.002256	2.629817
15	1	0	-3.549324	3.247396	1.896562
16	6	0	-5.300719	0.467098	1.314827
17	1	0	-5.754021	0.820458	0.583473
18	6	0	-4.001912	-0.590995	3.509773
19	1	0	-3.561669	-0.948234	4.247172
20	6	0	-3.352643	-0.565059	2.266253
21	6	0	-5.340093	-2.690118	-1.938757
22	1	0	-6.213047	-3.009821	-1.927115
23	6	0	-3.239989	0.059982	-0.210069
24	6	0	-5.939548	0.424855	2.554070
25	1	0	-6.807180	0.746825	2.637851
26	6	0	-3.995744	-0.009489	1.140999
27	6	0	-4.738827	1.530724	-1.725792
28	1	0	-5.272600	0.789814	-1.900313
29	6	0	-2.833970	2.529034	-0.662244
30	6	0	-0.699925	-0.964724	3.508975
31	1	0	-1.255246	-1.274126	4.255707
32	6	0	-3.177781	3.758444	-1.223575
33	1	0	-2.652914	4.506767	-1.050375
34	6	0	-5.064227	2.756173	-2.308949
35	1	0	-5.796246	2.817735	-2.878437
36	6	0	-1.997936	-3.044284	2.072403
37	1	0	-1.172254	-3.499981	1.807364
38	6	0	-3.630193	1.387339	-0.885512

39	6	0	-4.982113	-1.629900	-1.110692
40	1	0	-5.621718	-1.261735	-0.545281
41	6	0	-5.290076	-0.092274	3.658747
42	1	0	-5.709168	-0.107013	4.489935
43	6	0	-3.084558	-3.496396	1.100751
44	1	0	-3.186989	-4.449759	1.155643
45	1	0	-2.836970	-3.251424	0.205987
46	1	0	-3.914011	-3.072883	1.330188
47	6	0	-2.374639	-3.573776	3.467980
48	1	0	-3.208651	-3.185989	3.743407
49	1	0	-1.689325	-3.336150	4.096275
50	1	0	-2.461494	-4.529577	3.434330
51	6	0	-3.115644	-2.771435	-2.799728
52	1	0	-2.483847	-3.154087	-3.366548
53	6	0	-0.750968	-1.148162	-4.740497
54	1	0	-1.580024	-1.620407	-4.840874
55	1	0	-0.038712	-1.776973	-4.607887
56	1	0	-0.578243	-0.631117	-5.530824
57	6	0	1.502649	-2.065440	-2.315231
58	1	0	1.815103	-1.592208	-1.539649
59	1	0	1.549957	-1.489740	-3.081720
60	1	0	2.053171	-2.837709	-2.460536
61	6	0	-2.747844	-1.699193	-1.980183
62	6	0	-0.325574	0.487045	3.757235
63	1	0	0.179496	0.553496	4.571506
64	1	0	-1.124499	1.014869	3.832211
65	1	0	0.203405	0.811036	3.024982
66	6	0	-0.022549	-3.492168	-0.929395
67	1	0	0.581790	-4.220856	-1.087339
68	1	0	-0.916832	-3.829177	-0.851393
69	1	0	0.221701	-3.043661	-0.116590
70	6	0	-1.487758	3.224594	1.824152
71	1	0	-0.808956	2.902562	2.452414
72	6	0	0.050193	-2.507521	-2.095661
73	1	0	-0.255203	-2.969370	-2.904599
74	6	0	0.580691	-1.821703	3.461949
75	1	0	1.123702	-1.546872	2.719257
76	1	0	0.343951	-2.746055	3.359005
77	1	0	1.073156	-1.706308	4.278167
78	6	0	-0.838007	-0.212835	-3.526978
79	1	0	0.005710	0.283396	-3.493229
80	6	0	5.552067	0.484633	3.317571
81	1	0	5.929145	1.302376	3.676051
82	1	0	5.908135	-0.261935	3.825577
83	6	0	7.315816	0.488607	1.718843
84	1	0	7.801006	-0.186282	2.219940
85	1	0	7.613666	1.363018	2.015963
86	6	0	-1.299822	4.739239	1.722486

87	1	0	-1.914962	5.096379	1.078526
88	1	0	-0.400500	4.932966	1.446202
89	1	0	-1.464279	5.140526	2.579276
90	6	0	-4.406596	-3.272724	-2.778249
91	1	0	-4.643071	-3.990150	-3.321219
92	6	0	-0.039374	3.319208	-0.609736
93	1	0	-0.364441	4.240727	-0.526365
94	6	0	5.211785	3.482161	-0.977128
95	1	0	4.717915	4.251132	-1.301884
96	1	0	6.092941	3.493459	-1.381554
97	6	0	5.431388	-3.446517	-1.561156
98	1	0	4.909694	-4.171249	-1.941774
99	1	0	6.257089	-3.817878	-1.214349
100	6	0	1.307915	3.224629	0.107122
101	1	0	1.676736	2.348031	-0.020042
102	1	0	1.184523	3.386169	1.045478
103	1	0	1.909864	3.882193	-0.252694
104	6	0	4.068393	0.517784	3.442582
105	1	0	3.721485	1.265472	2.948807
106	1	0	3.827230	0.606058	4.366826
107	1	0	3.699349	-0.296154	3.090825
108	6	0	7.581088	0.327433	0.244385
109	1	0	7.263162	-0.529819	-0.046117
110	1	0	8.524717	0.391569	0.080971
111	1	0	7.123341	1.019454	-0.239674
112	6	0	-1.943089	0.817273	-3.782952
113	1	0	-1.701239	1.365393	-4.533243
114	1	0	-2.051741	1.370207	-3.005635
115	1	0	-2.768224	0.362999	-3.969832
116	6	0	0.135799	3.014067	-2.094347
117	1	0	0.816189	3.583836	-2.459410
118	1	0	-0.692505	3.169693	-2.553507
119	1	0	0.395576	2.095831	-2.203060
120	6	0	5.338946	3.557421	0.519011
121	1	0	4.464517	3.536775	0.915276
122	1	0	5.781619	4.374392	0.762325
123	1	0	5.851605	2.809564	0.835438
124	6	0	4.081567	2.325066	-2.694760
125	1	0	4.843965	2.383314	-3.292513
126	1	0	3.527624	3.108279	-2.831847
127	6	0	-4.305306	3.877919	-2.045170
128	1	0	-4.540148	4.701034	-2.407612
129	6	0	5.733516	-2.440262	-2.609574
130	1	0	4.912970	-2.089325	-2.961565
131	1	0	6.234523	-2.854135	-3.317077
132	1	0	6.248687	-1.726357	-2.227458
133	6	0	3.297851	1.090761	-2.994716
134	1	0	3.881903	0.327903	-2.972567

135	1	0	2.902512	1.166548	-3.865794
136	1	0	2.606298	0.983340	-2.337685
137	6	0	3.297906	-3.191439	1.321519
138	1	0	3.844961	-2.661537	1.906929
139	1	0	2.836541	-3.860832	1.835131
140	1	0	2.656223	-2.626817	0.883823
141	6	0	4.136732	-3.836024	0.327386
142	1	0	4.839780	-4.339808	0.765526
143	1	0	3.606577	-4.453089	-0.201928

Natural Population and Charge Analysis

Summary of Natural Population Analysis:

Atom	No	Charge	Core	Valence	Rydberg	Total
Fe	1	-1.46741	17.98394	9.44097	0.04249	27.46741
K	2	0.64775	17.99326	0.35849	0.00050	18.35225
P	3	1.27701	9.99593	3.65507	0.07199	13.72299
P	4	1.27393	9.99590	3.65705	0.07311	13.72607
P	5	1.26960	9.99597	3.66199	0.07244	13.73040
O	6	-0.62206	1.99980	6.60170	0.02056	8.62206
O	7	-0.62871	1.99981	6.61012	0.01878	8.62871
N	8	0.13757	1.99930	4.78375	0.07939	6.86243
N	9	-0.38115	1.99962	5.34359	0.03794	7.38115
O	10	-0.61888	1.99980	6.59853	0.02055	8.61888
C	11	0.03324	1.99900	3.94356	0.02420	5.96676
C	12	-0.58933	1.99939	4.58194	0.00799	6.58933
H	13	0.20074	0.00000	0.79796	0.00130	0.79926
H	14	0.21689	0.00000	0.78114	0.00197	0.78311
H	15	0.21007	0.00000	0.78860	0.00132	0.78993
C	16	-0.20245	1.99889	4.18565	0.01790	6.20245
H	17	0.19715	0.00000	0.80047	0.00238	0.80285
C	18	-0.19551	1.99919	4.18152	0.01480	6.19551
H	19	0.18943	0.00000	0.80850	0.00208	0.81057
C	20	-0.36151	1.99893	4.33351	0.02906	6.36151
C	21	-0.19506	1.99933	4.18256	0.01317	6.19506
H	22	0.19161	0.00000	0.80668	0.00171	0.80839
C	23	-0.24383	1.99889	4.20581	0.03913	6.24383
C	24	-0.19708	1.99933	4.18432	0.01343	6.19708
H	25	0.19149	0.00000	0.80686	0.00166	0.80851
C	26	0.03137	1.99899	3.94618	0.02346	5.96863
C	27	-0.21664	1.99913	4.20149	0.01602	6.21664
H	28	0.19763	0.00000	0.80004	0.00233	0.80237
C	29	-0.36260	1.99893	4.33489	0.02879	6.36260
C	30	-0.53199	1.99929	4.51377	0.01892	6.53199
H	31	0.20509	0.00000	0.79210	0.00281	0.79491

C	32	-0.17988	1.99894	4.16487	0.01608	6.17988
H	33	0.18683	0.00000	0.81093	0.00223	0.81317
C	34	-0.19064	1.99931	4.17808	0.01325	6.19064
H	35	0.19093	0.00000	0.80734	0.00173	0.80907
C	36	-0.52730	1.99926	4.51037	0.01768	6.52730
H	37	0.20537	0.00000	0.79253	0.00210	0.79463
C	38	0.03888	1.99897	3.93768	0.02447	5.96112
C	39	-0.20266	1.99890	4.18569	0.01808	6.20266
H	40	0.19621	0.00000	0.80127	0.00252	0.80379
C	41	-0.21185	1.99931	4.19886	0.01368	6.21185
H	42	0.19221	0.00000	0.80600	0.00180	0.80779
C	43	-0.58951	1.99940	4.58192	0.00819	6.58951
H	44	0.20163	0.00000	0.79705	0.00133	0.79837
H	45	0.21463	0.00000	0.78340	0.00198	0.78537
H	46	0.21065	0.00000	0.78794	0.00140	0.78935
C	47	-0.60288	1.99940	4.59489	0.00858	6.60288
H	48	0.20842	0.00000	0.78997	0.00161	0.79158
H	49	0.19819	0.00000	0.80052	0.00129	0.80181
H	50	0.20729	0.00000	0.79144	0.00127	0.79271
C	51	-0.18450	1.99894	4.16936	0.01620	6.18450
H	52	0.18808	0.00000	0.80963	0.00229	0.81192
C	53	-0.60314	1.99941	4.59520	0.00854	6.60314
H	54	0.20821	0.00000	0.79017	0.00162	0.79179
H	55	0.19684	0.00000	0.80188	0.00127	0.80316
H	56	0.20700	0.00000	0.79174	0.00126	0.79300
C	57	-0.59043	1.99941	4.58309	0.00792	6.59043
H	58	0.20584	0.00000	0.79087	0.00329	0.79416
H	59	0.20060	0.00000	0.79807	0.00134	0.79940
H	60	0.19874	0.00000	0.79959	0.00167	0.80126
C	61	-0.36574	1.99894	4.33721	0.02958	6.36574
C	62	-0.59173	1.99941	4.58456	0.00776	6.59173
H	63	0.19847	0.00000	0.80017	0.00135	0.80153
H	64	0.21141	0.00000	0.78727	0.00132	0.78859
H	65	0.21350	0.00000	0.78420	0.00230	0.78650
C	66	-0.58995	1.99940	4.58279	0.00775	6.58995
H	67	0.19510	0.00000	0.80351	0.00140	0.80490
H	68	0.21447	0.00000	0.78424	0.00129	0.78553
H	69	0.21245	0.00000	0.78575	0.00180	0.78755
C	70	-0.52833	1.99925	4.51129	0.01779	6.52833
H	71	0.20886	0.00000	0.78893	0.00221	0.79114
C	72	-0.53421	1.99929	4.51541	0.01950	6.53421
H	73	0.20462	0.00000	0.79260	0.00279	0.79538
C	74	-0.59659	1.99940	4.58966	0.00753	6.59659
H	75	0.21373	0.00000	0.78432	0.00195	0.78627
H	76	0.20192	0.00000	0.79687	0.00121	0.79808
H	77	0.20178	0.00000	0.79689	0.00133	0.79822
C	78	-0.53038	1.99926	4.51316	0.01796	6.53038
H	79	0.20219	0.00000	0.79557	0.00224	0.79781

C	80	-0.04176	1.99917	4.03024	0.01235	6.04176
H	81	0.17980	0.00000	0.81822	0.00198	0.82020
H	82	0.18048	0.00000	0.81756	0.00195	0.81952
C	83	-0.04055	1.99918	4.02912	0.01225	6.04055
H	84	0.18398	0.00000	0.81407	0.00195	0.81602
H	85	0.18176	0.00000	0.81610	0.00214	0.81824
C	86	-0.60429	1.99941	4.59648	0.00840	6.60429
H	87	0.20382	0.00000	0.79463	0.00155	0.79618
H	88	0.19918	0.00000	0.79960	0.00122	0.80082
H	89	0.20902	0.00000	0.78966	0.00131	0.79098
C	90	-0.21908	1.99933	4.20583	0.01391	6.21908
H	91	0.19181	0.00000	0.80641	0.00178	0.80819
C	92	-0.53192	1.99929	4.51319	0.01944	6.53192
H	93	0.20485	0.00000	0.79225	0.00291	0.79515
C	94	-0.04050	1.99917	4.02887	0.01245	6.04050
H	95	0.18419	0.00000	0.81373	0.00208	0.81581
H	96	0.17602	0.00000	0.82199	0.00198	0.82398
C	97	-0.04141	1.99921	4.02880	0.01339	6.04141
H	98	0.18298	0.00000	0.81479	0.00223	0.81702
H	99	0.17782	0.00000	0.82014	0.00204	0.82218
C	100	-0.59222	1.99940	4.58489	0.00793	6.59222
H	101	0.21333	0.00000	0.78348	0.00319	0.78667
H	102	0.20373	0.00000	0.79499	0.00127	0.79627
H	103	0.19554	0.00000	0.80292	0.00154	0.80446
C	104	-0.61128	1.99945	4.60495	0.00688	6.61128
H	105	0.21744	0.00000	0.78076	0.00180	0.78256
H	106	0.22131	0.00000	0.77775	0.00094	0.77869
H	107	0.21682	0.00000	0.78151	0.00168	0.78318
C	108	-0.61590	1.99944	4.60973	0.00673	6.61590
H	109	0.20825	0.00000	0.79001	0.00173	0.79175
H	110	0.22330	0.00000	0.77583	0.00088	0.77670
H	111	0.20956	0.00000	0.78844	0.00200	0.79044
C	112	-0.58856	1.99939	4.58096	0.00821	6.58856
H	113	0.20075	0.00000	0.79802	0.00124	0.79925
H	114	0.21848	0.00000	0.77936	0.00215	0.78152
H	115	0.20985	0.00000	0.78888	0.00127	0.79015
C	116	-0.59188	1.99940	4.58480	0.00768	6.59188
H	117	0.19375	0.00000	0.80484	0.00141	0.80625
H	118	0.21584	0.00000	0.78280	0.00135	0.78416
H	119	0.20764	0.00000	0.79076	0.00160	0.79236
C	120	-0.61677	1.99943	4.61060	0.00674	6.61677
H	121	0.22032	0.00000	0.77814	0.00154	0.77968
H	122	0.21640	0.00000	0.78267	0.00092	0.78360
H	123	0.20455	0.00000	0.79327	0.00218	0.79545
C	124	-0.04114	1.99918	4.02940	0.01256	6.04114
H	125	0.17691	0.00000	0.82114	0.00195	0.82309
H	126	0.18667	0.00000	0.81131	0.00202	0.81333
C	127	-0.21780	1.99933	4.20443	0.01404	6.21780

H 128	0.19017	0.00000	0.80811	0.00172	0.80983
C 129	-0.61559	1.99945	4.60971	0.00643	6.61559
H 130	0.21392	0.00000	0.78443	0.00165	0.78608
H 131	0.22119	0.00000	0.77791	0.00090	0.77881
H 132	0.20221	0.00000	0.79625	0.00154	0.79779
C 133	-0.61285	1.99945	4.60617	0.00723	6.61285
H 134	0.19711	0.00000	0.80130	0.00159	0.80289
H 135	0.22545	0.00000	0.77350	0.00105	0.77455
H 136	0.22507	0.00000	0.77309	0.00183	0.77493
C 137	-0.61910	1.99947	4.61242	0.00721	6.61910
H 138	0.20434	0.00000	0.79398	0.00168	0.79566
H 139	0.22460	0.00000	0.77445	0.00095	0.77540
H 140	0.22981	0.00000	0.76837	0.00182	0.77019
C 141	-0.04266	1.99914	4.03108	0.01244	6.04266
H 142	0.17873	0.00000	0.81929	0.00198	0.82127
H 143	0.18493	0.00000	0.81298	0.00209	0.81507

Natural Bond Orbital Analysis for Bonds of Interest

(Occupancy) Bond orbital/ Coefficients/ Hybrids

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1. (1.84620) BD (1)Fe 1 - P 3
   (25.00%) 0.5000*Fe 1 s(22.10%)p 2.97(65.54%)d 0.56(12.36%)
   f 0.00(0.01%)
   0.0000 0.0000 0.0018 -0.4700 0.0030
   0.0000 -0.0006 -0.1440 0.0154 0.0016
   -0.0079 0.0000 0.0003 -0.4789 0.0132
   -0.0005 -0.0004 0.0000 0.0014 0.6363
   -0.0072 0.0047 0.0020 0.0503 0.0003
   -0.0007 -0.1079 -0.0087 0.0016 -0.1041
   0.0224 -0.0069 -0.2673 -0.0003 -0.0053
   0.1624 -0.0056 0.0040 -0.0011 0.0011
   -0.0075 -0.0013 0.0018 -0.0005 -0.0016
   (75.00%) 0.8660* P 3 s(45.61%)p 1.19(54.37%)d 0.00(0.02%)
   0.0000 0.0009 0.6748 0.0261 0.0044
   -0.0013 0.0004 0.2963 -0.0194 0.0014
   0.0002 0.2694 -0.0281 0.0033 -0.0003
   -0.6165 0.0463 0.0044 0.0013 -0.0073
   -0.0067 -0.0023 0.0082
2. (1.84783) BD (1)Fe 1 - P 4
   (24.66%) 0.4966*Fe 1 s(22.28%)p 2.95(65.73%)d 0.54(11.98%)
   f 0.00(0.01%)
   0.0000 0.0000 0.0012 -0.4720 0.0029
   0.0000 -0.0004 0.0875 0.0133 0.0038
   -0.0055 0.0000 -0.0013 -0.3277 0.0023
   -0.0026 -0.0029 0.0000 -0.0005 -0.7360
   0.0174 0.0047 -0.0025 0.0104 0.0088

-0.0022 -0.0817 0.0103 -0.0062 0.0726
-0.0142 0.0036 -0.2421 -0.0118 -0.0018
0.2199 -0.0116 0.0064 -0.0014 0.0006
-0.0072 -0.0012 0.0020 -0.0015 -0.0022
(75.34%) 0.8680* P 4 s(46.11%)p 1.17(53.87%)d 0.00(0.02%)
0.0000 0.0008 0.6785 0.0271 0.0038
-0.0017 0.0003 0.1088 -0.0037 0.0030
0.0002 0.4019 -0.0288 -0.0074 0.0004
0.6016 -0.0503 0.0011 0.0019 0.0006
0.0097 -0.0040 0.0062
3. (1.84905) BD (1)Fe 1 - P 5
(24.92%) 0.4992*Fe 1 s(22.39%)p 2.91(65.15%)d 0.56(12.45%)
f 0.00(0.01%)
0.0000 0.0000 0.0018 -0.4732 0.0013
0.0000 -0.0002 -0.0073 0.0149 0.0020
-0.0063 0.0000 0.0010 0.8020 -0.0182
0.0024 0.0032 0.0000 -0.0012 0.0872
-0.0052 -0.0036 -0.0012 0.0023 -0.0101
0.0045 -0.0803 -0.0030 -0.0003 0.0345
-0.0077 0.0035 -0.3346 0.0087 -0.0083
0.0652 0.0176 -0.0019 -0.0011 0.0003
-0.0076 -0.0021 0.0012 -0.0013 -0.0024
(75.08%) 0.8665* P 5 s(45.74%)p 1.19(54.24%)d 0.00(0.02%)
0.0000 0.0008 0.6758 0.0266 0.0043
-0.0014 0.0004 0.1620 -0.0073 0.0026
-0.0004 -0.7133 0.0572 0.0020 0.0000
0.0627 0.0009 -0.0065 -0.0034 0.0000
-0.0020 -0.0112 -0.0053
4. (1.93106) BD (1)Fe 1 - N 8
(20.42%) 0.4519*Fe 1 s(18.42%)p 2.68(49.34%)d 1.75(32.18%)
f 0.00(0.06%)
0.0000 0.0000 0.0014 -0.4286 -0.0217
0.0000 -0.0003 0.6896 0.0616 -0.0002
-0.0021 0.0000 0.0000 -0.0237 -0.0021
0.0002 0.0016 0.0000 -0.0001 0.1161
0.0098 0.0012 -0.0010 -0.0345 -0.0021
-0.0003 0.1546 0.0061 0.0013 -0.0024
-0.0013 0.0002 0.4791 0.0198 0.0040
-0.2581 -0.0108 -0.0023 -0.0051 -0.0130
-0.0009 0.0078 -0.0001 0.0185 -0.0022
(79.58%) 0.8921* N 8 s(64.45%)p 0.55(35.55%)d 0.00(0.00%)
0.0000 0.8016 0.0435 -0.0028 -0.0001
-0.5864 0.0458 0.0048 0.0212 -0.0016
-0.0002 -0.0950 0.0043 0.0016 -0.0001
0.0004 0.0000 0.0019 -0.0009
5. (1.76371) BD (1)Fe 1 - C 23
(27.45%) 0.5240*Fe 1 s(14.70%)p 3.43(50.36%)d 2.38(34.92%)
f 0.00(0.03%)

0.0000 0.0000 0.0024 -0.3833 0.0068
0.0000 -0.0017 -0.6994 -0.0290 0.0077
-0.0040 0.0000 0.0001 0.0268 0.0008
-0.0002 -0.0014 0.0000 -0.0002 -0.1130
-0.0047 0.0025 0.0005 -0.0362 0.0015
-0.0002 0.1614 -0.0070 0.0025 -0.0047
-0.0002 -0.0003 0.4992 -0.0195 0.0072
-0.2682 0.0103 -0.0036 0.0020 0.0085
-0.0020 -0.0059 0.0005 -0.0120 0.0006
(72.55%) 0.8517* C 23 s(26.97%)p 2.71(73.03%)d 0.00(0.00%)
0.0007 0.5192 0.0058 0.0073 0.0001
0.8427 -0.0354 -0.0055 -0.0320 0.0006
0.0004 0.1334 -0.0063 -0.0012 0.0004
-0.0009 -0.0001 -0.0024 0.0012
1513. (0.04357) BD*(1)Fe 1 - P 3
(75.00%) 0.8660*Fe 1 s(22.10%)p 2.97(65.54%)d 0.56(12.36%)
f 0.00(0.01%)
0.0000 0.0000 0.0018 -0.4700 0.0030
0.0000 -0.0006 -0.1440 0.0154 0.0016
-0.0079 0.0000 0.0003 -0.4789 0.0132
-0.0005 -0.0004 0.0000 0.0014 0.6363
-0.0072 0.0047 0.0020 0.0503 0.0003
-0.0007 -0.1079 -0.0087 0.0016 -0.1041
0.0224 -0.0069 -0.2673 -0.0003 -0.0053
0.1624 -0.0056 0.0040 -0.0011 0.0011
-0.0075 -0.0013 0.0018 -0.0005 -0.0016
(25.00%) -0.5000* P 3 s(45.61%)p 1.19(54.37%)d 0.00(0.02%)
0.0000 0.0009 0.6748 0.0261 0.0044
-0.0013 0.0004 0.2963 -0.0194 0.0014
0.0002 0.2694 -0.0281 0.0033 -0.0003
-0.6165 0.0463 0.0044 0.0013 -0.0073
-0.0067 -0.0023 0.0082
1514. (0.04400) BD*(1)Fe 1 - P 4
(75.34%) 0.8680*Fe 1 s(22.28%)p 2.95(65.73%)d 0.54(11.98%)
f 0.00(0.01%)
0.0000 0.0000 0.0012 -0.4720 0.0029
0.0000 -0.0004 0.0875 0.0133 0.0038
-0.0055 0.0000 -0.0013 -0.3277 0.0023
-0.0026 -0.0029 0.0000 -0.0005 -0.7360
0.0174 0.0047 -0.0025 0.0104 0.0088
-0.0022 -0.0817 0.0103 -0.0062 0.0726
-0.0142 0.0036 -0.2421 -0.0118 -0.0018
0.2199 -0.0116 0.0064 -0.0014 0.0006
-0.0072 -0.0012 0.0020 -0.0015 -0.0022
(24.66%) -0.4966* P 4 s(46.11%)p 1.17(53.87%)d 0.00(0.02%)
0.0000 0.0008 0.6785 0.0271 0.0038
-0.0017 0.0003 0.1088 -0.0037 0.0030
0.0002 0.4019 -0.0288 -0.0074 0.0004

0.6016 -0.0503 0.0011 0.0019 0.0006
0.0097 -0.0040 0.0062
1515. (0.04386) BD*(1)Fe 1 - P 5
(75.08%) 0.8665*Fe 1 s(22.39%)p 2.91(65.15%)d 0.56(12.45%)
f 0.00(0.01%)
0.0000 0.0000 0.0018 -0.4732 0.0013
0.0000 -0.0002 -0.0073 0.0149 0.0020
-0.0063 0.0000 0.0010 0.8020 -0.0182
0.0024 0.0032 0.0000 -0.0012 0.0872
-0.0052 -0.0036 -0.0012 0.0023 -0.0101
0.0045 -0.0803 -0.0030 -0.0003 0.0345
-0.0077 0.0035 -0.3346 0.0087 -0.0083
0.0652 0.0176 -0.0019 -0.0011 0.0003
-0.0076 -0.0021 0.0012 -0.0013 -0.0024
(24.92%) -0.4992* P 5 s(45.74%)p 1.19(54.24%)d 0.00(0.02%)
0.0000 0.0008 0.6758 0.0266 0.0043
-0.0014 0.0004 0.1620 -0.0073 0.0026
-0.0004 -0.7133 0.0572 0.0020 0.0000
0.0627 0.0009 -0.0065 -0.0034 0.0000
-0.0020 -0.0112 -0.0053
1516. (0.08300) BD*(1)Fe 1 - N 8
(79.58%) 0.8921*Fe 1 s(18.42%)p 2.68(49.34%)d 1.75(32.18%)
f 0.00(0.06%)
0.0000 0.0000 0.0014 -0.4286 -0.0217
0.0000 -0.0003 0.6896 0.0616 -0.0002
-0.0021 0.0000 0.0000 -0.0237 -0.0021
0.0002 0.0016 0.0000 -0.0001 0.1161
0.0098 0.0012 -0.0010 -0.0345 -0.0021
-0.0003 0.1546 0.0061 0.0013 -0.0024
-0.0013 0.0002 0.4791 0.0198 0.0040
-0.2581 -0.0108 -0.0023 -0.0051 -0.0130
-0.0009 0.0078 -0.0001 0.0185 -0.0022
(20.42%) -0.4519* N 8 s(64.45%)p 0.55(35.55%)d 0.00(0.00%)
0.0000 0.8016 0.0435 -0.0028 -0.0001
-0.5864 0.0458 0.0048 0.0212 -0.0016
-0.0002 -0.0950 0.0043 0.0016 -0.0001
0.0004 0.0000 0.0019 -0.0009
1517. (0.09062) BD*(1)Fe 1 - C 23
(72.55%) 0.8517*Fe 1 s(14.70%)p 3.43(50.36%)d 2.38(34.92%)
f 0.00(0.03%)
0.0000 0.0000 0.0024 -0.3833 0.0068
0.0000 -0.0017 -0.6994 -0.0290 0.0077
-0.0040 0.0000 0.0001 0.0268 0.0008
-0.0002 -0.0014 0.0000 -0.0002 -0.1130
-0.0047 0.0025 0.0005 -0.0362 0.0015
-0.0002 0.1614 -0.0070 0.0025 -0.0047
-0.0002 -0.0003 0.4992 -0.0195 0.0072
-0.2682 0.0103 -0.0036 0.0020 0.0085

-0.0020 -0.0059 0.0005 -0.0120 0.0006
(27.45%) -0.5240* C 23 s(26.97%)p 2.71(73.03%)d 0.00(0.00%)
0.0007 0.5192 0.0058 0.0073 0.0001
0.8427 -0.0354 -0.0055 -0.0320 0.0006
0.0004 0.1334 -0.0063 -0.0012 0.0004
-0.0009 -0.0001 -0.0024 0.0012

(0.03482) BD*(1) C 11 - C 23
(48.70%)   0.6978* C 11 s(33.58%)p 1.98(66.38%)d 0.00(0.03%)
-0.0001 -0.5792 -0.0172 -0.0008 0.0009
-0.2099 0.0082 -0.0022 -0.6201 0.0243
0.0038 -0.4842 0.0106 0.0047 -0.0066
-0.0035 -0.0148 0.0080 0.0001
(51.30%) -0.7163* C 23 s(24.80%)p 3.03(75.13%)d 0.00(0.07%)
0.0002 -0.4979 0.0073 0.0026 0.0001
0.2526 0.0037 -0.0023 0.6602 0.0177
0.0084 0.5012 0.0072 0.0070 -0.0160
-0.0119 -0.0162 0.0080 -0.0005
1537. (0.03133) BD*(1) C 11 - C 39
(49.58%)   0.7041* C 11 s(33.03%)p 2.03(66.94%)d 0.00(0.02%)
0.0002 -0.5746 0.0136 0.0025 -0.0007
0.7661 0.0163 0.0115 0.2861 -0.0003
-0.0004 -0.0117 -0.0095 0.0016 -0.0089
-0.0019 0.0018 -0.0092 0.0076
(50.42%) -0.7101* C 39 s(33.98%)p 1.94(65.94%)d 0.00(0.08%)
-0.0002 -0.5829 -0.0049 -0.0014 -0.7523
0.0055 0.0184 -0.3044 -0.0110 0.0071
0.0055 -0.0137 -0.0018 -0.0173 0.0018
-0.0100 -0.0141 0.0134
1538. (0.31948) BD*(2) C 11 - C 39
(53.31%)   0.7301* C 11 s(0.01%)p 1.00(99.94%)d 0.00(0.05%)
0.0000 -0.0091 -0.0008 0.0005 0.0025
-0.2612 0.0062 -0.0044 0.6523 -0.0040
0.0005 -0.7110 0.0039 -0.0054 -0.0060
0.0132 0.0050 0.0137 0.0093
(46.69%) -0.6833* C 39 s(0.00%)p 1.00(99.97%)d 0.00(0.02%)
-0.0001 -0.0048 0.0023 0.0001 -0.2638
0.0066 0.0017 0.6482 -0.0144 -0.0055
-0.7138 0.0129 0.0081 0.0090 -0.0090
-0.0039 -0.0043 0.0067
1558. (0.03658) BD*(1) C 23 - C 26
(51.30%)   0.7162* C 23 s(23.91%)p 3.18(76.01%)d 0.00(0.07%)
-0.0003 0.4890 -0.0055 -0.0027 -0.0003
-0.4236 -0.0066 0.0002 -0.0470 0.0005
-0.0019 0.7603 0.0164 0.0102 0.0010
-0.0242 -0.0001 0.0069 0.0093
(48.70%) -0.6978* C 26 s(32.91%)p 2.04(67.05%)d 0.00(0.03%)
0.0002 0.5734 0.0183 0.0001 -0.0007

0.3768 -0.0128 0.0010 0.0404 0.0037
-0.0022 -0.7253 0.0264 0.0054 -0.0006
-0.0125 -0.0013 0.0037 0.0127

1559. (0.03587) BD*(1) C 23 - C 38
(51.26%) 0.7160* C 23 s(24.27%)p 3.12(75.66%)d 0.00(0.07%)
-0.0003 0.4926 -0.0058 -0.0027 0.0002
-0.2136 -0.0013 0.0027 0.7478 0.0151
0.0099 -0.3889 -0.0133 -0.0023 -0.0168
0.0086 -0.0151 -0.0112 -0.0028
(48.74%) -0.6981* C 38 s(33.14%)p 2.02(66.83%)d 0.00(0.03%)
0.0002 0.5754 0.0159 0.0008 -0.0006
0.1860 -0.0064 0.0016 -0.7162 0.0203
0.0055 0.3463 -0.0171 -0.0001 -0.0052
0.0044 -0.0119 -0.0114 -0.0037

Second-order perturbation analysis: donor-acceptor interactions involving the Fe-C σ bond:

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
5. BD (1)Fe 1 - C 23	/263. RY*(1)Fe 1	0.57	0.86	0.021
5. BD (1)Fe 1 - C 23	/266. RY*(4)Fe 1	0.87	0.93	0.027
5. BD (1)Fe 1 - C 23	/300. RY*(2) P 3	0.63	1.49	0.029
5. BD (1)Fe 1 - C 23	/303. RY*(5) P 3	1.04	1.17	0.033
5. BD (1)Fe 1 - C 23	/305. RY*(7) P 3	1.11	1.45	0.038
5. BD (1)Fe 1 - C 23	/315. RY*(3) P 4	0.53	1.36	0.025
5. BD (1)Fe 1 - C 23	/317. RY*(5) P 4	0.90	1.14	0.030
5. BD (1)Fe 1 - C 23	/319. RY*(7) P 4	1.72	1.38	0.046
5. BD (1)Fe 1 - C 23	/328. RY*(2) P 5	0.57	1.51	0.028
5. BD (1)Fe 1 - C 23	/329. RY*(3) P 5	0.63	1.36	0.028
5. BD (1)Fe 1 - C 23	/331. RY*(5) P 5	0.67	1.18	0.027
5. BD (1)Fe 1 - C 23	/333. RY*(7) P 5	1.90	1.44	0.050
5. BD (1)Fe 1 - C 23	/371. RY*(3) N 8	3.86	1.19	0.064
5. BD (1)Fe 1 - C 23	/378. RY*(10) N 8	1.14	1.87	0.044
5. BD (1)Fe 1 - C 23	/412. RY*(2) C 11	2.10	1.13	0.046
5. BD (1)Fe 1 - C 23	/432. RY*(8) C 12	3.50	0.47	0.038
5. BD (1)Fe 1 - C 23	/434. RY*(10) C 12	1.29	1.63	0.044
5. BD (1)Fe 1 - C 23	/453. RY*(5) H 15	0.80	2.95	0.046
5. BD (1)Fe 1 - C 23	/496. RY*(6) C 20	13.77	0.19	0.048
5. BD (1)Fe 1 - C 23	/512. RY*(8) C 21	3.90	0.42	0.039
5. BD (1)Fe 1 - C 23	/513. RY*(9) C 21	3.23	0.66	0.044
5. BD (1)Fe 1 - C 23	/524. RY*(1) C 23	3.81	1.47	0.071
5. BD (1)Fe 1 - C 23	/531. RY*(8) C 23	2.41	3.06	0.082
5. BD (1)Fe 1 - C 23	/545. RY*(8) C 24	0.62	1.10	0.025

5. BD (1)Fe 1 - C 23	/548. RY*(11) C 24	1.47	0.68	0.030
5. BD (1)Fe 1 - C 23	/569. RY*(13) C 26	0.56	1.46	0.027
5. BD (1)Fe 1 - C 23	/584. RY*(14) C 27	4.48	0.63	0.051
5. BD (1)Fe 1 - C 23	/588. RY*(4) H 28	2.49	1.14	0.051
5. BD (1)Fe 1 - C 23	/615. RY*(12) C 30	5.84	0.42	0.047
5. BD (1)Fe 1 - C 23	/631. RY*(9) C 32	1.63	1.14	0.041
5. BD (1)Fe 1 - C 23	/652. RY*(12) C 34	5.10	0.35	0.040
5. BD (1)Fe 1 - C 23	/676. RY*(3) H 37	0.51	1.83	0.029
5. BD (1)Fe 1 - C 23	/677. RY*(4) H 37	1.46	1.03	0.037
5. BD (1)Fe 1 - C 23	/700. RY*(8) C 39	0.63	2.53	0.038
5. BD (1)Fe 1 - C 23	/735. RY*(6) C 43	2.67	0.62	0.038
5. BD (1)Fe 1 - C 23	/736. RY*(7) C 43	0.80	0.84	0.025
5. BD (1)Fe 1 - C 23	/739. RY*(10) C 43	0.59	1.10	0.024
5. BD (1)Fe 1 - C 23	/743. RY*(14) C 43	3.25	1.35	0.063
5. BD (1)Fe 1 - C 23	/754. RY*(1) H 46	5.82	0.38	0.045
5. BD (1)Fe 1 - C 23	/757. RY*(4) H 46	0.80	1.10	0.028
5. BD (1)Fe 1 - C 23	/764. RY*(6) C 47	1.28	1.17	0.037
5. BD (1)Fe 1 - C 23	/776. RY*(4) H 48	0.65	0.54	0.018
5. BD (1)Fe 1 - C 23	/785. RY*(3) H 50	4.77	0.96	0.064
5. BD (1)Fe 1 - C 23	/794. RY*(7) C 51	0.55	1.71	0.029
5. BD (1)Fe 1 - C 23	/795. RY*(8) C 51	3.39	0.73	0.047
5. BD (1)Fe 1 - C 23	/804. RY*(4) H 52	0.60	1.90	0.032
5. BD (1)Fe 1 - C 23	/808. RY*(3) C 53	2.92	0.71	0.043
5. BD (1)Fe 1 - C 23	/822. RY*(3) H 54	0.82	2.33	0.042
5. BD (1)Fe 1 - C 23	/827. RY*(3) H 55	0.52	2.36	0.033
5. BD (1)Fe 1 - C 23	/833. RY*(4) H 56	0.55	0.49	0.016
5. BD (1)Fe 1 - C 23	/846. RY*(12) C 57	0.67	2.21	0.037
5. BD (1)Fe 1 - C 23	/848. RY*(14) C 57	7.14	0.79	0.071
5. BD (1)Fe 1 - C 23	/850. RY*(2) H 58	1.26	0.70	0.028
5. BD (1)Fe 1 - C 23	/854. RY*(1) H 59	1.34	0.76	0.030
5. BD (1)Fe 1 - C 23	/857. RY*(4) H 59	3.54	0.54	0.041
5. BD (1)Fe 1 - C 23	/859. RY*(1) H 60	0.65	0.91	0.023
5. BD (1)Fe 1 - C 23	/861. RY*(3) H 60	1.22	1.97	0.047
5. BD (1)Fe 1 - C 23	/864. RY*(1) C 61	0.88	1.33	0.032
5. BD (1)Fe 1 - C 23	/890. RY*(13) C 62	0.72	1.59	0.032
5. BD (1)Fe 1 - C 23	/891. RY*(14) C 62	0.55	1.73	0.029
5. BD (1)Fe 1 - C 23	/901. RY*(5) H 64	3.15	1.83	0.072
5. BD (1)Fe 1 - C 23	/910. RY*(4) C 66	2.18	0.96	0.044
5. BD (1)Fe 1 - C 23	/918. RY*(12) C 66	2.46	1.24	0.053
5. BD (1)Fe 1 - C 23	/928. RY*(3) H 68	13.25	0.43	0.071
5. BD (1)Fe 1 - C 23	/930. RY*(5) H 68	0.91	2.71	0.047
5. BD (1)Fe 1 - C 23	/931. RY*(1) H 69	1.12	0.98	0.032
5. BD (1)Fe 1 - C 23	/932. RY*(2) H 69	10.78	0.55	0.074
5. BD (1)Fe 1 - C 23	/935. RY*(5) H 69	1.12	2.62	0.051
5. BD (1)Fe 1 - C 23	/961. RY*(7) C 72	0.76	0.74	0.023
5. BD (1)Fe 1 - C 23	/966. RY*(12) C 72	19.18	0.24	0.065
5. BD (1)Fe 1 - C 23	/978. RY*(5) C 74	1.79	0.86	0.037
5. BD (1)Fe 1 - C 23	/979. RY*(6) C 74	5.12	0.75	0.059

5. BD (1)Fe 1 - C 23	/980. RY*(7) C 74	1.45	0.87	0.034
5. BD (1)Fe 1 - C 23	/982. RY*(9) C 74	4.59	0.92	0.062
5. BD (1)Fe 1 - C 23	/985. RY*(12) C 74	2.97	1.37	0.061
5. BD (1)Fe 1 - C 23	/992. RY*(5) H 75	1.19	2.22	0.049
5. BD (1)Fe 1 - C 23	/***. RY*(6) C 78	3.08	1.03	0.054
5. BD (1)Fe 1 - C 23	/***. RY*(12) C 78	0.96	1.33	0.034
5. BD (1)Fe 1 - C 23	/***. RY*(2) C 86	1.36	0.77	0.031
5. BD (1)Fe 1 - C 23	/***. RY*(5) C 86	1.23	0.97	0.033
5. BD (1)Fe 1 - C 23	/***. RY*(7) C 86	0.81	1.27	0.030
5. BD (1)Fe 1 - C 23	/***. RY*(8) C 86	0.51	0.98	0.021
5. BD (1)Fe 1 - C 23	/***. RY*(9) C 86	1.16	1.40	0.038
5. BD (1)Fe 1 - C 23	/***. RY*(1) H 89	0.54	0.92	0.021
5. BD (1)Fe 1 - C 23	/***. RY*(2) H 89	9.27	0.67	0.075
5. BD (1)Fe 1 - C 23	/***. RY*(4) C 90	10.95	0.31	0.055
5. BD (1)Fe 1 - C 23	/***. RY*(9) C 90	0.77	0.85	0.024
5. BD (1)Fe 1 - C 23	/***. RY*(11) C 90	0.73	0.75	0.022
5. BD (1)Fe 1 - C 23	/***. RY*(13) C 92	1.62	0.85	0.035
5. BD (1)Fe 1 - C 23	/***. RY*(4) H 102	1.02	0.67	0.025
5. BD (1)Fe 1 - C 23	/***. RY*(5) H 103	0.88	2.79	0.047
5. BD (1)Fe 1 - C 23	/***. RY*(4) C 112	2.27	0.90	0.043
5. BD (1)Fe 1 - C 23	/***. RY*(6) C 112	2.37	0.65	0.037
5. BD (1)Fe 1 - C 23	/***. RY*(7) C 112	2.49	0.74	0.041
5. BD (1)Fe 1 - C 23	/***. RY*(8) C 112	0.58	1.91	0.032
5. BD (1)Fe 1 - C 23	/***. RY*(4) H 113	2.34	0.39	0.029
5. BD (1)Fe 1 - C 23	/***. RY*(6) C 116	4.87	0.49	0.047
5. BD (1)Fe 1 - C 23	/***. RY*(7) C 116	10.17	0.31	0.053
5. BD (1)Fe 1 - C 23	/***. RY*(4) H 117	2.79	0.41	0.032
5. BD (1)Fe 1 - C 23	/***. RY*(1) H 119	0.79	0.89	0.025
5. BD (1)Fe 1 - C 23	/***. RY*(4) H 119	1.65	0.92	0.037
5. BD (1)Fe 1 - C 23	/***. RY*(4) C 127	4.63	0.83	0.059
5. BD (1)Fe 1 - C 23	/***. RY*(3) H 128	3.11	1.36	0.062
5. BD (1)Fe 1 - C 23	/***. BD*(1)Fe 1 - P 3	7.31	0.66	0.065
5. BD (1)Fe 1 - C 23	/***. BD*(1)Fe 1 - P 4	6.04	0.64	0.058
5. BD (1)Fe 1 - C 23	/***. BD*(1)Fe 1 - P 5	7.73	0.66	0.067
5. BD (1)Fe 1 - C 23	/***. BD*(1)Fe 1 - N 8	8.40	0.63	0.068
5. BD (1)Fe 1 - C 23	/***. BD*(1)Fe 1 - C 23	4.92	0.55	0.048
5. BD (1)Fe 1 - C 23	/***. BD*(1) P 3 - C 20	2.43	0.53	0.034
5. BD (1)Fe 1 - C 23	/***. BD*(1) P 3 - C 30	3.29	0.49	0.037
5. BD (1)Fe 1 - C 23	/***. BD*(1) P 3 - C 36	0.77	0.47	0.018
5. BD (1)Fe 1 - C 23	/***. BD*(1) P 4 - C 61	2.52	0.53	0.034
5. BD (1)Fe 1 - C 23	/***. BD*(1) P 4 - C 72	3.78	0.48	0.040
5. BD (1)Fe 1 - C 23	/***. BD*(1) P 4 - C 78	0.93	0.47	0.019
5. BD (1)Fe 1 - C 23	/***. BD*(1) P 5 - C 29	2.49	0.53	0.034
5. BD (1)Fe 1 - C 23	/***. BD*(1) P 5 - C 70	0.95	0.47	0.020
5. BD (1)Fe 1 - C 23	/***. BD*(1) P 5 - C 92	3.17	0.48	0.036
5. BD (1)Fe 1 - C 23	/***. BD*(1) C 11 - C 39	6.70	0.86	0.071
5. BD (1)Fe 1 - C 23	/***. BD*(2) C 11 - C 39	1.46	0.31	0.019
5. BD (1)Fe 1 - C 23	/***. BD*(1) C 20 - C 26	5.95	0.43	0.048

5. BD (1)Fe 1 - C 23	/***. BD*(1) C 23 - C 26	1.21	0.68	0.027
5. BD (1)Fe 1 - C 23	/***. BD*(1) C 23 - C 38	4.61	0.55	0.048
5. BD (1)Fe 1 - C 23	/***. BD*(1) C 27 - C 38	5.99	0.86	0.068
5. BD (1)Fe 1 - C 23	/***. BD*(2) C 27 - C 38	2.45	0.32	0.026
5. BD (1)Fe 1 - C 23	/***. BD*(1) C 66 - H 67	9.18	0.27	0.047
5. BD (1)Fe 1 - C 23	/***. BD*(1) C 66 - C 72	2.11	0.49	0.031
5. BD (1)Fe 1 - C 23	/***. BD*(1) C 74 - H 75	2.73	0.68	0.041
5. BD (1)Fe 1 - C 23	/***. BD*(1) C 112 - H 113	0.68	0.82	0.022
5. BD (1)Fe 1 - C 23	/***. BD*(1) C 116 - H 117	3.29	0.51	0.039