Protonation of Ferrous Dinitrogen Complexes Containing a Diphosphine Ligand with a Pendent Amine

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Supporting Information

Index

1) Molecular Structures

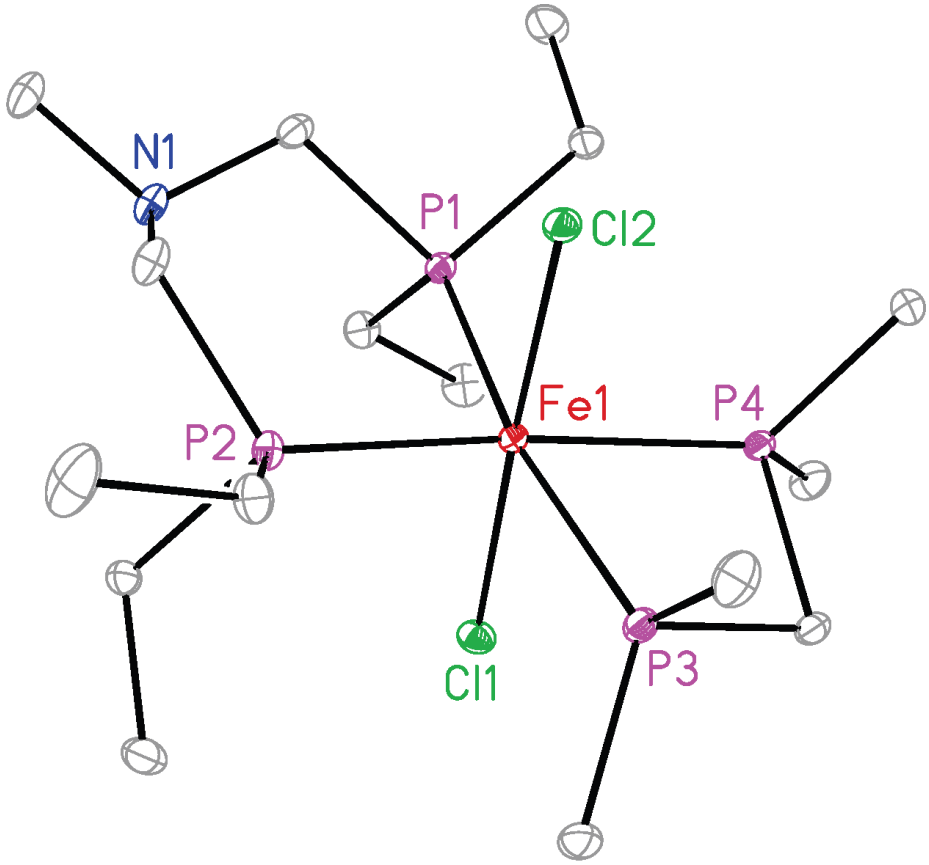


Figure S1. Molecular structure of $FeCl_2(P^{Et}N^{Me}P^{Et})$(dmpm) (**1(Cl)**). Thermal ellipsoids are drawn at 30 % probability.

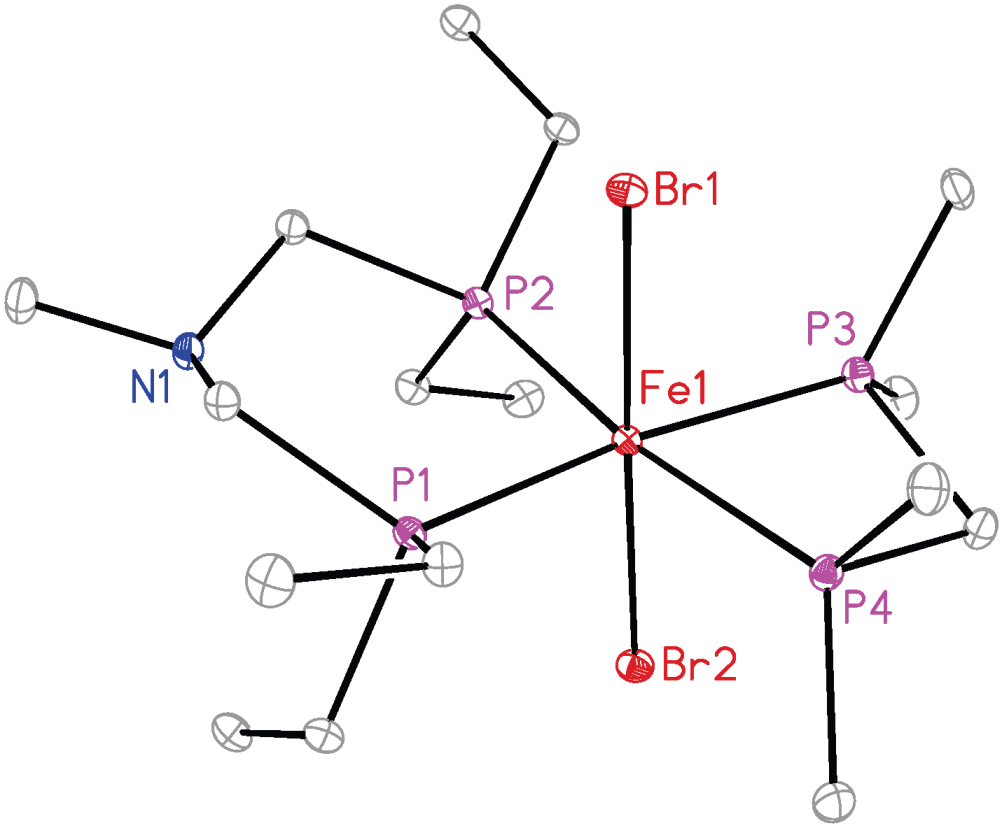


Figure S2. Molecular structures of $FeBr_2(P^{Et}N^{Me}P^{Et})$(dmpm) (**2(Br)**). Thermal ellipsoids are drawn at 30 % probability.

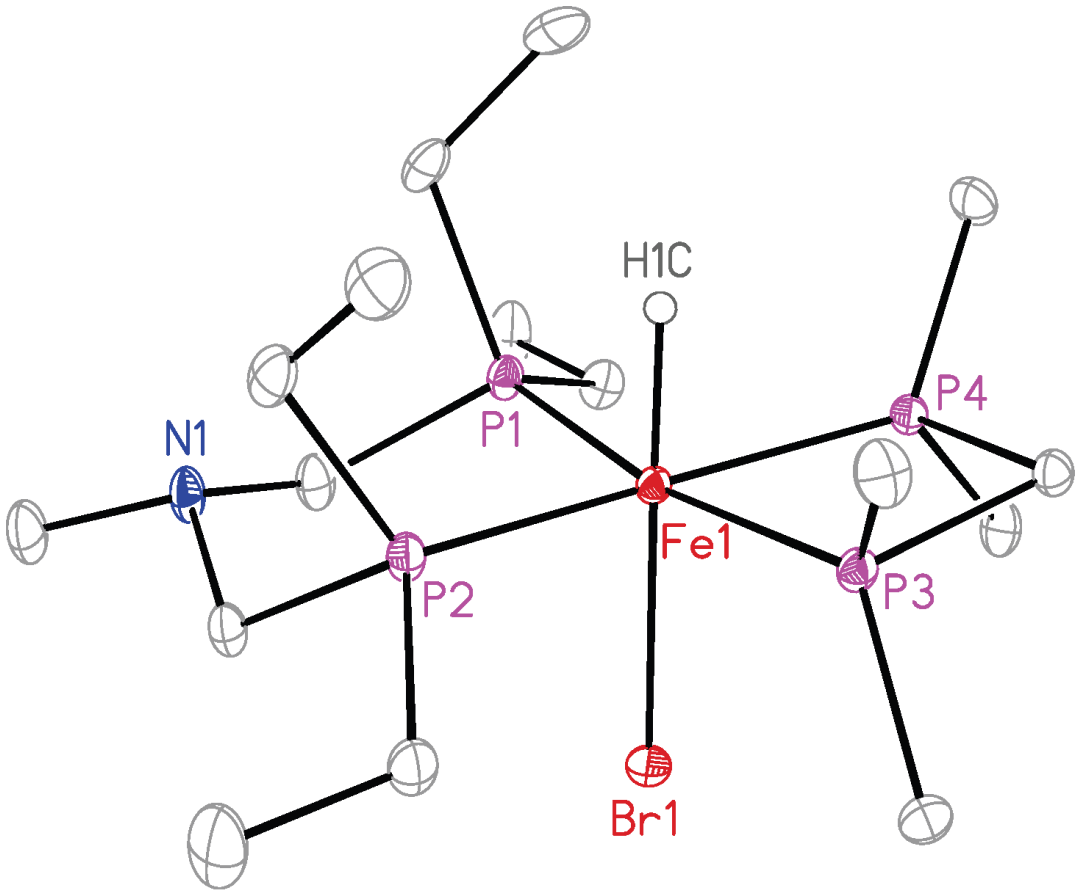


Figure S3. Molecular structure of FeHBr($P^{Et}N^{Me}P^{Et}$)(dmpm) (**2(H)**). Thermal ellipsoids are drawn at 30 % probability.

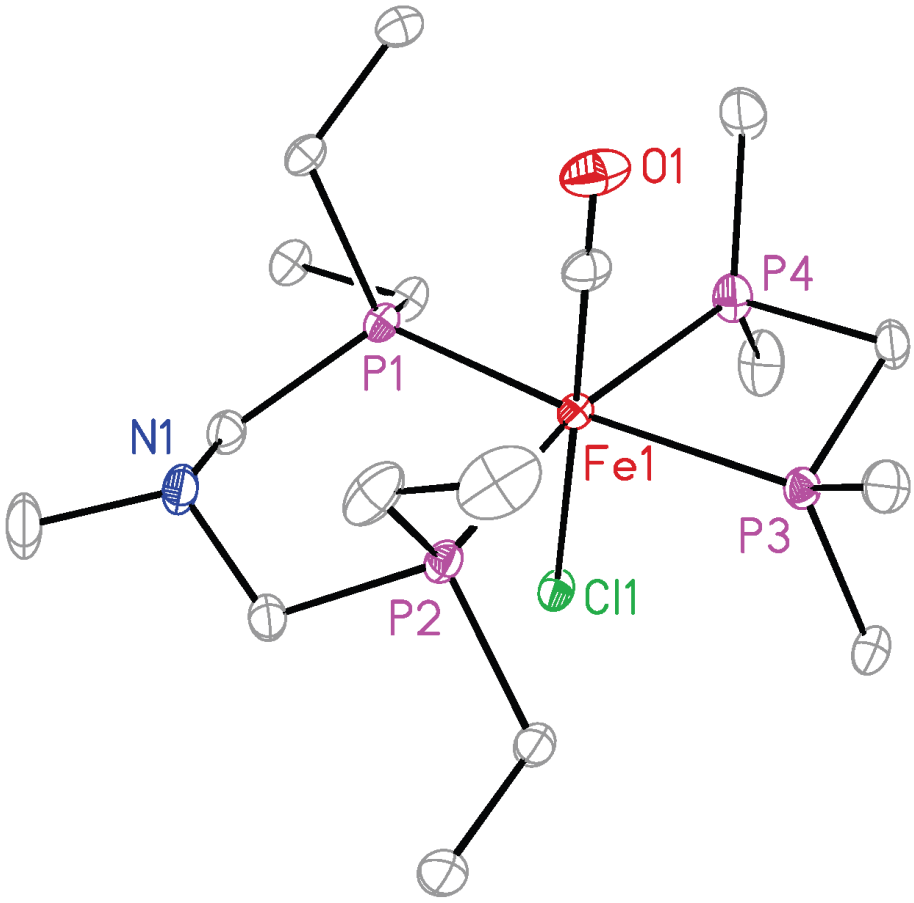


Figure S4. Molecular structure of the cation $[FeCl(CO)(P^{Et}N^{Me}P^{Et})(dmpm)]^+$ (**[1(CO)]$^+$**). The thermal ellipsoids are drawn at 30% and the BPh_4^- anions are removed for clarity.

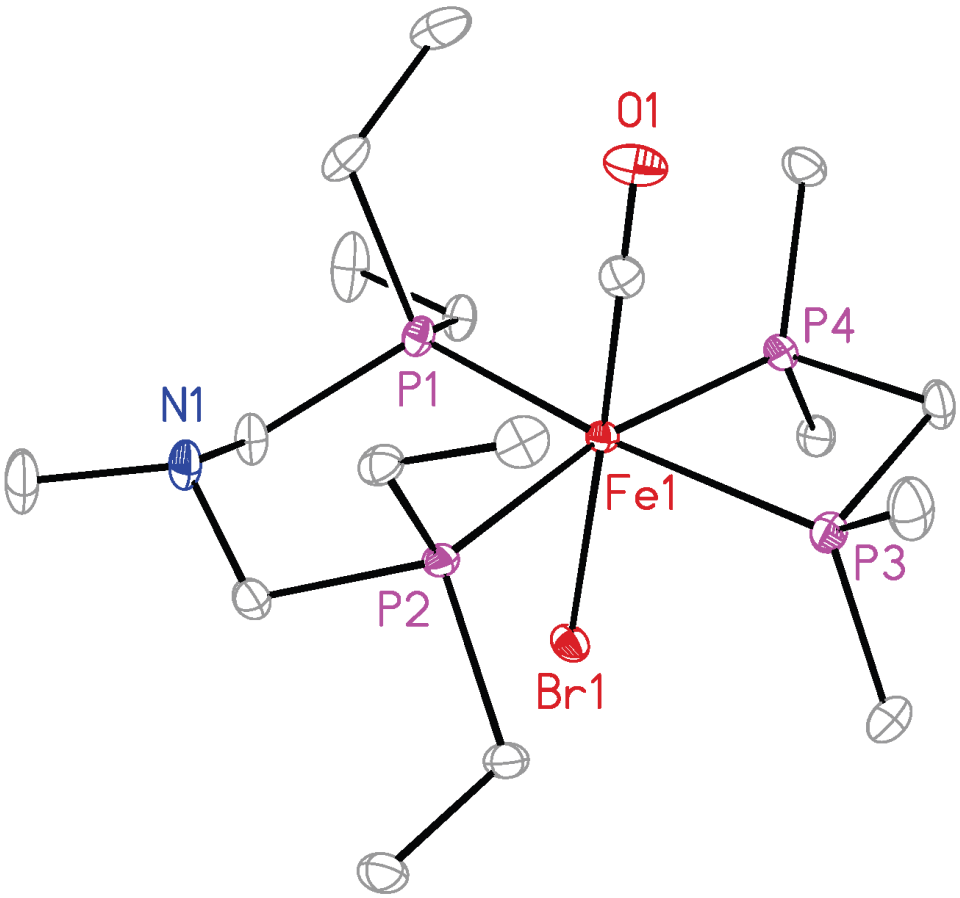


Figure S5. Molecular structure of the cation $[FeBr(CO)(P^{Et}N^{Me}P^{Et})(dmpm)]^+$ (**[2(CO)]$^+$**). The thermal ellipsoids are drawn at 30% and the BPh_4^- anions are removed for clarity.

2) X-ray diffraction studies

X-ray structural analysis for **1(Cl)**: A single green block (0.10 × 0.18 × 0.20 mm) was mounted using NVH immersion oil onto a nylon fiber and cooled to the data collection temperature of 100(2) K. Data were collected on a Brüker-AXS Kappa APEX II CCD diffractometer with 0.71073 Å Mo-K□ radiation. Unit cell parameters were obtained from 60 data frames, 0.5º Φ, from three different sections of the Ewald sphere yielding a = 13.415(1), b = 10.529(1), c = 18.091(2) Å, β = 105.94(1)°, V = 2457.2(3) Å^3. 49678 reflections (R_{int} = 0.0356) were collected (9365 unique) over θ = 2.26 to 33.16°. The systematic absences in the data were consistent with the centrosymmetric, monoclinic space group *P*2(1)/*c*. The data-set was treated with SADABS absorption corrections based on redundant multi-scan data T_{max}/T_{min} = 1.11. The asymmetric unit contains one (PNP)Fe(dmpm)Cl_2 molecule located on a general position yielding Z = 4. One of the ethyl groups on the PNP ligand was disordered over two positions which were located from the difference map and refined using SIMU, DELU, and SAME commands. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were treated as idealized contributions. The goodness of fit on F^2 was 1.019 with *R*1(*wR*2) 0.0257(0.0603) for [*I*□>2(*I*)] and with largest difference peak and hole of 0.674 and –0.525 e/Å^3.

X-ray structural analysis for **2(Br)**: A single yellow plate (0.04 × 0.10 × 0.16 mm) was mounted using NVH immersion oil onto a nylon fiber and cooled to the data collection temperature of 100(2) K. Data were collected on a Brüker-AXS Kappa APEX II CCD diffractometer with 0.71073 Å Mo-K□ radiation. Unit cell parameters were obtained from 60 data frames, 0.5º Φ, from three different sections of the Ewald sphere yielding a = 15.559(1), b = 9.979(1), c = 15.830(1) Å, β = 99.67(1)°, V = 2458(2) Å^3. 46183 reflections (R_{int} = 0.0585) were collected (9394 unique) over θ = 1.31 to 33.19°. The systematic absences in the data were consistent with the centrosymmetric, monoclinic space group *P*2(1)/*c*. The data-set was treated with SADABS absorption corrections based on redundant multi-scan data T_{max}/T_{min} = 1.53. The asymmetric unit contains one (PNP)Fe(dmpm)Br_2 molecule located on a general position yielding Z = 4. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were treated as idealized contributions. The goodness of fit on F^2 was 1.008 with *R*1(*wR*2) 0.0343(0.0577) for [*I*□>2(*I*)] and with largest difference peak and hole of 0.608 and –0.530 e/Å^3.

X-ray structural analysis for **2(H)**: An orange needle (0.03 × 0.20 × 0.22 mm) was mounted using NVH immersion oil onto a nylon fiber and cooled to the data collection temperature of 110(2) K. Data were collected on a Brüker-AXS Kappa APEX II CCD diffractometer with 0.71073 Å Mo-K□ radiation. Unit cell parameters were obtained from 60 data frames, 0.5º Φ, from three different sections of the Ewald sphere yielding a = 16.431(2), b = 19.339(3), c = 7.469(1) Å, V = 2430.8(5) Å^3. 43048 reflections (R_{int} = 0.0785) were collected (8709 unique) over θ = 1.63 to 33.17°. The systematic absences in the data were consistent with the non-centrosymmetric, orthorhombic space group *Pna*2(1). The data-set was treated with SADABS absorption corrections based on redundant multi-scan data (Sheldrick, G,.Bruker-AXS, 2001) T_{max}/T_{min} = 1.66. The asymmetric unit contains one (PNP)(dmpm)Fe(H)Br molecule located on a general position yielding Z = 8. The hydride ligand was located from the difference map and allowed to refine freely. The solution crystallized in a non-centrosymmetric space group but the flack parameter would not refine to 0. Therefore racemic twinning was modeled using TWIN and a BASF command to account for this. All non-hydrogen atoms were refined with anisotropic displacement parameters. All

other hydrogen atoms were treated as idealized contributions. The goodness of fit on F^2 was 1.011 with $R1(wR2)$ 0.0424(0.0613) for [I□>2(I)] and with largest difference peak and hole of 0.492 and –0.533 e/Å^3.

X-ray structural analysis for **[3(N$_2$)]B(C$_6$F$_5$)$_4$**: A single yellow block (0.14 × 0.20 × 0.28 mm) was mounted using NVH immersion oil onto a nylon fiber and cooled to the data collection temperature of 110(2) K. Data were collected on a Brüker-AXS Kappa APEX II CCD diffractometer with 0.71073 Å Mo-K□ radiation. Unit cell parameters were obtained from 60 data frames, 0.5º Φ, from three different sections of the Ewald sphere yielding a = 17.144(2), b = 13.525(1), c = 19.908(2) Å, β = 90.71(1)°, V = 4615.8(5) Å^3. 83409 reflections (R_{int} = 0.0309) were collected (16739 unique) over θ = 1.82 to 32.62°. The systematic absences in the data were consistent with the centrosymmetric, monoclinic space group $P2(1)/c$. The data-set was treated with SADABS absorption corrections based on redundant multi-scan data T_{max}/T_{min} = 1.08. The asymmetric unit contains one [Fe(H)(PNP)(dmpm)N$_2$]$^+$ cation and one [B(C$_6$F$_5$)$_4$]$^-$ anion located on general positions yielding Z = 4. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were treated as idealized contributions. The goodness of fit on F^2 was 1.012 with $R1(wR2)$ 0.0331(0.0845) for [I□>2(I)] and with largest difference peak and hole of 0.567 and –0.312 e/Å^3.

X-ray structural analysis for **[3(NH$_3$)]B(C$_6$F$_5$)$_4$**: A single yellow plate (0.03 × 0.10 × 0.26 mm) was mounted using NVH immersion oil onto a nylon fiber and cooled to the data collection temperature of 120(2) K. Data were collected on a Brüker-AXS Kappa APEX II CCD diffractometer with 0.71073 Å Mo-K□ radiation. Unit cell parameters were obtained from 60 data frames, 0.5º Φ, from three different sections of the Ewald sphere yielding a = 17.261(2), b = 13.467(2), c = 19.843(3) Å, β = 90.52(1)°, V = 4612(1) Å^3. 55276 reflections (R_{int} = 0.0715) were collected (11338 unique) over θ = 1.83 to 28.39°. The systematic absences in the data were consistent with the centrosymmetric, monoclinic space group $P2(1)/c$. The data-set was treated with SADABS absorption corrections based on redundant multi-scan data T_{max}/T_{min} = 1.14. The asymmetric unit contains one [Fe(PNP)(dmpm)(H)(NH$_3$)]$^+$ cation and one [B(C$_6$F$_5$)$_4$]$^-$ anion located on general positions yielding Z = 4. The hydride ligand was located from the difference map and allowed to refine freely. The protons on the ammonia ligand were located from the difference map and refined using a riding model that chose their position by maximizing electron density while allowing the individual N-H bond lengths to vary. All non-hydrogen atoms were refined with anisotropic displacement parameters. All other hydrogen atoms were treated as idealized contributions. The goodness of fit on F^2 was 1.013 with $R1(wR2)$ 0.0526(0.1080) for [I□>2(I)] and with largest difference peak and hole of 0.794 and –0.533 e/Å^3.

X-ray structural analysis for **[1(CO)]BPh$_4$**: A single yellow needle (0.08 × 0.20 × 0.30 mm) was mounted using NVH immersion oil onto a nylon fiber and cooled to the data collection temperature of 100(2) K. Data were collected on a Brüker-AXS Kappa APEX II CCD diffractometer with 0.71073 Å Mo-K□ radiation. Unit cell parameters were obtained from 60 data frames, 0.5º Φ, from three different sections of the Ewald sphere yielding a = 19.253(3), b = 9.943(2), c = 23.458(4) Å, β = 99.04(1)°, V = 4435(2) Å^3. 77894 reflections (R_{int} = 0.0389) were collected (16808 unique) over θ = 1.49 to 33.20°. The systematic absences in the data were consistent with the centrosymmetric, monoclinic space group $P2(1)/n$. The data-set was treated with SADABS absorption corrections based on redundant multi-scan data T_{max}/T_{min} =

1.13. The asymmetric unit contains one $[(PNP)Fe(dmpm)(CO)Cl]^+$ cation, one $[BPh_4]^-$ anion located on general positions and a molecule of THF solvent located on a special position yielding Z = 4. The molecule of THF was disordered about the special position. Modeling using the PART -1 command was attempted but the model would not survive refinement with chemically reasonable bond lengths and angles. The solvent is not interacting with the cation or anion so it was removed using Platon SQUEEZE and the empirical formula was altered to include this solvent. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were treated as idealized contributions. The goodness of fit on F^2 was 1.040 with $R1(wR2)$ 0.0467(0.1201) for [I□>2(I)] and with largest difference peak and hole of 1.393 and –0.581 e/Å^3.

X-ray structural analysis for **[2(CO)]BPh$_4$**: A single yellow blade (0.05 × 0.20 × 0.22 mm) was mounted using NVH immersion oil onto a nylon fiber and cooled to the data collection temperature of 100(2) K. Data were collected on a Brüker-AXS Kappa APEX II CCD diffractometer with 0.71073 Å Mo-K□ radiation. Unit cell parameters were obtained from 60 data frames, 0.5º Φ, from three different sections of the Ewald sphere yielding a = 19.399(2), b = 9.895(1), c = 23.439(2) Å, β = 98.60(1)°, V = 4448.5(5) Å^3. 86850 reflections (R_{int} = 0.0499) were collected (16809 unique) over θ = 1.48 to 33.16°. The systematic absences in the data were consistent with the centrosymmetric, monoclinic space group $P2(1)/n$. The data-set was treated with SADABS absorption corrections based on redundant multi-scan data T_{max}/T_{min} = 1.25. The asymmetric unit contains one $[(PNP)Fe(dmpm)Br(CO)]^+$ cation, one $[BPh_4]^-$ anion located on general positions and a molecule of THF solvent located on a special position yielding Z = 4. The THF solvent is disordered over two positions about the inversion center. One position of the THF molecule was located from the difference map and refined using PART -1 and the occupancy for this solvent was set at 0.5. SIMU and DELU commands were used to keep the thermal parameters of this THF molecule in check. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were treated as idealized contributions. The goodness of fit on F^2 was 1.007 with $R1(wR2)$ 0.0407(0.0901) for [I□>2(I)] and with largest difference peak and hole of 0.876 and –0.409 e/Å^3.

X-ray structural analysis for **4**: A single orange blade (0.10 × 0.12 × 0.14 mm) was mounted using NVH immersion oil onto a nylon fiber and cooled to the data collection temperature of 110(2) K. Data were collected on a Brüker-AXS Kappa APEX II CCD diffractometer with 0.71073 Å Mo-K□ radiation. Unit cell parameters were obtained from 60 data frames, 0.5º Φ, from three different sections of the Ewald sphere yielding a = 10.202(2), b = 16.764(2), c = 16.945(2) Å, α = 88.39(1), β = 89.90(1), γ = 85.78(1)°, V = 2889(1) Å^3. 60504 reflections (R_{int} = 0.0359) were collected (21921 unique) over θ = 1.69 to 33.24°. The data was consistent with the centrosymmetric, triclinic space group P-1. The data-set was treated with SADABS absorption corrections based on redundant multi-scan data, T_{max}/T_{min} = 1.03. The asymmetric unit contains two independent molecules of $(PNP)_2Fe$ located on general positions yielding Z = 4. The hydride ligands were located from the difference map and allowed to refine freely. All non-hydrogen atoms were refined with anisotropic displacement parameters. All other hydrogen atoms were treated as idealized contributions. The goodness of fit on F^2 was 1.012 with $R1(wR2)$ 0.0384(0.0766) for [I□>2(I)] and with largest difference peak and hole of 0.508 and –0.414 e/Å^3.

3) ^{15}N NMR of [3(N_2)]B(C_6F_5)$_4$ in THF-d_8

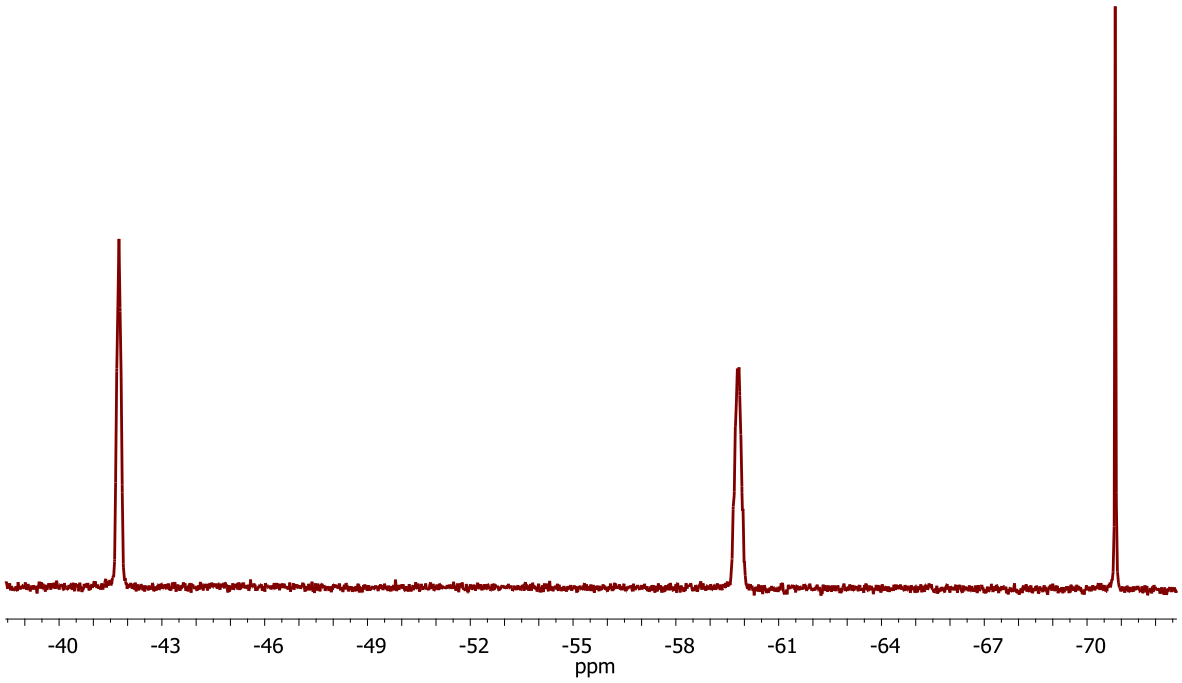


Figure S6. ^{15}N NMR of **[3(N_2)]B(C_6F_5)$_4$** in THF-d_8. The peak at -70.8 ppm is free $^{15}N_2$.

4) Multinuclear NMR of $[3(N_2)]B(C_6F_5)_4$ with 1 eq HOTf in THF-d_8

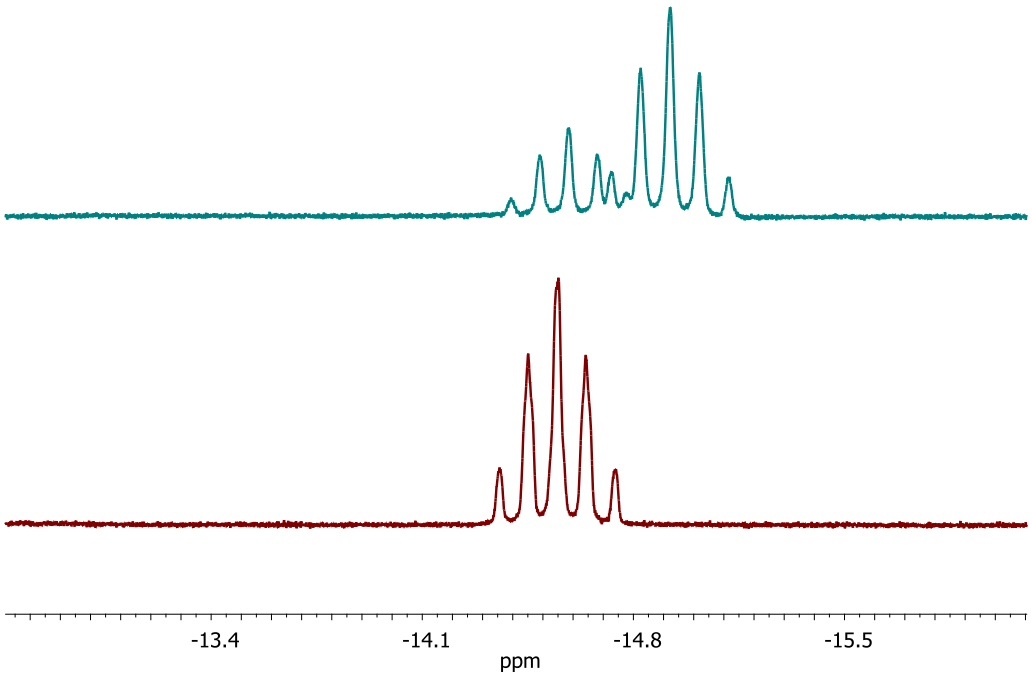


Figure S7. ^{1}H NMR of the hydride region of (bottom spectrum) **$[3(N_2)]B(C_6F_5)_4$** and (top spectrum) **$[3(N_2)]B(C_6F_5)_4$** with one eq HOTf in THF-d_8 at -30 °C.

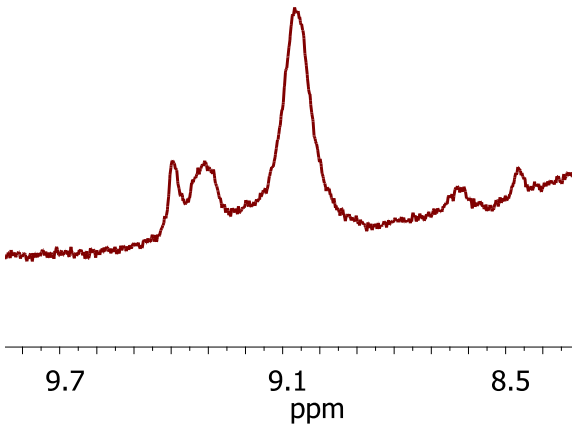


Figure S8. ^{1}H NMR of the ammonium region of **$[3(N_2)]B(C_6F_5)_4$** with one eq HOTf in THF-d_8 at -30 °C.

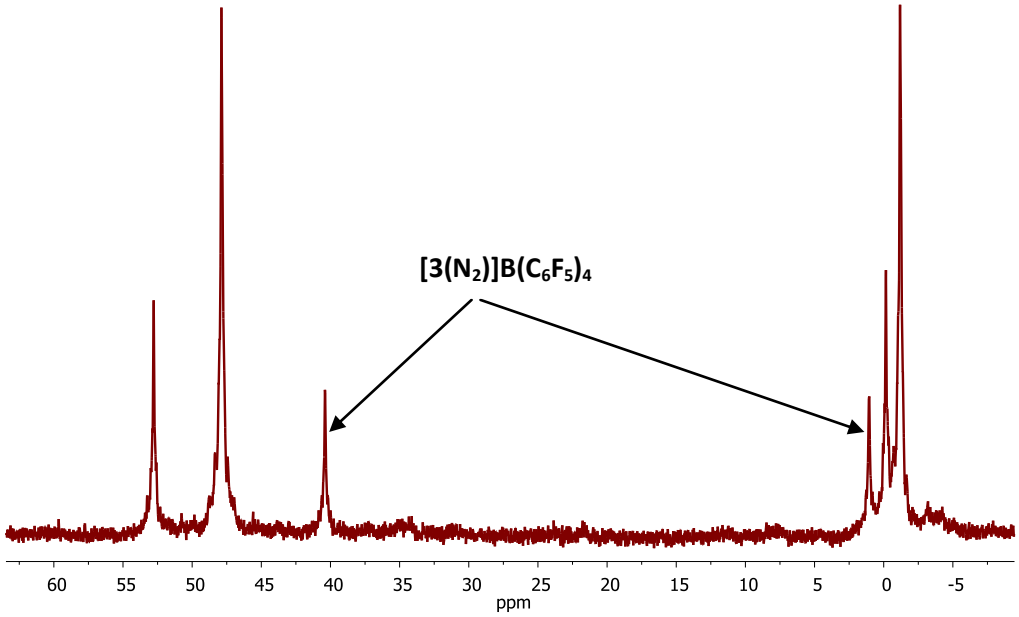


Figure S9. ^{31}P NMR of **[3(N$_2$)]B(C$_6$F$_5$)$_4$** with 0.9 eq HOTf in THF-d_8 at -30 °C.

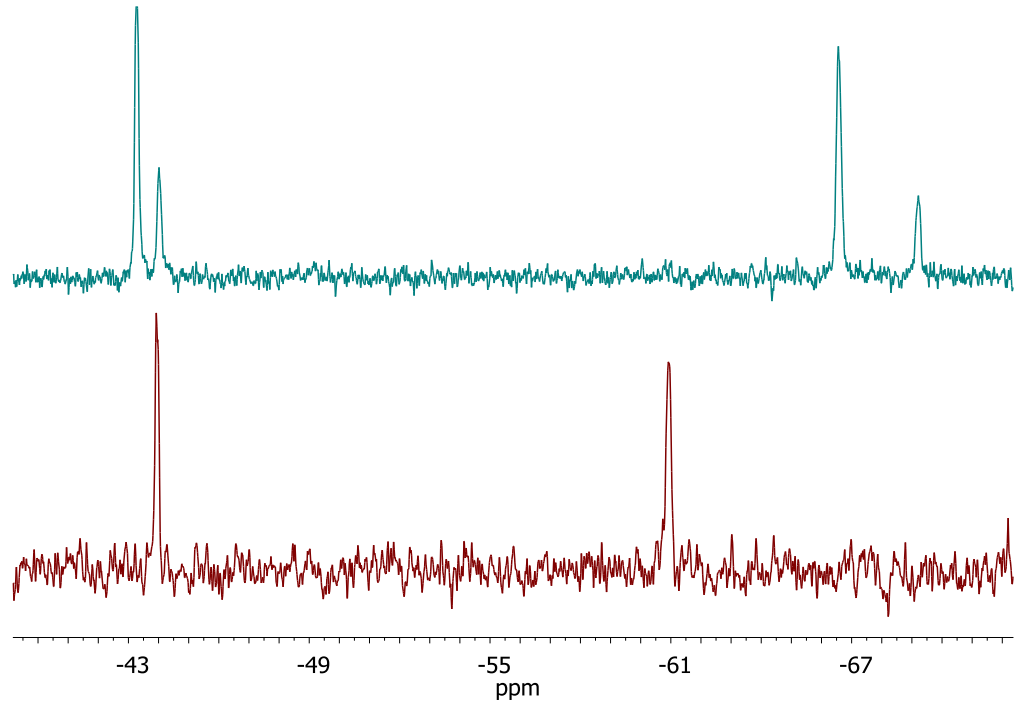


Figure S10. ^{15}N NMR of (bottom spectrum) **[3(N$_2$)]B(C$_6$F$_5$)$_4$** and (top spectrum) **[3(N$_2$)]B(C$_6$F$_5$)$_4$** with one eq HOTf in THF-d_8 at -30 °C.

5) In situ IR plots of Addition of $H(OEt_2)_2B(C_6F_5)_4$ to $[3(N_2)]B(C_6F_5)_4$

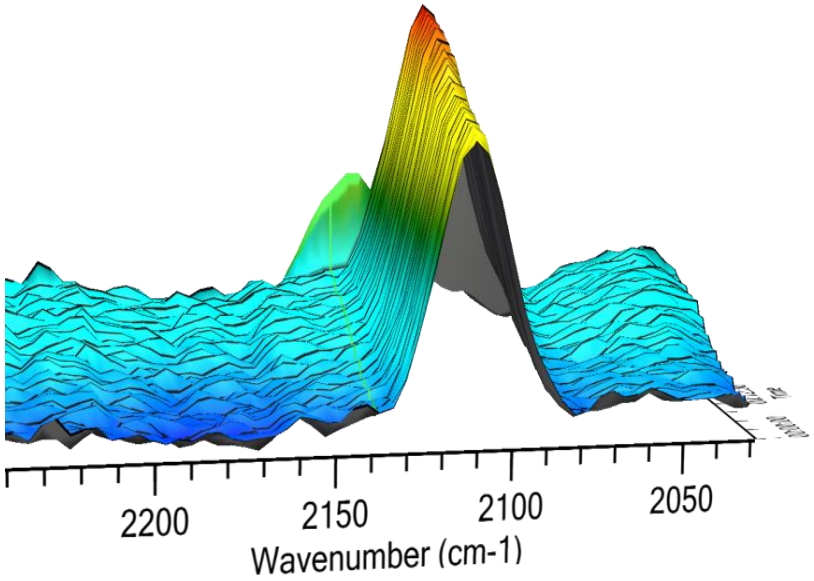


Figure S11. *In situ* IR data (left) addition of 1 equivalent of $H(OEt_2)_2B(C_6F_5)_4$ to **$[3(N_2)]BPh_4$** in fluorobenzene at 25 °C.

6) In situ IR plots of N_2-CO exchange for $[3(N_2)]B(C_6F_5)_4$

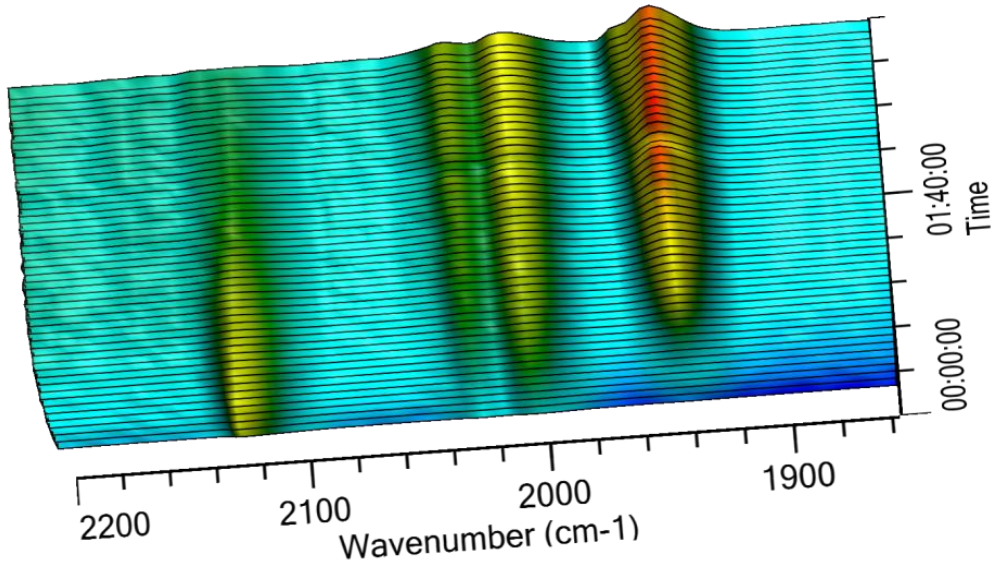


Figure S12. *In situ* IR data showing the reaction of **$[3(N_2)]^+$** with 1 atmosphere of CO in fluorobenzene to generate **$[3(CO)]^+$**. The two peaks at 2010 and 2030 cm^{-1} are attributed to the formation of $[Fe(CO)_2(P^{Et}N^{Me}P^{Et})(dmpm)]^{2+}$.

7) In situ IR plots of protonation reactions of $[1(N_2)]BPh_4$ and $[2(N_2)]BPh_4$

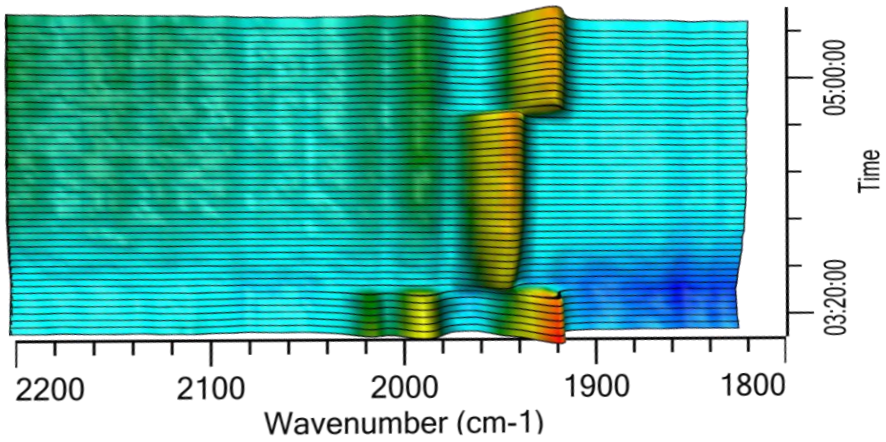


Figure S13. Treatment of **[3(CO)]**$^+$ with 1 equivalent of $H(OEt_2)_2B(C_6F_5)_4$ followed by 1 equivalent of Et_3N in fluorobenzene.

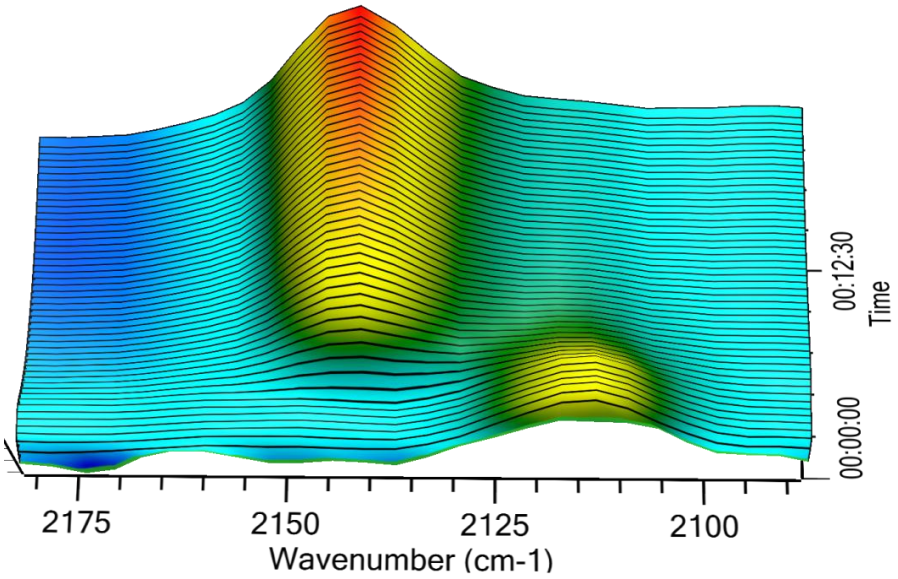


Figure S14. Addition of one equivalent of acid to **$[1(N_2)]B(C_6F_5)_4$** in fluorobenzene (shift by 23 cm^{-1}).

8) Cyclic Voltammograms of $[3(N_2)]BPh_4$ and $[FeH(N_2)(dmpe)_2]BPh_4$

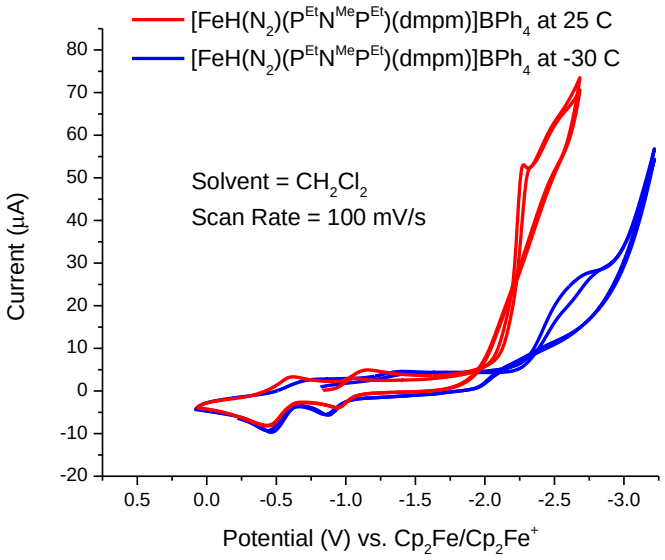


Figure S15. Comparison of the cyclic voltammogram of $\mathbf{[3(N_2)]^+}$ (red) in CH_2Cl_2 at 25 °C (red) and -30 °C (blue). Electrolyte = $Bu_4NB(C_6F_5)_4$ (0.1 M); scan rate = 100 mV/s.

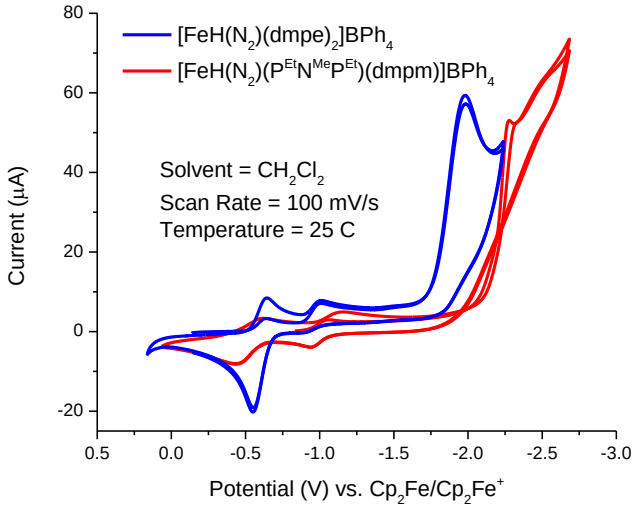


Figure S16. Comparison of the cyclic voltammogram of $[FeH(N_2)(dmpe)_2]BPh_4$ (blue) to $\mathbf{[3(N_2)]BPh_4}$ (red) in CH_2Cl_2 at 25 °C. Electrolyte = $Bu_4NB(C_6F_5)_4$ (0.1 M); scan rate = 100 mV/s.

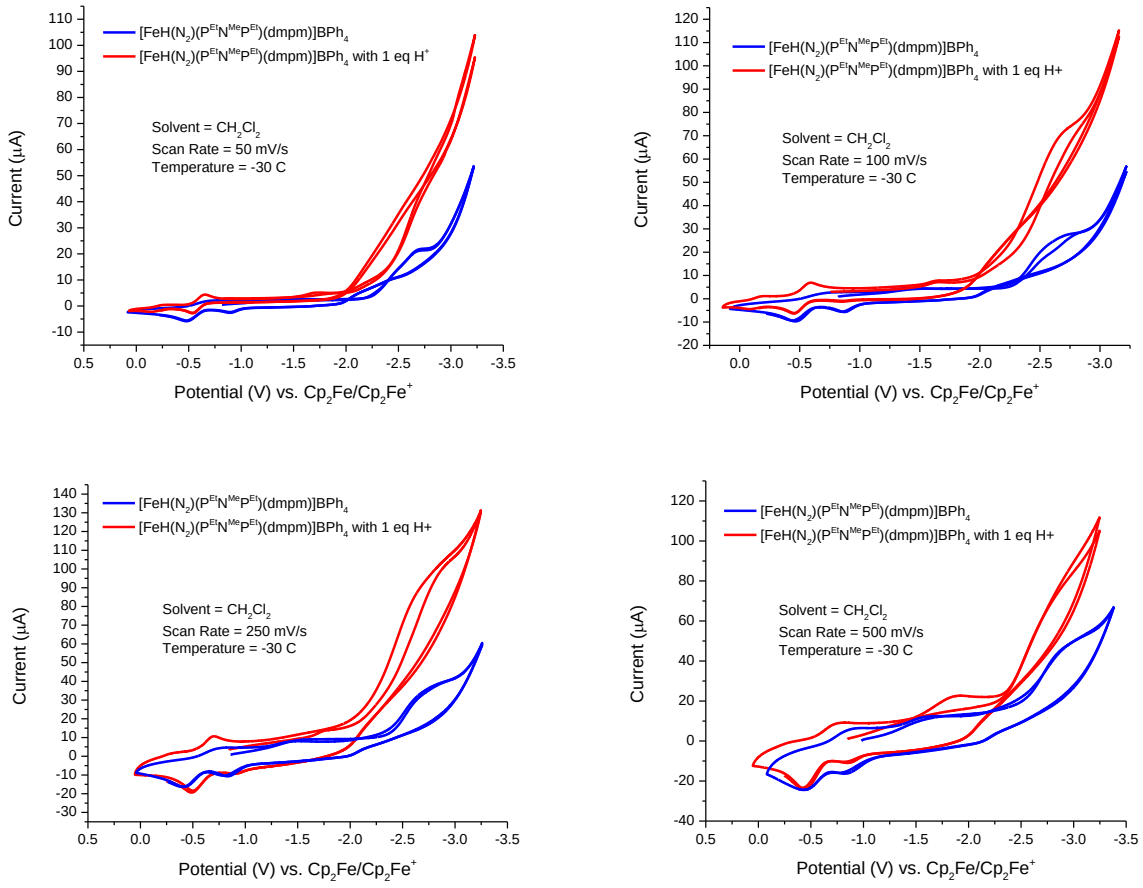


Figure S17. Comparison of cyclic voltammograms of **[3(N$_2$)]BPh$_4$** both before and after the addition of one equivalent of $H(OEt_2)_2B(C_6F_5)_4$ in CH_2Cl_2 at different scan rates (top left) 50 mV/s, (top right) 100 mV/s, (bottom left) 250 mV/s, and (bottom right) 500 mV/s. Electrolyte = $Bu_4NB(C_6F_5)_4$ (0.1 M); Temperature = -30 °C.

9) Cyclic Voltammograms of [3(CO)]$^+$

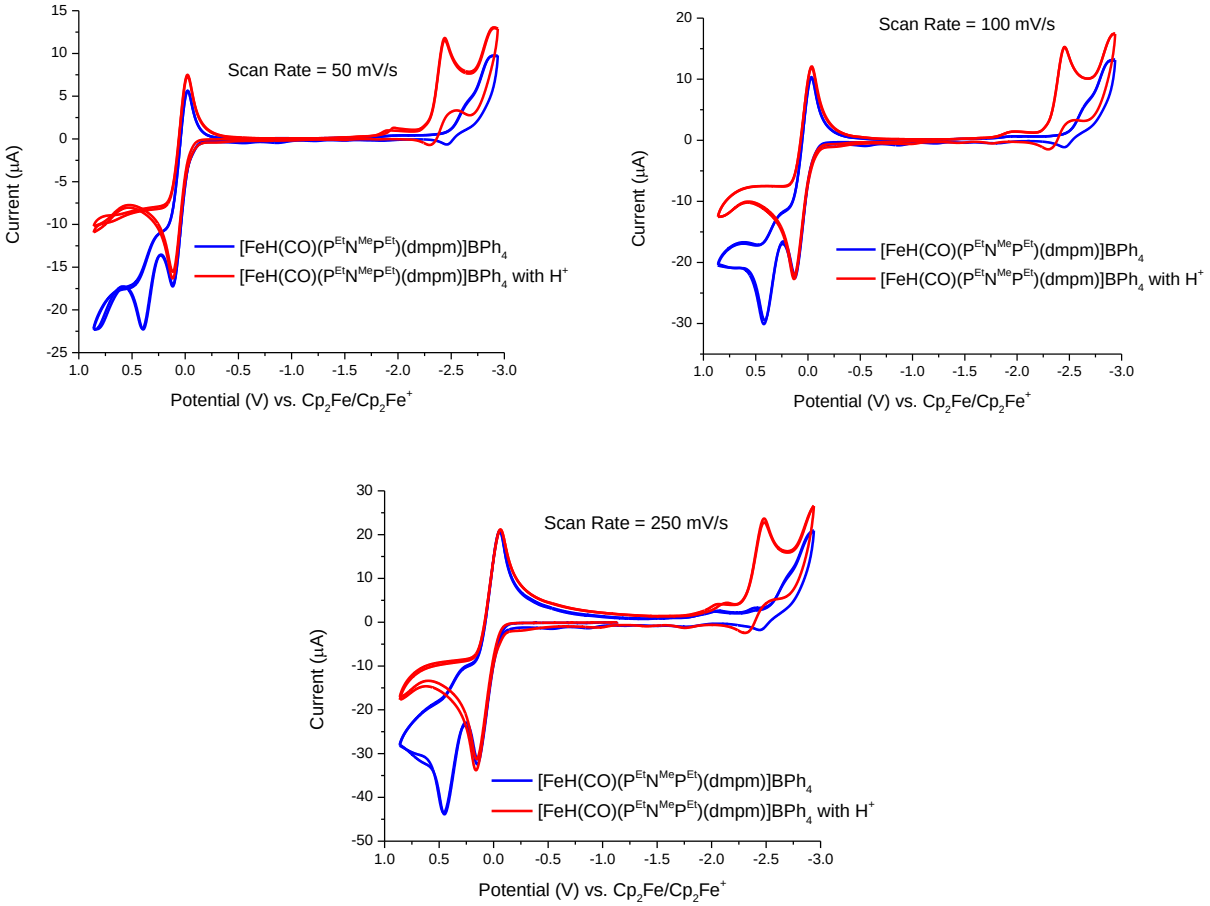


Figure S18. Comparison of cyclic voltammograms of **[3(CO)]$^+$** both before and after the addition of one equivalent of $H(OEt_2)_2B(C_6F_5)_4$ in CH_2Cl_2 at different scan rates (top left) 50 mV/s, (top right) 100 mV/s, and (bottom) 250 mV/s. Electrolyte = $Bu_4NB(C_6F_5)_4$ (0.1 M); Temperature = 25 °C.

10) NMR and Structural Characterization of $[3(^{15}NH_3)]^+$

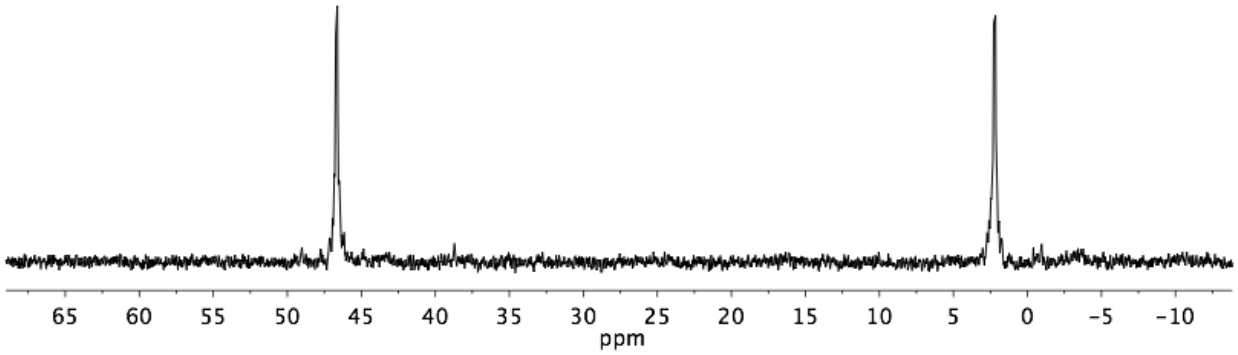


Figure S19. ^{31}P NMR (202 MHz, THF-d_8) of **$[3(^{15}NH_3)]^+$**.

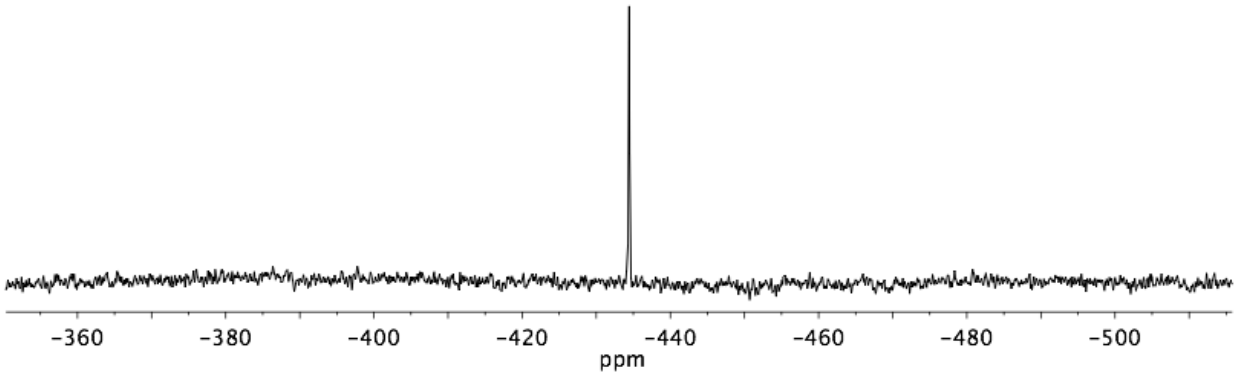


Figure S20. ^{15}N NMR (51 MHz, THF-d_8) of **$[3(^{15}NH_3)]^+$**.

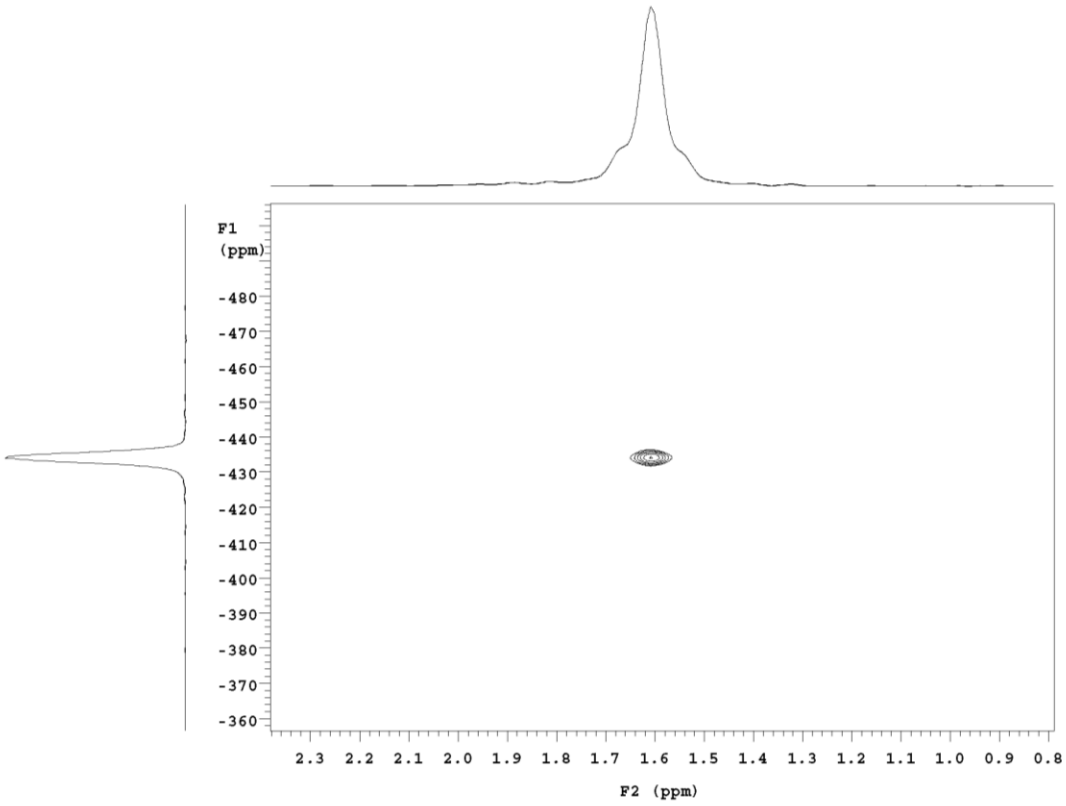


Figure S21. ^{15}N-^{1}H HSQC NMR spectrum of (THF-d_8) of **[3(**^{15}**NH$_3$)]$^+$**.

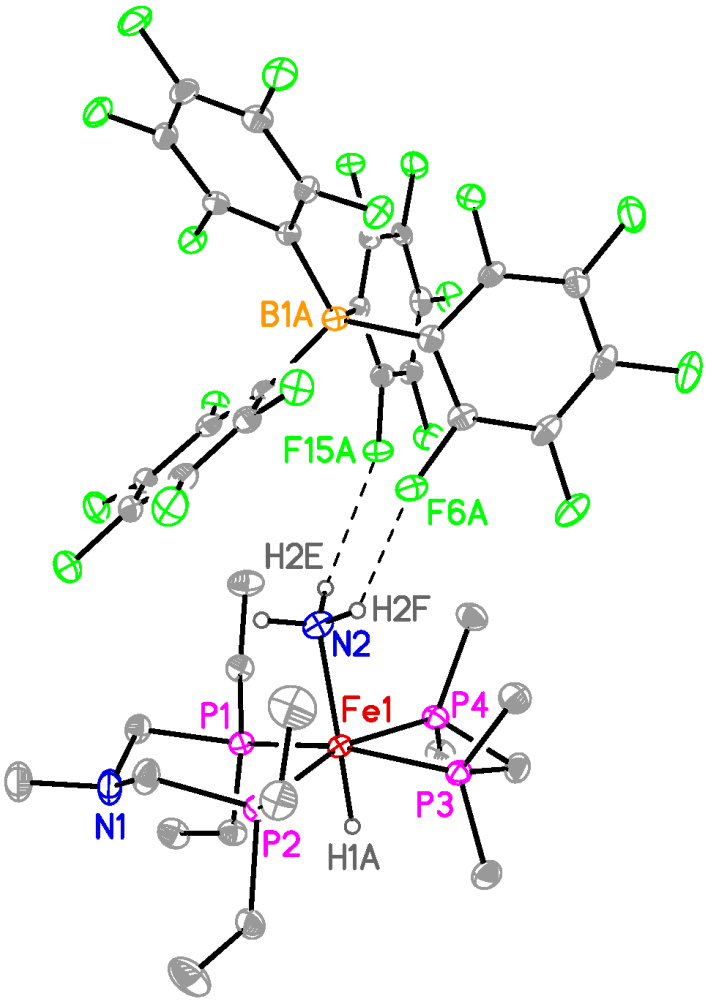


Figure S22. Molecular structure of **[3($^{15}NH_3$)]B(C_6F_5)$_4$** showing the hydrogen bonding interaction between B(C_6F_5)$_4$ and the bound NH_3. Thermal ellipsoids are drawn at 30% probability.

11) Frontier Molecular Orbitals for $[3(N_2)]^+$

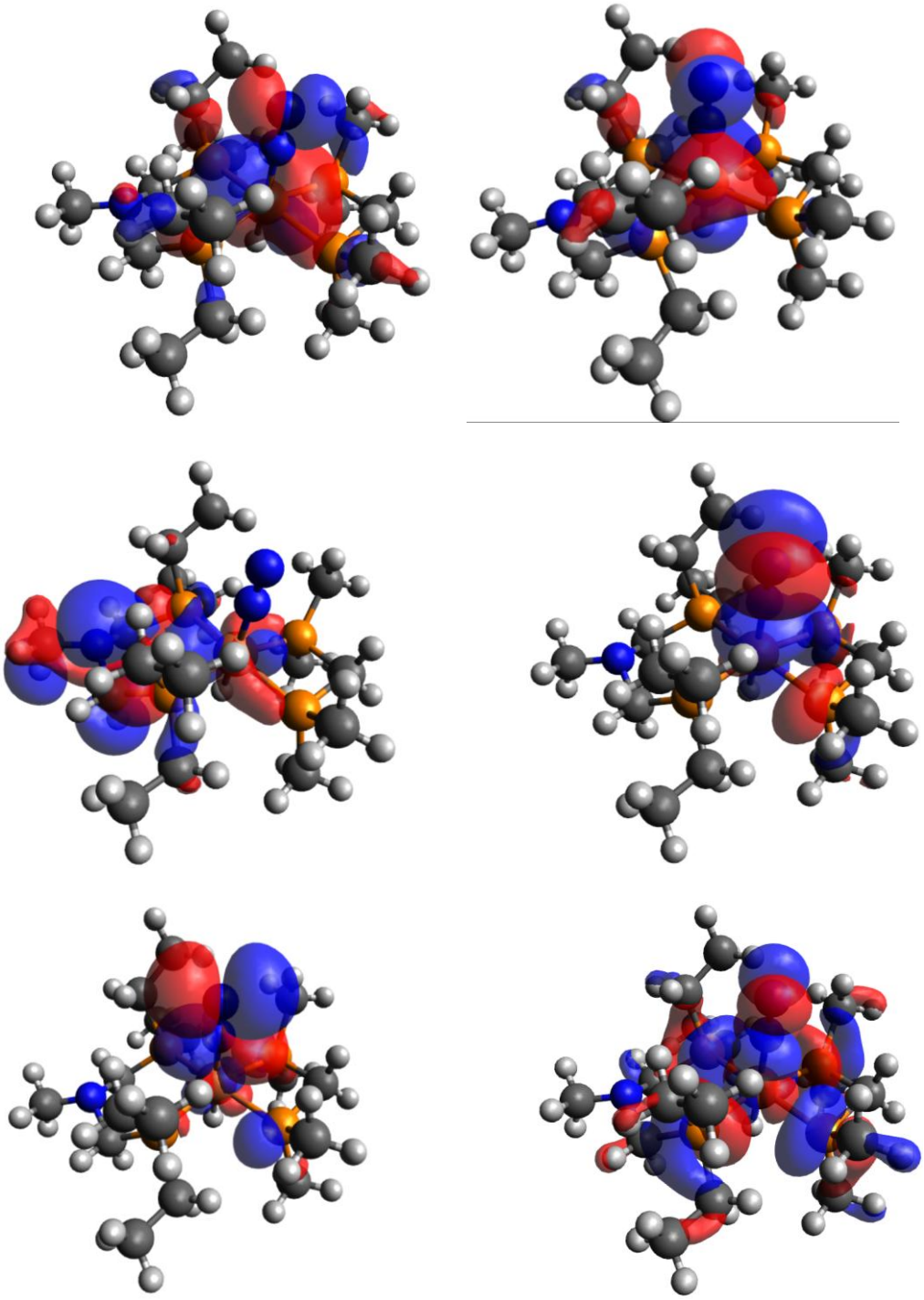


Figure S23. Frontier molecular orbitals of **$[3(N_2)]^+$** (top left) HOMO-2, (top right) HOMO-1, (middle left) HOMO, (middle right) LUMO, (bottom left) LUMO+1, (bottom right) LUMO+2. Phosphorus = orange, nitrogen = blue, carbon = gray, hydrogen = white, iron = metallic orange.

12) Frontier Molecular Orbitals for $[1(N_2)]^+$

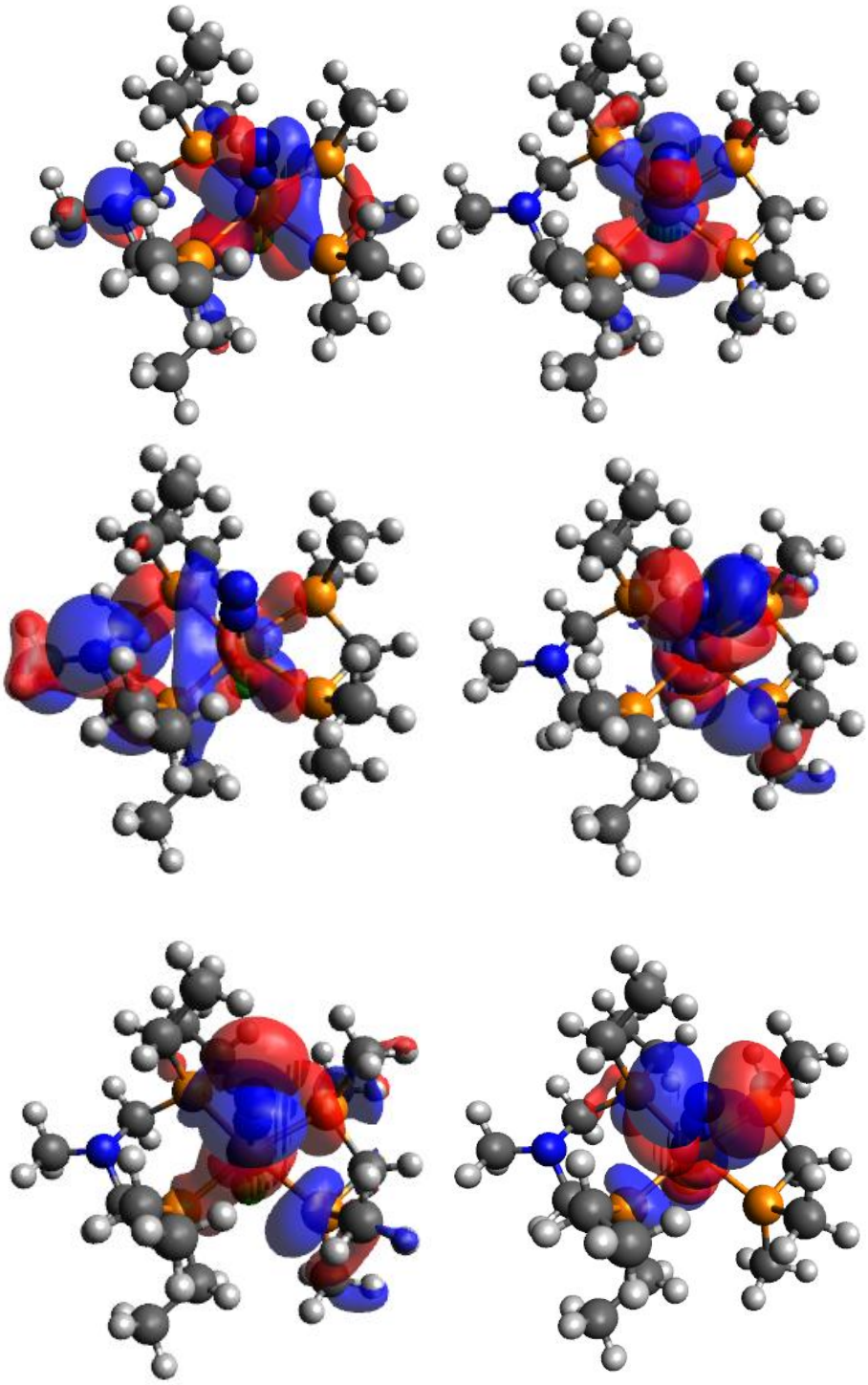


Figure S24. Frontier molecular orbitals of **$[1(N_2)]^+$** (top left) HOMO-2, (top right) HOMO-1, (middle left) HOMO, (middle right) LUMO, (bottom left) LUMO+1, (bottom right) LUMO+2. Phosphorus = orange, nitrogen = blue, carbon = gray, hydrogen = white, iron = metallic orange.

13) NBO Analysis of Fe(II) and Fe(0) Complexes

Table S1. NBO analysis for Fe(II) complexes and hypothetical Fe(0) complexes, where L = N_2, CO.

Fe(II) Complex	E(2) (kcal/mol)		d(Å)	WBI	q(X)	q(Fe)
	Fe(d)-L(σ)	Fe(d)-L(π*)				
$[FeH(N_2)(PNP)(dmpm)]^+$	150	13	1.121	2.70	-0.07	-0.56
$[FeH(N_2)(PN\mathbf{H}P)(dmpm)]^{2+}$	145	12	1.118	2.74	-0.05	-0.58
$[FeH(CO)(PNP)(dmpm)]^+$	313	36	1.161	2.06	0.27	-0.73
$[FeH(CO)(PN\mathbf{H}P)(dmpm)]^{2+}$	287	30	1.156	2.10	0.29	-0.74
Fe(0) Complex						
$[Fe(N_2)(PNP)(dmpm)]$	93	37	1.136	2.54	-0.34	-0.58
$[Fe(CO)(PNP)(dmpm)]$	214	63	1.181	1.89	-0.04	-0.76

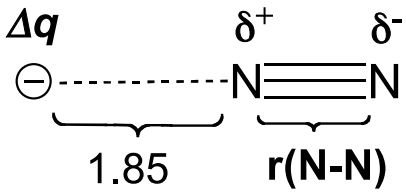
*E(2) is the stabilization energy for the interaction of the natural bonding orbitals; d denotes the bond distance of N_2/CO; WBI denotes Wiberg bond index; q(X) denotes the net charge on N_2 or CO in the complexes; q(Fe) denotes the natural atomic charge on Fe center of the complexes.

14) Charge Model for N_2 Bond Polarization

Charge Model for N_2 bond polarization induced by charge Metal atom site.

In this simple test calculation we employ the following scheme:

Scheme S1. Charge model for N_2 bond polarization.



The value of Δq obtained from NBO population analysis is on the order of -0.6 electrons and δq=0.1e- as obtained from our SSD/6-31G* and cc-PVTZ calculations. We note that this large negative charge on Fe is more a reflection of the excess charge build up (into very diffuse orbitals) from both the Fe and phosphine. In this context we ascribe the large negative charge on Fe to be a reflection of the pileup of electron density at this metal rich center and not a reflection of the oxidation state.

Table S2. Calculated relative energies, N-N bond distance, N_2 vibrational frequencies and net charge on N(δ+) atom based on the above charge model.

Δq	ΔE(kcal/mol)	Δν(cm^{-1})	N(δ+)	r(N-N) Å
0.0	0.0	0	0.000	1.104
-0.5	0.8	-31	0.112	1.107
-1.0	-5.3	-77	0.224	1.111
-1.5	-17.8	-139	0.333	1.116
-2.0	-36.1	-220	0.442	1.226
-2.5	-60.0	-321	0.550	1.131

In general for Fe(II) species a charge of approximately -0.6 electrons on the metal center is expected to provide a polarization of N_2 leading to a value of δ+/δ- of $0.1e^-$ in good accord with

the observations form the full calculations. It is noted however that unlike the case of Cr(0) species, where our model was more quantitative, the predicted red shift of the N_2 stretching mode for these Fe(II) complexes is only on the order of 50 cm^{-1} as opposed to the observed 190 cm^{-1} and the lengthening of r(N-N) is underestimated by ca 0.01 Å. For Fe(0) species the NBO analysis above indicates that the bound N_2 can act a π acceptor and thus this purely electrostatic model is not appropriate.

15) 3D Coordinates for all optimized structures

$[Fe(N_2H)Cl(P^{Et}N^{Me}P^{Et})(dmpm)]^{2+}$ (**$[1(N_2)H''])^{2+}$**)

Fe	0.479047	-0.082242	0.078257
N	-3.249356	0.635435	-0.385303
P	-0.823146	1.847620	-0.003434
P	-1.448024	-1.399789	0.037938
P	2.029811	-1.813978	-0.309938
P	2.604093	0.929681	-0.156430
C	-1.369508	2.436358	1.658410
H	-2.193081	3.140901	1.499416
H	-1.814902	1.576032	2.168254
C	-0.276066	3.095689	2.496543
H	-0.642510	3.298023	3.506642
H	0.031787	4.055469	2.074525
H	0.626993	2.480536	2.581535
C	-0.008335	3.293923	-0.793342
H	0.857916	3.539469	-0.170516
H	0.371875	2.944332	-1.757324
C	-0.893665	4.529628	-0.972321
H	-0.285778	5.352660	-1.356618
H	-1.339786	4.868894	-0.033479
H	-1.694212	4.360417	-1.695313
C	-2.409962	1.681302	-0.930982
H	-2.913920	2.644560	-0.805144
H	-2.183513	1.560439	-2.003388
C	-4.673449	0.909500	-0.605027
H	-5.271275	0.136726	-0.116976
H	-4.943476	0.942347	-1.671254
H	-4.934317	1.867132	-0.149080
C	-2.866503	-0.666527	-0.892767
H	-2.618787	-0.667086	-1.967757
H	-3.697760	-1.362349	-0.745555
C	-1.237814	-3.031395	-0.788445
H	-0.790996	-2.822511	-1.765014
H	-0.497398	-3.586056	-0.202198
C	-2.511403	-3.865244	-0.944665
H	-2.252859	-4.843423	-1.358144
H	-3.221467	-3.405777	-1.635310
H	-3.018619	-4.040591	0.007650
C	-2.178354	-1.783495	1.690916
H	-2.230382	-0.844603	2.251526
H	-3.218511	-2.079401	1.516072
C	-1.453531	-2.867520	2.487531
H	-1.928713	-2.987521	3.464401
H	-0.400776	-2.630638	2.664922
H	-1.503479	-3.838251	1.988043
C	2.566263	-2.785826	1.139950
H	1.797270	-3.516212	1.404472
H	2.737734	-2.140782	2.004479
H	3.490606	-3.323103	0.908108
C	1.995775	-3.001307	-1.692741
H	1.401925	-3.881420	-1.444631
H	3.025326	-3.318578	-1.886859
H	1.591801	-2.520068	-2.585267
C	3.396516	-0.644863	-0.696704
H	4.349188	-0.873866	-0.209985
H	3.549498	-0.617542	-1.779679
C	3.086448	2.154050	-1.420809
H	2.870106	3.171403	-1.092520
H	2.557832	1.947724	-2.353396
H	4.164222	2.065159	-1.588859
C	3.495935	1.447520	1.353782
H	3.101756	2.401582	1.713979
H	4.560203	1.575838	1.136250

H	3.389296	0.704304	2.147539
Cl	0.366951	0.003979	-2.208715
N	0.589346	-0.136273	1.701158
N	0.748557	-0.286117	2.860601
H	0.392856	0.381416	3.556723

$[Fe(N_2)Cl(P^{Et}NH^{Me}P^{Et})(dmpm)]^{2+}$
($[1(N_2)H']^{2+}$)

Fe	0.513161	-0.000857	0.052269
N	-3.358844	0.004248	-0.460962
P	-1.076130	1.642334	0.131325
P	-1.080461	-1.639955	0.130688
P	2.366373	-1.391790	-0.292223
P	2.368855	1.386437	-0.293931
C	-1.784475	2.118427	1.778838
H	-2.751079	2.612493	1.625342
H	-1.977995	1.195743	2.339799
C	-0.868958	3.030008	2.600517
H	-1.300332	3.191303	3.591033
H	-0.753391	4.010390	2.132544
H	0.124588	2.599078	2.744908
C	-0.679508	3.255464	-0.673658
H	0.157629	3.653789	-0.090421
H	-0.279735	3.001890	-1.660396
C	-1.788681	4.301583	-0.776439
H	-1.364414	5.240809	-1.140317
H	-2.259427	4.515621	0.187065
H	-2.567373	4.018068	-1.488894
C	-2.622689	1.256846	-0.842242
H	-3.328859	2.082168	-0.731695
H	-2.343444	1.155513	-1.894243
C	-4.734712	0.006157	-1.067028
H	-5.269091	-0.886234	-0.740543
H	-4.630720	0.006101	-2.152418
H	-5.266690	0.899930	-0.740403
C	-2.625916	-1.250041	-0.842875
H	-2.346315	-1.148942	-1.894802
H	-3.334235	-2.073582	-0.732772
C	-0.687891	-3.253942	-0.674537
H	-0.287282	-3.001281	-1.661172
H	0.148092	-3.654558	-0.091240
C	-1.799789	-4.297124	-0.777642
H	-1.377969	-5.237327	-1.141844
H	-2.577776	-4.011361	-1.489976
H	-2.271066	-4.510241	0.185799
C	-1.790345	-2.114507	1.777995
H	-1.981690	-1.191382	2.338997
H	-2.758119	-2.606205	1.624275
C	-0.877226	-3.028345	2.599841
H	-1.309433	-3.188978	3.590101
H	0.117184	-2.599622	2.744826
H	-0.763571	-4.008847	2.131651
C	3.229531	-2.109934	1.154341
H	2.662292	-2.958463	1.546428
H	3.334402	-1.372994	1.953645
H	4.224530	-2.461652	0.867756
C	2.532754	-2.673880	-1.585563
H	2.132103	-3.631948	-1.250521
H	3.594201	-2.806200	-1.814907
H	2.007691	-2.351448	-2.487094
C	3.431243	-0.003991	-0.872000
H	4.461866	-0.004739	-0.505328
H	3.440648	-0.004605	-1.966314
C	2.537475	2.666367	-1.589154
H	2.138884	3.625729	-1.255386
H	2.011552	2.343706	-2.490098
H	3.599148	2.796164	-1.818882
C	3.233038	2.105369	1.151618
H	2.667580	2.956086	1.541528
H	4.229087	2.454062	0.864997
H	3.335507	1.369879	1.952570
Cl	0.224716	-0.001081	-2.249080
N	0.753462	-0.001107	1.840637
N	0.910571	-0.001359	2.946835
H	-3.488338	0.004145	0.556213

$[Fe(N_2)Cl(P^{Et}N^{Me}P^{Et})(dmpm)]^{+}$ **($[1(N_2)]^{+}$)**

Fe	-0.479330	-0.000053	0.042392
N	3.326653	0.001499	-0.305165
P	1.134355	-1.632835	0.043722
P	1.132985	1.633998	0.043477
P	-2.339604	1.387914	-0.207753
P	-2.337612	-1.390284	-0.208907
C	1.767323	-2.190286	1.692505
H	2.724517	-2.697987	1.530825
H	1.996594	-1.286503	2.265486
C	0.818378	-3.098140	2.471732
H	1.231382	-3.314128	3.460646
H	0.669452	-4.056503	1.966419
H	-0.162470	-2.640071	2.624497

C	0.669848	-3.201030	-0.812465
H	-0.159653	-3.625026	-0.236947
H	0.260180	-2.896312	-1.780478
C	1.768785	-4.247399	-0.988437
H	1.346832	-5.158889	-1.421028
H	2.235429	-4.524968	-0.038718
H	2.554533	-3.906285	-1.666465
C	2.704841	-1.198940	-0.834485
H	3.386078	-2.040779	-0.680547
H	2.490314	-1.133377	-1.915673
C	4.767357	0.002138	-0.544092
H	5.214854	0.885115	-0.080778
H	5.027366	0.002085	-1.615957
H	5.215668	-0.880278	-0.080494
C	2.703713	1.201231	-0.834811
H	2.489078	1.135118	-1.915934
H	3.384245	2.043711	-0.681242
C	0.666974	3.201641	-0.812904
H	0.257603	2.896455	-1.780894
H	-0.162931	3.624874	-0.237414
C	1.764878	4.249081	-0.988954
H	1.342085	5.159960	-1.422014
H	2.551199	3.908575	-1.666630
H	2.230954	4.527492	-0.039199
C	1.765591	2.192255	1.692086
H	1.996206	1.288748	2.264968
H	2.722043	2.701301	1.530248
C	0.815499	3.098758	2.471497
H	1.228207	3.315074	3.460461
H	-0.164778	2.639422	2.624128
H	0.665377	4.057027	1.966362
C	-3.149624	2.105218	1.274383
H	-2.574622	2.965402	1.627888
H	-3.188523	1.372016	2.083318
H	-4.166553	2.434494	1.043941
C	-2.603565	2.666676	-1.491899
H	-2.185644	3.626828	-1.185373
H	-3.676711	2.789937	-1.663693
H	-2.120435	2.340638	-2.415363
C	-3.438754	-0.001756	-0.728499
H	-4.449792	-0.002664	-0.310579
H	-3.498511	-0.001349	-1.820865
C	-2.600024	-2.668326	-1.494091
H	-2.180863	-3.628229	-1.188509
H	-2.117464	-2.340843	-2.417342
H	-3.673049	-2.792770	-1.665808
C	-3.146471	-2.109902	1.272744
H	-2.569865	-2.969156	1.625914
H	-4.162752	-2.441005	1.042057
H	-3.186840	-1.377165	2.082032
Cl	-0.356086	0.000436	-2.279297
N	-0.603095	-0.000310	1.826924
N	-0.695425	-0.000505	2.942623

$[FeCl(P^{Et}NH^{Me}P^{Et})(dmpm)]^{2+}$

Fe	-0.530642	-0.000006	0.084804
N	3.328633	0.000046	-0.433854
P	1.052032	-1.624929	0.219038
P	1.051986	1.624967	0.219044
P	-2.407220	1.380056	-0.108492
P	-2.407165	-1.380133	-0.108565
C	1.765535	-2.029281	1.880429
H	2.560719	-2.773444	1.760906
H	2.233995	-1.122218	2.283502
C	0.711724	-2.530695	2.869495
H	1.169647	-2.721870	3.842609
H	0.259307	-3.468335	2.536057
H	-0.088164	-1.798969	3.020325
C	0.645714	-3.269847	-0.516883
H	-0.175146	-3.649045	0.101916
H	0.215302	-3.049347	-1.499177
C	1.749750	-4.320300	-0.619555
H	1.316676	-5.262958	-0.963748
H	2.231014	-4.524737	0.340638
H	2.520052	-4.050756	-1.346471
C	2.585954	-1.259733	-0.782419
H	3.297311	-2.081189	-0.674764
H	2.284619	-1.174114	-1.830138
C	4.680949	0.000064	-1.091438
H	5.226037	0.893127	-0.785244
H	4.535960	0.000070	-2.172070
H	5.226056	-0.892992	-0.785257
C	2.585930	1.259816	-0.782398
H	2.284611	1.174216	-1.830123
H	3.297270	2.081284	-0.674716
C	0.645606	3.269859	-0.516905
H	0.215146	3.049324	-1.499170
H	-0.175225	3.649064	0.101927
C	1.749620	4.320328	-0.619669
H	1.316506	5.262979	-0.963830

H	2.519864	4.050791	-1.346649
H	2.230960	4.524776	0.340482
C	1.765463	2.029369	1.880435
H	2.234003	1.122345	2.283502
H	2.560586	2.773596	1.760909
C	0.711618	2.530692	2.869509
H	1.169535	2.721914	3.842617
H	-0.088202	1.798894	3.020351
H	0.259114	3.468290	2.536072
C	-3.216288	2.014005	1.410551
H	-2.655653	2.865661	1.804408
H	-3.251601	1.244011	2.185053
H	-4.237541	2.339868	1.193535
C	-2.642566	2.718338	-1.332623
H	-2.224182	3.661267	-0.976357
H	-3.712924	2.859316	-1.508234
H	-2.158451	2.436132	-2.270289
C	-3.477040	-0.000044	-0.697851
H	-4.515150	-0.000073	-0.352663
H	-3.460711	-0.000015	-1.792503
C	-2.642423	-2.718342	-1.332793
H	-2.224019	-3.661280	-0.976573
H	-2.158284	-2.436057	-2.270422
H	-3.712770	-2.859345	-1.508451
C	-3.216227	-2.014230	1.410419
H	-2.655560	-2.865891	1.804220
H	-4.237461	-2.340123	1.193363
H	-3.251586	-1.244296	2.184978
Cl	-0.290964	0.000031	-2.196525
H	3.496589	0.000038	0.577313

[FeCl($P^{Et}NH^{Me}P^{Et}$)(dmpm)]$^{+}$

Fe	-0.488011	-0.000074	0.050569
N	3.319279	0.001224	-0.227591
P	1.115166	-1.610647	0.114501
P	1.114133	1.611473	0.115173
P	-2.363298	1.379559	-0.038715
P	-2.362619	-1.380617	-0.037443
C	1.726164	-2.055584	1.801358
H	2.351329	-2.952174	1.722594
H	2.391551	-1.238193	2.098938
C	0.618879	-2.261481	2.830208
H	1.039887	-2.501448	3.810338
H	-0.046610	-3.085039	2.553244
H	0.005238	-1.361268	2.949308
C	0.655358	-3.223636	-0.660634
H	-0.122587	-3.650362	-0.016841
H	0.173115	-2.965172	-1.608693
C	1.770762	-4.242876	-0.881195
H	1.348102	-5.181130	-1.251250
H	2.313679	-4.475804	0.039658
H	2.493487	-3.901220	-1.625911
C	2.702637	-1.206046	-0.750165
H	3.382000	-2.045492	-0.574638
H	2.502703	-1.157249	-1.834736
C	4.762864	0.001668	-0.449742
H	5.205117	0.884662	0.018751
H	5.035357	0.002041	-1.518094
H	5.205582	-0.881353	0.018257
C	2.702033	1.208477	-0.749442
H	2.502363	1.160338	-1.834098
H	3.380845	2.048217	-0.573171
C	0.653435	3.224669	-0.659025
H	0.171677	2.966535	-1.607420
H	-0.125020	3.650403	-0.015178
C	1.768178	4.244853	-0.878558
H	1.344968	5.183055	-1.248117
H	2.491380	3.904206	-1.623274
H	2.310645	4.477552	0.042616
C	1.724513	2.055594	1.802473
H	2.391506	1.239086	2.098900
H	2.347929	2.953487	1.724737
C	0.616999	2.258052	2.831759
H	1.037698	2.497479	3.812155
H	0.005066	1.356523	2.949763
H	-0.050092	3.080713	2.556006
C	-3.138043	2.013438	1.503258
H	-2.569960	2.869220	1.876975
H	-3.133861	1.244236	2.279471
H	-4.169889	2.328045	1.323118
C	-2.680955	2.717969	-1.248361
H	-2.237502	3.659123	-0.918593
H	-3.758885	2.858917	-1.367873
H	-2.241820	2.430180	-2.206248
C	-3.464166	-0.001061	-0.580014
H	-4.488639	-0.001142	-0.195651
H	-3.482798	-0.001563	-1.674222
C	-2.680142	-2.720565	-1.245422
H	-2.236050	-3.661133	-0.914830
H	-2.241607	-2.433655	-2.203848

H	-3.758050	-2.862203	-1.364300
C	-3.136579	-2.012868	1.505586
H	-2.567614	-2.867494	1.880604
H	-4.168160	-2.328707	1.326090
H	-3.133028	-1.242414	2.280564
Cl	-0.447534	-0.000387	-2.249529

$[Fe(N_2H)H(P^{Et}N^{Me}P^{Et})(dmpm)]^{2+}$
($[3(N_2)H'']^{2+}$)

Fe	-0.146645	-0.481679	0.111525
N	0.989352	3.106365	-0.442827
P	1.918925	0.527217	-0.047390
P	-1.222685	1.506720	-0.176830
P	-2.033970	-1.798142	-0.179936
P	0.574582	-2.583383	-0.494167
C	2.715394	0.865039	1.583109
H	3.539225	1.564970	1.408403
H	1.981207	1.405785	2.189296
C	3.230169	-0.373560	2.312705
H	3.599112	-0.099376	3.304180
H	4.060929	-0.842991	1.779538
H	2.454836	-1.134845	2.445684
C	3.186438	-0.391658	-1.029259
H	3.286816	-1.387187	-0.588156
H	2.751462	-0.528468	-2.025672
C	4.563544	0.265822	-1.135538
H	5.238764	-0.392856	-1.687706
H	5.015725	0.444828	-0.156798
H	4.529868	1.213543	-1.676845
C	1.994989	2.172166	-0.893700
H	2.984646	2.577406	-0.663848
H	1.963300	1.995850	-1.986167
C	1.408665	4.497079	-0.640151
H	0.651360	5.167246	-0.227759
H	1.564597	4.751137	-1.699811
H	2.339537	4.675485	-0.097546
C	-0.288802	2.830941	-1.060506
H	-0.213756	2.568075	-2.132261
H	-0.917526	3.723292	-0.990042
C	-2.796095	1.443780	-1.135522
H	-2.562670	0.963174	-2.091099
H	-3.467544	0.769272	-0.593778
C	-3.491269	2.787434	-1.363260
H	-4.454179	2.617841	-1.851708
H	-2.914631	3.445326	-2.016695
H	-3.692193	3.317480	-0.428838
C	-1.656467	2.325905	1.419115
H	-0.751635	2.323943	2.033904
H	-1.864627	3.376360	1.187247
C	-2.831527	1.706448	2.169469
H	-2.979827	2.231822	3.116155
H	-2.662346	0.653679	2.407850
H	-3.765666	1.788936	1.607193
C	-3.356332	-1.954116	1.071660
H	-4.019441	-1.086384	1.035548
H	-2.928045	-2.017377	2.074549
H	-3.948233	-2.853841	0.879778
C	-2.915208	-1.903347	-1.779913
H	-3.657355	-1.110036	-1.873349
H	-3.430845	-2.866312	-1.840656
H	-2.211896	-1.819509	-2.610805
C	-1.054320	-3.359035	-0.123224
H	-1.038578	-3.745581	0.901282
H	-1.376903	-4.159397	-0.796089
C	0.947126	-2.998126	-2.231284
H	1.933578	-2.621513	-2.508024
H	0.208287	-2.546051	-2.895384
H	0.938709	-4.084121	-2.362275
C	1.792802	-3.543510	0.478737
H	2.816020	-3.220906	0.278950
H	1.707148	-4.601347	0.211247
H	1.594762	-3.432348	1.546802
N	-0.151793	-0.510810	1.772370
N	-0.231118	-0.340213	2.941379
H	-0.161133	-0.296877	-1.391757
H	0.179406	-1.005625	3.609582

$[Fe(N_2)H(P^{Et}NH^{Me}P^{Et})(dmpm)]^{2+}$
($[3(N_2)H']^{2+}$)

Fe	0.000147	-0.502190	0.006684
N	-0.001384	3.332041	-0.460973
P	1.631672	1.016655	-0.027538
P	-1.632440	1.015388	-0.027867
P	-1.365348	-2.306718	-0.381098
P	1.367030	-2.305484	-0.381666
C	2.266648	1.681769	1.586806
H	2.812646	2.615181	1.406961
H	1.393599	1.929453	2.204343
C	3.161385	0.701670	2.347745
H	3.435304	1.125495	3.316637

H	4.089939	0.501011	1.807283
H	2.661601	-0.250366	2.538249
C	3.169694	0.623858	-0.981529
H	3.576859	-0.272471	-0.501627
H	2.830934	0.310318	-1.974948
C	4.257018	1.692265	-1.084379
H	5.136768	1.268375	-1.575302
H	4.581372	2.055908	-0.105898
H	3.949401	2.550471	-1.687413
C	1.247398	2.626938	-0.905474
H	2.073474	3.325349	-0.756259
H	1.138743	2.439951	-1.977094
C	-0.001944	4.758781	-0.930920
H	-0.895402	5.257713	-0.554799
H	-0.001658	4.761850	-2.021332
H	0.890830	5.258577	-0.554324
C	-1.249189	2.625673	-0.906213
H	-1.139608	2.438451	-1.977694
H	-2.076025	3.323346	-0.757761
C	-3.170335	0.621302	-0.981544
H	-2.831528	0.307958	-1.975013
H	-3.576692	-0.275324	-0.501513
C	-4.258522	1.688837	-1.084307
H	-5.137998	1.264206	-1.575082
H	-3.951677	2.547239	-1.687458
H	-4.583044	2.052297	-0.105819
C	-2.267717	1.680686	1.586301
H	-1.394786	1.929351	2.203625
H	-2.814533	2.613562	1.406150
C	-3.161492	0.700136	2.347792
H	-3.435656	1.124119	3.316545
H	-2.660853	-0.251386	2.538609
H	-4.089945	0.498436	1.807539
C	-2.684945	-2.886879	0.752304
H	-3.581260	-2.268419	0.661120
H	-2.338204	-2.839765	1.787435
H	-2.955517	-3.920466	0.517873
C	-2.056565	-2.624545	-2.045859
H	-2.947128	-2.017025	-2.217204
H	-2.334602	-3.678079	-2.140562
H	-1.317486	-2.374423	-2.809425
C	0.001424	-3.533637	-0.204419
H	0.001854	-3.929814	0.816594
H	0.001632	-4.373198	-0.905959
C	2.057978	-2.622592	-2.046673
H	2.948187	-2.014560	-2.218057
H	1.318613	-2.372690	-2.810032
H	2.336572	-3.675952	-2.141661
C	2.687521	-2.884701	0.751202
H	3.583230	-2.265373	0.659993
H	2.959014	-3.917960	0.516383
H	2.340997	-2.838246	1.786437
N	0.000343	-0.752988	1.824839
N	0.000477	-0.915431	2.931379
H	0.000029	-0.306986	-1.496715
H	-0.001721	3.360484	0.564230

$[Fe(N_2)H(P^{Et}N^{Me}P^{Et})(dmpm)]^+$ (**[3(N$_2$)]$^+$**)

Fe	0.000090	-0.495075	0.007129
N	-0.001234	3.285815	-0.410627
P	1.616284	1.065921	-0.080489
P	-1.617056	1.064792	-0.080814
P	-1.360998	-2.284609	-0.334798
P	1.362578	-2.283419	-0.335453
C	2.281984	1.694021	1.531234
H	2.834055	2.620526	1.338292
H	1.411961	1.974449	2.133598
C	3.163523	0.705005	2.289026
H	3.459350	1.125075	3.254113
H	4.082044	0.477160	1.739950
H	2.646846	-0.236532	2.489530
C	3.137364	0.603246	-1.033338
H	3.542234	-0.296114	-0.556780
H	2.781051	0.294460	-2.022265
C	4.236076	1.656355	-1.163075
H	5.099667	1.233539	-1.684298
H	4.586210	2.009864	-0.189341
H	3.908287	2.524407	-1.739995
C	1.197065	2.658415	-0.931786
H	2.041329	3.334729	-0.769692
H	1.136038	2.464660	-2.020601
C	-0.001798	4.723451	-0.662976
H	-0.885050	5.175508	-0.204687
H	-0.001588	4.972662	-1.737904
H	0.880783	5.176286	-0.204162
C	-1.198694	2.657327	-0.932428
H	-1.136814	2.463332	-2.021145
H	-2.043605	3.332996	-0.771031
C	-3.137930	0.600941	-1.033409
H	-2.781544	0.292205	-2.022329

H	-3.542112	-0.298617	-0.556632
C	-4.237388	1.653260	-1.163196
H	-5.100695	1.229775	-1.684348
H	-3.910249	2.521491	-1.740216
H	-4.587737	2.006607	-0.189484
C	-2.283043	1.693050	1.530724
H	-1.413147	1.974471	2.132808
H	-2.835904	2.619016	1.337450
C	-3.163667	0.703641	2.289063
H	-3.459811	1.123926	3.253961
H	-2.646156	-0.237343	2.489997
H	-4.082024	0.474714	1.740158
C	-2.682424	-2.862509	0.804187
H	-3.571833	-2.234058	0.713182
H	-2.329155	-2.802308	1.836561
H	-2.961019	-3.896643	0.582243
C	-2.060567	-2.655081	-1.988945
H	-2.939111	-2.035689	-2.178371
H	-2.351521	-3.707330	-2.055358
H	-1.316363	-2.432053	-2.756035
C	0.001360	-3.521092	-0.141312
H	0.001809	-3.893697	0.888499
H	0.001537	-4.374594	-0.826311
C	2.061786	-2.653261	-1.989885
H	2.939667	-2.033043	-2.179693
H	1.317058	-2.430968	-2.756679
H	2.353709	-3.705235	-2.056369
C	2.684884	-2.860398	0.803010
H	3.573511	-2.230787	0.712429
H	2.964746	-3.894039	0.580363
H	2.331576	-2.801340	1.835441
N	0.000283	-0.652308	1.819972
N	0.000430	-0.762055	2.935465
H	-0.000032	-0.328162	-1.501919

$[FeH(P^{Et}NH^{Me}P^{Et})(dmpm)]^{2+}$

Fe	0.537524	0.000019	0.036881
N	-3.293560	-0.000114	-0.503464
P	-0.985048	1.607463	0.048820
P	-0.984936	-1.607531	0.048834
P	2.373587	-1.370256	-0.181874
P	2.373500	1.370411	-0.181862
C	-1.696710	2.107521	1.690283
H	-2.482420	2.855900	1.538273
H	-2.177079	1.223804	2.131976
C	-0.638010	2.634655	2.659307
H	-1.094064	2.880208	3.621078
H	-0.164705	3.545445	2.283135
H	0.146579	1.894741	2.844683
C	-0.581889	3.218527	-0.774233
H	0.298155	3.589950	-0.237876
H	-0.233618	2.956077	-1.779396
C	-1.648969	4.309702	-0.832756
H	-1.217680	5.214008	-1.269798
H	-2.023928	4.583261	0.156820
H	-2.499664	4.036913	-1.462752
C	-2.566923	1.255411	-0.895304
H	-3.270078	2.079407	-0.754835
H	-2.339674	1.169549	-1.961287
C	-4.687912	-0.000163	-1.062660
H	-5.210010	-0.893323	-0.718686
H	-4.622278	-0.000171	-2.151052
H	-5.210066	0.892970	-0.718703
C	-2.566848	-1.255605	-0.895276
H	-2.339619	-1.169759	-1.961266
H	-3.269948	-2.079641	-0.754774
C	-0.581668	-3.218570	-0.774213
H	-0.233402	-2.956098	-1.779373
H	0.298394	-3.589937	-0.237846
C	-1.648680	-4.309811	-0.832748
H	-1.217327	-5.214093	-1.269775
H	-2.499379	-4.037076	-1.462763
H	-2.023642	-4.583386	0.156823
C	-1.696543	-2.107629	1.690308
H	-2.176989	-1.223948	2.131991
H	-2.482187	-2.856080	1.538315
C	-0.637789	-2.634653	2.659333
H	-1.093814	-2.880234	3.621110
H	0.146735	-1.894665	2.844694
H	-0.164402	-3.545405	2.283170
C	2.932933	-2.659102	1.002047
H	2.323738	-3.561933	0.910930
H	2.851415	-2.292960	2.028357
H	3.974892	-2.927050	0.804515
C	2.736320	-2.116491	-1.815435
H	2.124201	-3.006360	-1.974829
H	3.789593	-2.405934	-1.870216
H	2.514950	-1.399579	-2.608371
C	3.602115	0.000116	-0.009085
H	4.014422	0.000125	1.005704

H	4.434195	0.000145	-0.719768
C	2.736195	2.116689	-1.815412
H	2.124021	3.006521	-1.974801
H	2.514879	1.399771	-2.608358
H	3.789450	2.406201	-1.870182
C	2.932754	2.659277	1.002080
H	2.323492	3.562066	0.910981
H	3.974694	2.927305	0.804552
H	2.851263	2.293111	2.028384
H	0.430991	0.000016	-1.437211
H	-3.387619	-0.000106	0.517602

$[FeH(P^{Et}N^{Me}P^{Et})(dmpm)]^{+}$

Fe	0.525641	-0.000068	0.010012
N	-3.258961	-0.000082	-0.392808
P	-1.036761	1.593543	-0.023351
P	-1.036790	-1.593609	-0.023647
P	2.339099	-1.364937	-0.148171
P	2.338853	1.365030	-0.148958
C	-1.684131	2.090453	1.639360
H	-2.299484	2.990707	1.531864
H	-2.363590	1.283622	1.935153
C	-0.600069	2.299234	2.691996
H	-1.041624	2.560348	3.657709
H	0.085062	3.107083	2.418087
H	-0.003140	1.391919	2.838573
C	-0.575352	3.192396	-0.842450
H	0.264894	3.594579	-0.264578
H	-0.169442	2.913047	-1.820885
C	-1.656536	4.258872	-1.000629
H	-1.224449	5.168499	-1.427401
H	-2.109913	4.536368	-0.044920
H	-2.454823	3.937012	-1.673841
C	-2.629575	1.207365	-0.895247
H	-3.306742	2.047895	-0.715450
H	-2.435757	1.169853	-1.983896
C	-4.695553	-0.000130	-0.652137
H	-5.150388	-0.883509	-0.196560
H	-4.939832	0.000140	-1.727837
H	-5.150523	0.882937	-0.196089
C	-2.629363	-1.207191	-0.895837
H	-2.435275	-1.169004	-1.984405
H	-3.306506	-2.047880	-0.716700
C	-0.575093	-3.192353	-0.842768
H	-0.168771	-2.912867	-1.820992
H	0.264924	-3.594592	-0.264588
C	-1.656232	-4.258783	-1.001512
H	-1.224020	-5.168372	-1.428238
H	-2.454251	-3.936804	-1.674988
H	-2.109995	-4.536387	-0.046014
C	-1.684629	-2.090691	1.638825
H	-2.364334	-1.283982	1.934377
H	-2.299763	-2.991072	1.531126
C	-0.600868	-2.299278	2.691808
H	-1.042685	-2.560388	3.657405
H	-0.004085	-1.391887	2.838512
H	0.084441	-3.107063	2.418155
C	2.898505	-2.653761	1.043841
H	2.289769	-3.556113	0.942137
H	2.791868	-2.286728	2.067631
H	3.944654	-2.919908	0.866979
C	2.760987	-2.130233	-1.763078
H	2.145504	-3.015707	-1.933737
H	3.814263	-2.424288	-1.786059
H	2.561532	-1.416926	-2.565086
C	3.578614	0.000219	0.039221
H	3.972750	0.000542	1.061186
H	4.421303	0.000094	-0.659423
C	2.760288	2.129237	-1.764499
H	2.144807	3.014652	-1.935499
H	2.560489	1.415441	-2.565981
H	3.813573	2.423213	-1.788019
C	2.898335	2.654823	1.041982
H	2.289663	3.557137	0.939550
H	3.944490	2.920768	0.864853
H	2.791728	2.288645	2.066081
H	0.497763	-0.000160	-1.470197

$[Fe(CO)H(P^{Et}NH^{Me}P^{Et})(dmpm)]^{2+}$
($[3(CO)H']^{2+}$)

Fe	-0.003620	-0.508588	0.002061
N	0.024980	3.325078	-0.520187
P	1.629914	1.001782	-0.020974
P	-1.614438	1.025750	-0.021435
P	-1.379026	-2.286040	-0.401110
P	1.344905	-2.306257	-0.401683
C	2.237235	1.699893	1.588160
H	2.815361	2.610489	1.392419
H	1.354720	1.991653	2.172193
C	3.079616	0.719556	2.405977

H	3.356061	1.176474	3.358958
H	4.007264	0.457099	1.890770
H	2.535869	-0.199583	2.633031
C	3.184908	0.589134	-0.939118
H	3.567844	-0.315390	-0.455335
H	2.865020	0.286429	-1.942084
C	4.291354	1.640431	-1.009982
H	5.171083	1.207064	-1.492658
H	4.606457	1.984397	-0.021621
H	4.009344	2.512135	-1.606102
C	1.267443	2.594565	-0.938931
H	2.100685	3.286661	-0.800508
H	1.163160	2.381692	-2.006154
C	0.035582	4.733865	-1.041794
H	-0.853804	5.253041	-0.683823
H	0.035579	4.697357	-2.131595
H	0.932413	5.239762	-0.683394
C	-1.228239	2.613239	-0.939002
H	-1.127117	2.398952	-2.006244
H	-2.050987	3.317760	-0.800551
C	-3.175326	0.636329	-0.940016
H	-2.860232	0.329676	-1.943307
H	-3.571308	-0.262788	-0.456617
C	-4.266298	1.703754	-1.009881
H	-5.152463	1.283544	-1.492434
H	-3.971838	2.571518	-1.605719
H	-4.575929	2.051877	-0.021236
C	-2.212762	1.731920	1.587534
H	-1.326734	2.010698	2.172512
H	-2.777613	2.650770	1.391687
C	-3.069673	0.763355	2.404244
H	-3.338825	1.223030	3.357984
H	-2.539765	-0.164202	2.629766
H	-4.001368	0.515648	1.889047
C	-2.695158	-2.850146	0.742159
H	-3.580387	-2.213351	0.671633
H	-2.331455	-2.820346	1.772005
H	-2.989930	-3.874965	0.498613
C	-2.088113	-2.585867	-2.061752
H	-2.970980	-1.965120	-2.224771
H	-2.382640	-3.634972	-2.157030
H	-1.350407	-2.344522	-2.829494
C	-0.026197	-3.529109	-0.244544
H	-0.029141	-3.946001	0.768008
H	-0.032330	-4.351887	-0.965267
C	2.048203	-2.616588	-2.062857
H	2.940081	-2.009096	-2.226658
H	1.313508	-2.364211	-2.829936
H	2.326995	-3.669959	-2.158442
C	2.652846	-2.890576	0.740769
H	3.548047	-2.268054	0.669316
H	2.931133	-3.920052	0.497470
H	2.290371	-2.854532	1.770852
C	-0.005677	-0.786094	1.749609
O	-0.007321	-0.992793	2.887374
H	0.025460	3.391630	0.503305
H	-0.002155	-0.294720	-1.515266

$[Fe(CO)H(P^{Et}N^{Me}P^{Et})(dmpm)]^+$ (**[3(CO)]$^+$**)

Fe	0.000156	-0.498982	0.003784
N	-0.000669	3.277935	-0.455421
P	1.611055	1.061384	-0.076811
P	-1.611482	1.060704	-0.076672
P	-1.356010	-2.273730	-0.349620
P	1.357004	-2.273247	-0.349263
C	2.260859	1.725028	1.525382
H	2.842187	2.628460	1.309806
H	1.385679	2.049935	2.097224
C	3.098663	0.741111	2.336656
H	3.405420	1.198067	3.281325
H	4.010754	0.450434	1.806509
H	2.541828	-0.165802	2.582498
C	3.141752	0.588082	-1.009100
H	3.533873	-0.315624	-0.530888
H	2.795523	0.286188	-2.003688
C	4.251612	1.631582	-1.120248
H	5.113131	1.204957	-1.641791
H	4.600507	1.968915	-0.140534
H	3.937119	2.509964	-1.688841
C	1.196646	2.637174	-0.960701
H	2.042235	3.314208	-0.808891
H	1.138141	2.420231	-2.045271
C	-0.000952	4.709020	-0.742138
H	-0.883927	5.172025	-0.294377
H	-0.001098	4.932261	-1.822723
H	0.881943	5.172341	-0.294548
C	-1.197850	2.636760	-0.960478
H	-1.139513	2.419964	-2.045088
H	-2.043669	3.313447	-0.808399
C	-3.141966	0.586778	-1.009000

H	-2.795580	0.284994	-2.003564
H	-3.533761	-0.317057	-0.530772
C	-4.252213	1.629859	-1.120232
H	-5.113597	1.202863	-1.641693
H	-3.938050	2.508286	-1.688939
H	-4.601202	1.967185	-0.140548
C	-2.261602	1.723938	1.525569
H	-1.386579	2.049096	2.097509
H	-2.843221	2.627191	1.310029
C	-3.099142	0.739687	2.336713
H	-3.406134	1.196502	3.281374
H	-2.542029	-0.167048	2.582573
H	-4.011089	0.448731	1.806472
C	-2.676403	-2.835254	0.796192
H	-3.558407	-2.195123	0.716179
H	-2.311559	-2.782277	1.824765
H	-2.970872	-3.864350	0.571429
C	-2.061631	-2.646204	-2.001047
H	-2.935691	-2.021421	-2.193019
H	-2.360883	-3.696592	-2.061119
H	-1.316369	-2.433085	-2.769980
C	0.000700	-3.514986	-0.158753
H	0.000616	-3.894004	0.868427
H	0.000949	-4.361429	-0.851981
C	2.063075	-2.645444	-2.000567
H	2.937005	-2.020416	-2.192336
H	1.317901	-2.432470	-2.769626
H	2.362620	-3.695747	-2.060650
C	2.677395	-2.834207	0.796814
H	3.558993	-2.193462	0.717237
H	2.972609	-3.863056	0.571904
H	2.312200	-2.781708	1.825288
C	0.000066	-0.678748	1.753460
O	-0.000016	-0.823156	2.905058
H	0.000216	-0.304066	-1.517821

$[Fe(CO)Cl(P^{Et}NH^{Me}P^{Et})(dmpm)]^{2+}$

Fe	-0.514235	-0.000002	0.045168
N	3.350252	0.000022	-0.505279
P	1.074104	-1.628326	0.137186
P	1.074061	1.628363	0.137100
P	-2.353357	1.390782	-0.297329
P	-2.353261	-1.390911	-0.297426
C	1.812515	-2.084938	1.775615
H	2.759978	-2.609150	1.603885
H	2.047102	-1.156009	2.309809
C	0.896672	-2.950619	2.644576
H	1.366192	-3.121918	3.615901
H	0.719804	-3.929437	2.192326
H	-0.068199	-2.474232	2.831504
C	0.666210	-3.252480	-0.640223
H	-0.176596	-3.634447	-0.053922
H	0.273755	-3.012972	-1.633416
C	1.766607	-4.309941	-0.718721
H	1.337111	-5.248325	-1.078704
H	2.222363	-4.519169	0.252776
H	2.557143	-4.041787	-1.424017
C	2.605280	-1.253302	-0.865416
H	3.311251	-2.079506	-0.760070
H	2.307510	-1.158205	-1.912856
C	4.708088	0.000022	-1.150956
H	5.250365	0.893126	-0.839803
H	4.572638	-0.000002	-2.232845
H	5.250388	-0.893055	-0.839766
C	2.605245	1.253306	-0.865485
H	2.307470	1.158147	-1.912919
H	3.311205	2.079522	-0.760185
C	0.666087	3.252492	-0.640354
H	0.273707	3.012964	-1.633572
H	-0.176791	3.634392	-0.054110
C	1.766374	4.310073	-0.718773
H	1.336792	5.248420	-1.078748
H	2.556971	4.042036	-1.424044
H	2.222058	4.519324	0.252753
C	1.812469	2.085035	1.775513
H	2.046982	1.156125	2.309777
H	2.759968	2.609178	1.603775
C	0.896667	2.950849	2.644387
H	1.366164	3.122171	3.615718
H	-0.068251	2.474555	2.831309
H	0.719898	3.929653	2.192068
C	-3.176971	2.177142	1.135358
H	-2.583974	3.024835	1.489302
H	-3.282332	1.469886	1.960947
H	-4.167796	2.542085	0.851015
C	-2.517997	2.628360	-1.633584
H	-2.107961	3.593879	-1.333539
H	-3.580944	2.760942	-1.856268
H	-2.002887	2.271496	-2.527701
C	-3.447525	-0.000083	-0.811698

H	-4.449106	-0.000133	-0.371895
H	-3.537693	-0.000051	-1.902183
C	-2.517865	-2.628398	-1.633774
H	-2.107842	-3.593940	-1.333793
H	-2.002744	-2.271471	-2.527858
H	-3.580810	-2.760958	-1.856482
C	-3.176799	-2.177433	1.135216
H	-2.583731	-3.025107	1.489088
H	-4.167604	-2.542431	0.850871
H	-3.282192	-1.470245	1.960858
Cl	-0.220857	0.000005	-2.269387
C	-0.783719	-0.000012	1.763466
O	-0.987129	0.000067	2.900698
H	3.509372	0.000052	0.507741

$[Fe(CO)Cl(P^{Et}N^{Me}P^{Et})(dmpm)]^{+}$ (**[1(CO)]$^{+}$**)

Fe	0.482537	-0.000013	0.036086
N	-3.314441	-0.000091	-0.342785
P	-1.125200	1.626936	0.046849
P	-1.125125	-1.627016	0.046773
P	2.324427	-1.389301	-0.207915
P	2.324228	1.389485	-0.208268
C	-1.788771	2.174752	1.685545
H	-2.725759	2.712218	1.502567
H	-2.059946	1.267922	2.234833
C	-0.838888	3.041465	2.508520
H	-1.286629	3.269842	3.479341
H	-0.630774	3.995482	2.015630
H	0.112898	2.541159	2.703403
C	-0.644501	3.200937	-0.789383
H	0.186054	3.612648	-0.206164
H	-0.235341	2.903775	-1.759874
C	-1.734717	4.258035	-0.955887
H	-1.304621	5.168967	-1.381564
H	-2.197595	4.532388	-0.003570
H	-2.523849	3.929519	-1.636182
C	-2.681700	1.199779	-0.859589
H	-3.362617	2.043168	-0.712643
H	-2.448825	1.136998	-1.936869
C	-4.750373	-0.000128	-0.608809
H	-5.206760	-0.882872	-0.153807
H	-4.990034	-0.000103	-1.685351
H	-5.206814	0.882560	-0.153752
C	-2.681631	-1.199891	-0.859664
H	-2.448755	-1.137034	-1.936938
H	-3.362500	-2.043329	-0.712768
C	-0.644300	-3.200958	-0.789492
H	-0.235054	-2.903739	-1.759928
H	0.186212	-3.612663	-0.206209
C	-1.734475	-4.258076	-0.956141
H	-1.304315	-5.168981	-1.381811
H	-2.523550	-3.929552	-1.636499
H	-2.197438	-4.532480	-0.003880
C	-1.788706	-2.174917	1.685438
H	-2.059981	-1.268119	2.234727
H	-2.725639	-2.712470	1.502430
C	-0.838765	-3.041551	2.508430
H	-1.286495	-3.269957	3.479248
H	0.112980	-2.541169	2.703315
H	-0.630572	-3.995554	2.015546
C	3.087654	-2.174698	1.263102
H	2.486434	-3.032910	1.575307
H	3.122741	-1.469590	2.096748
H	4.101308	-2.519174	1.040730
C	2.595041	-2.624802	-1.532728
H	2.164543	-3.591037	-1.265953
H	3.670078	-2.751489	-1.690092
H	2.129234	-2.262120	-2.451378
C	3.454544	0.000116	-0.658264
H	4.431376	0.000249	-0.165799
H	3.598542	-0.000012	-1.742638
C	2.594697	2.624690	-1.533387
H	2.164141	3.590958	-1.266832
H	2.128895	2.261749	-2.451937
H	3.669722	2.751415	-1.690805
C	3.087345	2.175347	1.262559
H	2.485987	3.033528	1.574583
H	4.100942	2.519942	1.040109
H	3.122552	1.470423	2.096357
Cl	0.349569	-0.000155	-2.299086
C	0.616653	0.000033	1.759602
O	0.732758	0.000088	2.912923

$Fe(N_2)(P^{Et}N^{Me}P^{Et})_2$

Fe	-0.000027	0.000101	0.480830
P	1.061777	-1.512803	-0.691818
P	1.927095	1.107887	0.666111
C	0.273531	-2.647089	-1.972121
C	-0.110766	-2.013122	-3.304814
C	1.877407	-2.858492	0.340669

C	3.040277	-3.657907	-0.237639
N	3.535711	-0.212117	-1.139332
C	2.497075	-0.999462	-1.786884
C	4.722481	-0.150713	-1.976619
C	3.083922	1.126500	-0.790958
C	3.089204	0.419694	1.948332
C	4.337573	1.223201	2.299162
C	1.939942	2.920847	1.099407
C	1.297907	3.212497	2.453483
P	-1.061940	1.512589	-0.692224
P	-1.927139	-1.107547	0.666619
C	-0.273314	2.645943	-1.973150
C	0.110550	2.011089	-3.305538
C	-1.877114	2.859018	0.339635
C	-3.039972	3.658258	-0.238890
N	-3.535873	0.211699	-1.139272
C	-2.497277	0.998945	-1.787004
C	-4.722533	0.149842	-1.976684
C	-3.083955	-1.126740	-0.790394
C	-3.088991	-0.418929	1.948783
C	-4.337880	-1.221764	2.299271
C	-1.939973	-2.920373	1.100503
C	-1.298107	-3.211620	2.454738
H	-0.621309	-3.064346	-1.498851
H	0.947627	-3.494386	-2.149361
H	-0.703362	-1.105585	-3.159748
H	-0.706126	-2.707272	-3.907654
H	0.767305	-1.742521	-3.897778
H	1.054635	-3.528825	0.620636
H	2.182661	-2.371357	1.271106
H	2.789197	-4.138081	-1.189656
H	3.343008	-4.453539	0.452030
H	3.911816	-3.017674	-0.402505
H	2.070638	-0.458138	-2.652051
H	2.960374	-1.910020	-2.182649
H	5.086589	-1.163227	-2.176183
H	5.515169	0.397241	-1.457941
H	4.541278	0.345243	-2.949191
H	2.591099	1.637845	-1.639779
H	3.960656	1.725589	-0.521257
H	2.495139	0.222642	2.844562
H	3.380239	-0.554011	1.541988
H	4.096150	2.183750	2.763450
H	4.962266	1.422377	1.422710
H	4.955132	0.666385	3.011714
H	2.973198	3.288359	1.074974
H	1.400194	3.454826	0.310590
H	1.851268	2.743729	3.272319
H	0.275531	2.829091	2.494824
H	1.269516	4.289928	2.645514
H	-0.946947	3.493530	-2.150768
H	0.621760	3.062881	-1.500064
H	-0.767720	1.741475	-3.898665
H	0.701873	1.102805	-3.160001
H	0.707001	2.704256	-3.908429
H	-2.182219	2.372501	1.270449
H	-1.054135	3.529362	0.618956
H	-3.911612	3.018066	-0.403375
H	-2.788942	4.138007	-1.191137
H	-3.342574	4.454197	0.450487
H	-2.070729	0.457402	-2.651985
H	-2.960648	1.909330	-2.183089
H	-5.086751	1.162237	-2.176641
H	-5.515210	-0.398040	-1.457915
H	-4.541135	-0.346427	-2.949059
H	-2.591008	-1.638359	-1.638984
H	-3.960643	-1.725822	-0.520519
H	-3.379389	0.555078	1.542716
H	-2.494838	-0.222435	2.845088
H	-4.962771	-1.419908	1.422732
H	-4.954966	-0.664969	3.012248
H	-4.097102	-2.182787	2.762918
H	-1.400063	-3.454492	0.311890
H	-2.973190	-3.287992	1.076021
H	-0.275835	-2.827970	2.496209
H	-1.269492	-4.289009	2.646976
H	-1.851761	-2.742857	3.273382
N	0.000210	0.000143	2.250056
N	0.000388	0.000229	3.389562

$Fe(P^{Et}N^{Me}P^{Et})_2$

Fe	-0.000006	0.000005	0.112317
P	-1.277408	1.534458	-0.684011
P	-1.730738	-1.205827	0.683355
C	-0.650377	2.616024	-2.080914
C	0.068511	1.858003	-3.188802
C	-2.048836	2.851322	0.419990
C	-2.723208	4.068379	-0.207690
N	-3.757594	0.308748	-0.532469
C	-2.870123	0.958459	-1.486573

C	-5.136867	0.343066	-0.987718
C	-3.358605	-1.052949	-0.231410
C	-2.257793	-0.762263	2.421050
C	-1.351656	-1.341931	3.504879
C	-1.732493	-3.079260	0.795488
C	-2.956688	-3.790902	1.368411
P	1.277427	-1.534505	-0.683854
P	1.730709	1.205876	0.683325
C	0.650440	-2.616189	-2.080686
C	-0.068418	-1.858260	-3.188657
C	2.048836	-2.851271	0.420276
C	2.723236	-4.068375	-0.207285
N	3.757602	-0.308765	-0.532349
C	2.870160	-0.958560	-1.486422
C	5.136885	-0.343103	-0.987567
C	3.358592	1.052951	-0.231402
C	2.257738	0.762405	2.421052
C	1.351599	1.342147	3.504840
C	1.732451	3.079315	0.795363
C	2.956641	3.790994	1.368248
H	0.026873	3.349976	-1.629499
H	-1.491321	3.187664	-2.491903
H	0.881006	1.254483	-2.773230
H	0.486136	2.545900	-3.932520
H	-0.606492	1.174264	-3.712047
H	-1.264068	3.174499	1.111329
H	-2.773914	2.286489	1.017439
H	-2.010031	4.702173	-0.742928
H	-3.195082	4.688803	0.562532
H	-3.509979	3.786468	-0.915085
H	-2.630934	0.301248	-2.344308
H	-3.388407	1.834695	-1.891791
H	-5.449050	1.379067	-1.150265
H	-5.790067	-0.090659	-0.223835
H	-5.296613	-0.215710	-1.929918
H	-3.272665	-1.668858	-1.152359
H	-4.143595	-1.505780	0.384366
H	-2.256528	0.330654	2.469443
H	-3.294788	-1.084207	2.576555
H	-0.303369	-1.089728	3.322050
H	-1.423749	-2.432893	3.552772
H	-1.623597	-0.953387	4.491978
H	-1.536256	-3.441530	-0.219716
H	-0.841869	-3.338476	1.377762
H	-3.840102	-3.661514	0.736950
H	-3.210895	-3.432009	2.370371
H	-2.773731	-4.868136	1.446736
H	1.491397	-3.187860	-2.491604
H	-0.026821	-3.350105	-1.629228
H	0.606601	-1.174568	-3.711943
H	-0.880922	-1.254700	-2.773157
H	-0.486028	-2.546218	-3.932327
H	2.773893	-2.286383	1.017699
H	1.264051	-3.174398	1.111620
H	3.510018	-3.786514	-0.914688
H	2.010078	-4.702224	-0.742483
H	3.195102	-4.688726	0.563001
H	2.630988	-0.301422	-2.344217
H	3.388460	-1.834826	-1.891555
H	5.449084	-1.379113	-1.150028
H	5.790064	0.090689	-0.223705
H	5.296644	0.215603	-1.929808
H	3.272661	1.668788	-1.152398
H	4.143567	1.505837	0.384354
H	3.294736	1.084343	2.576550
H	2.256455	-0.330509	2.469506
H	1.423707	2.433111	3.552673
H	1.623526	0.953655	4.491963
H	0.303310	1.089948	3.322017
H	0.841827	3.338549	1.377629
H	1.536204	3.441535	-0.219857
H	3.210861	3.432142	2.370220
H	2.773670	4.868229	1.446534
H	3.840050	3.661594	0.736785

$Fe(P^{Et}N^{Me}P^{Et})_2$-CH activation (**4**)

Fe	-0.302883	-0.020104	0.069102
H	-1.231459	0.082302	1.259093
N	-3.150483	0.079288	-0.651681
N	3.363378	-0.981606	-0.019388
P	-1.263488	1.909278	-0.088289
P	-1.305694	-1.916322	0.116315
P	1.263477	-0.030217	1.580462
P	1.186551	-0.172697	-1.540615
C	-0.800946	3.383094	-1.140199
H	-0.559338	2.985952	-2.133291
H	-1.678381	4.029198	-1.269865
C	0.371616	4.189259	-0.590870
H	0.667292	4.984236	-1.283390
H	1.244409	3.553169	-0.419187

H	0.121353	4.663789	0.363213
C	-1.778354	2.768741	1.486581
H	-2.312103	1.996007	2.049387
H	-0.861225	2.967013	2.053930
C	-2.624280	4.033477	1.383546
H	-2.915596	4.384225	2.379466
H	-3.546759	3.860969	0.820288
H	-2.089138	4.852945	0.894793
C	-2.908481	1.491813	-0.873980
H	-3.738336	2.097782	-0.486428
H	-2.814056	1.729494	-1.955759
C	-4.324151	-0.377948	-1.368550
H	-4.499638	-1.435213	-1.151163
H	-4.223072	-0.269920	-2.467434
H	-5.210345	0.186004	-1.056250
C	-1.945925	-0.657952	-0.971896
H	-1.847257	-0.882581	-2.046028
C	-2.513062	-2.343441	1.454161
H	-1.948675	-2.568427	2.366423
H	-3.019891	-1.387629	1.625432
C	-3.522934	-3.447155	1.159538
H	-4.241339	-3.538251	1.981145
H	-3.046667	-4.424537	1.035103
H	-4.091993	-3.237191	0.248746
C	-1.015347	-3.525650	-0.771716
H	-1.976081	-3.972149	-1.051432
H	-0.501449	-3.270848	-1.704780
C	-0.175866	-4.513679	0.034687
H	0.007237	-5.434814	-0.528248
H	-0.671563	-4.793977	0.970123
H	0.795723	-4.082215	0.296964
C	0.816089	-0.711399	3.254139
H	0.370899	-1.693387	3.059471
H	1.731740	-0.882712	3.833898
C	-0.159705	0.153388	4.043205
H	-0.430097	-0.325533	4.989944
H	-1.075123	0.319395	3.469000
H	0.267799	1.133159	4.281311
C	2.189244	1.525335	2.040553
H	2.699125	1.832010	1.120613
H	1.419331	2.284206	2.220476
C	3.179140	1.488741	3.200548
H	3.653538	2.466993	3.333783
H	3.981846	0.764419	3.031959
H	2.693413	1.231750	4.146578
C	2.685483	-1.197385	1.250657
H	3.425181	-1.090233	2.052158
H	2.274731	-2.224684	1.327932
C	4.649558	-1.659087	-0.028971
H	5.178435	-1.440782	-0.961901
H	4.561496	-2.758313	0.065233
H	5.265770	-1.297177	0.799872
C	2.564520	-1.378676	-1.171953
H	2.112970	-2.381397	-1.039326
H	3.228676	-1.436219	-2.041207
C	2.203240	1.319994	-2.005457
H	1.486890	2.077196	-2.339468
H	2.612875	1.688479	-1.060414
C	3.322851	1.157462	-3.027972
H	3.792338	2.124010	-3.240226
H	2.961485	0.756937	-3.980258
H	4.109371	0.492323	-2.660760
C	0.710766	-0.803039	-3.232200
H	1.607061	-1.129620	-3.773524
H	0.096634	-1.696272	-3.075931
C	-0.066642	0.215169	-4.062255
H	-0.431897	-0.233580	-4.991702
H	0.556657	1.072265	-4.335451
H	-0.931698	0.593380	-3.509730

$[FeH(N_2)(dmpe)_2]^+$

Fe	-0.000011	-0.000020	0.032265
C	1.749003	-2.790858	-1.367865
C	2.207848	-2.314180	1.407201
P	1.714056	-1.435001	-0.131772
C	3.258600	-0.500964	-0.560443
C	3.213214	0.860539	0.122567
P	1.545311	1.604804	-0.188905
C	1.777471	2.347858	-1.850707
C	1.559747	3.073953	0.914839
C	-1.559634	-3.074094	0.914899
C	-1.777718	-2.347787	-1.850539
P	-1.545262	-1.604822	-0.188708
C	-3.213159	-0.860620	0.122967
C	-3.258635	0.500757	-0.560352
P	-1.714162	1.434904	-0.131811
C	-2.207839	2.314237	1.407109
C	-1.749101	2.790663	-1.368017
N	0.000153	0.000310	1.855704
N	0.000300	0.000637	2.976092

H	-0.000163	-0.000073	-1.480865
H	1.033221	-3.574089	-1.107366
H	2.744997	-3.241406	-1.405401
H	1.497439	-2.397190	-2.355178
H	1.386811	-2.939144	1.766553
H	2.442233	-1.591734	2.192812
H	3.083460	-2.946157	1.235010
H	3.278755	-0.386088	-1.650082
H	4.145284	-1.077692	-0.278071
H	3.329198	0.755244	1.207667
H	4.009422	1.525705	-0.227587
H	0.879098	2.881127	-2.163428
H	1.960871	1.554234	-2.578042
H	2.621264	3.043824	-1.850706
H	0.713565	3.728870	0.691419
H	2.480737	3.650043	0.787674
H	1.482350	2.756866	1.957994
H	-1.482297	-2.757100	1.958103
H	-0.713433	-3.728974	0.691476
H	-2.480609	-3.650183	0.787644
H	-1.962617	-1.554276	-2.577618
H	-2.620674	-3.044775	-1.850046
H	-0.878923	-2.879910	-2.164005
H	-3.328931	-0.755043	1.208064
H	-4.009432	-1.525855	-0.226897
H	-3.278661	0.385628	-1.649968
H	-4.145404	1.077460	-0.278205
H	-2.443292	1.591888	2.192488
H	-3.082768	2.947091	1.234637
H	-1.386350	2.938331	1.766924
H	-1.497065	2.396980	-2.355209
H	-1.033656	3.574121	-1.107316
H	-2.745230	3.240880	-1.405948

$[FeH(N_2H)(dmpe)_2]^{2+}$

Fe	-0.005471	0.007752	0.133184
C	1.306711	-2.826315	-1.671140
C	1.824414	-2.709166	1.155786
P	1.506696	-1.642625	-0.295956
C	3.148218	-0.866448	-0.627954
C	3.280435	0.414158	0.186610
P	1.772017	1.430536	-0.107233
C	2.085963	2.136142	-1.765717
C	1.955594	2.856418	1.023195
C	-1.952264	-2.852793	1.006205
C	-2.131640	-2.087280	-1.768395
P	-1.790036	-1.408941	-0.103748
C	-3.298655	-0.399619	0.221821
C	-3.175947	0.898523	-0.566520
P	-1.529045	1.662873	-0.234064
C	-1.836726	2.677198	1.261453
C	-1.350834	2.899864	-1.564767
N	0.068012	-0.067194	1.790209
N	0.253105	-0.265223	2.942757
H	-0.006339	0.009797	-1.378448
H	0.547097	-3.575112	-1.438130
H	2.254671	-3.352148	-1.820856
H	1.037974	-2.309628	-2.594496
H	0.920266	-3.243612	1.453008
H	2.157661	-2.110354	2.006432
H	2.599830	-3.441165	0.912275
H	3.212624	-0.659671	-1.701506
H	3.938718	-1.586132	-0.391622
H	3.347766	0.198902	1.258884
H	4.176633	0.979544	-0.088693
H	1.323930	2.866202	-2.037728
H	2.081821	1.347701	-2.520899
H	3.059329	2.635238	-1.773101
H	1.221820	3.632844	0.794031
H	2.952589	3.292722	0.912125
H	1.827638	2.544066	2.062316
H	-1.757266	-2.570863	2.043523
H	-1.250869	-3.639983	0.719513
H	-2.963931	-3.263197	0.937783
H	-2.146389	-1.285786	-2.509643
H	-3.102362	-2.591557	-1.765517
H	-1.371540	-2.808262	-2.067990
H	-3.360970	-0.208020	1.298853
H	-4.195502	-0.961343	-0.058913
H	-3.250185	0.713562	-1.643403
H	-3.964954	1.612528	-0.308785
H	-2.226258	2.048086	2.065779
H	-2.574244	3.454851	1.042249
H	-0.918039	3.154600	1.607308
H	-1.099808	2.417116	-2.511280
H	-0.582704	3.635564	-1.317823
H	-2.298689	3.434524	-1.679220
H	-0.221995	0.282599	3.671949

$[Fe(N_2)H(P^{Et}N^{Me}P^{Et})(dmpm)]^{0}$

Fe	-0.118078	-0.205363	0.258496
N	3.061215	1.471839	-0.702039
P	1.911047	-1.028269	-0.199802
P	0.426128	1.922448	0.062064
P	-3.758868	0.381712	-0.290891
P	-1.558637	-1.855821	-0.022429
C	3.094096	-1.433674	1.178728
H	4.098119	-1.615698	0.775362
H	3.159027	-0.523740	1.785144
C	2.643457	-2.610241	2.039660
H	3.329462	-2.765389	2.878679
H	2.615947	-3.542411	1.465225
H	1.646413	-2.440649	2.453629
C	2.039483	-2.548079	-1.275600
H	1.486330	-3.332912	-0.746093
H	1.445258	-2.313509	-2.166613
C	3.420694	-3.062117	-1.672988
H	3.336425	-3.971714	-2.277394
H	4.030554	-3.309181	-0.798743
H	3.974605	-2.330632	-2.268365
C	2.996295	0.108504	-1.209820
H	4.012230	-0.300632	-1.207140
H	2.634703	0.078446	-2.257237
C	4.273481	2.135346	-1.156280
H	4.335831	3.134441	-0.714854
H	4.327367	2.242299	-2.256173
H	5.149794	1.568796	-0.827779
C	1.881863	2.251948	-1.048270
H	1.558733	2.074234	-2.092539
H	2.136394	3.313747	-0.962075
C	-0.855230	2.988727	-0.756525
H	-1.019661	2.522669	-1.734687
H	-1.783872	2.821274	-0.200072
C	-0.564370	4.479230	-0.905666
H	-1.398995	4.983899	-1.403667
H	0.330783	4.668426	-1.506223
H	-0.422819	4.967697	0.063059
C	0.911193	2.920844	1.551562
H	1.729667	2.368886	2.025857
H	1.324873	3.884414	1.228829
C	-0.231434	3.134766	2.540931
H	0.118241	3.678729	3.424266
H	-0.649289	2.184240	2.879870
H	-1.045758	3.716403	2.097342
C	-5.604343	0.268937	-0.106856
H	-6.062641	1.184462	-0.492618
H	-5.863154	0.192132	0.953134
H	-6.034345	-0.588251	-0.637156
C	-3.639461	0.236513	-2.133237
H	-4.085407	1.126738	-2.586982
H	-4.149259	-0.649640	-2.527695
H	-2.583645	0.209067	-2.416046
C	-3.332792	-1.350058	0.243679
H	-3.488492	-1.369847	1.329327
H	-4.010852	-2.092667	-0.200735
C	-1.669352	-2.729601	-1.641979
H	-0.728141	-3.251549	-1.829175
H	-1.815316	-2.002621	-2.442222
H	-2.487158	-3.457516	-1.653303
C	-1.499606	-3.309141	1.119791
H	-0.573033	-3.864604	0.949908
H	-2.349976	-3.984273	0.978716
H	-1.490393	-2.952196	2.153020
N	-0.089814	-0.337449	2.036138
N	-0.091875	-0.434012	3.162990
H	-0.304093	-0.017064	-1.273192

$[Fe(N_2)H(P^{Et}NH^{Me}P^{Et})(dmpm)]^+$

Fe	0.050460	-0.217884	0.225306
N	2.862046	1.835365	-0.137604
P	2.108350	-0.859623	-0.210570
P	0.064208	1.957487	-0.042809
P	-3.700266	-0.009208	-0.245899
P	-1.271643	-2.021769	-0.054638
C	3.275058	-1.465780	1.112008
H	4.290282	-1.565139	0.710032
H	3.310665	-0.688906	1.887084
C	2.820869	-2.780000	1.742359
H	3.496561	-3.071476	2.550910
H	2.816123	-3.595087	1.012185
H	1.815997	-2.693759	2.163165
C	2.399086	-2.069412	-1.588550
H	1.912894	-2.994696	-1.257977
H	1.793046	-1.700997	-2.423712
C	3.831623	-2.358760	-2.027663
H	3.837069	-3.099407	-2.832476
H	4.438962	-2.763936	-1.213611
H	4.337471	-1.468312	-2.413928
C	3.176073	0.553398	-0.873248
H	4.243708	0.360921	-0.741024

H	2.975623	0.722931	-1.932807
C	4.065706	2.700927	0.014244
H	3.805200	3.575796	0.611078
H	4.399903	3.012583	-0.975642
H	4.854014	2.134106	0.510744
C	1.698233	2.588839	-0.734878
H	1.733692	2.450829	-1.816975
H	1.847772	3.647420	-0.508038
C	-1.079598	2.681442	-1.302655
H	-0.856256	2.142377	-2.230107
H	-2.073557	2.333820	-0.997394
C	-1.059480	4.191778	-1.513474
H	-1.770522	4.468658	-2.297059
H	-0.078385	4.561417	-1.829764
H	-1.348421	4.737140	-0.611061
C	-0.110489	3.103474	1.410571
H	0.668264	2.830304	2.134398
H	0.081796	4.137941	1.102416
C	-1.481841	2.986740	2.073798
H	-1.533916	3.629688	2.956453
H	-1.684034	1.961107	2.391498
H	-2.284150	3.286299	1.393998
C	-5.404628	-0.130355	0.467116
H	-6.005742	0.707811	0.103635
H	-5.356181	-0.053687	1.556731
H	-5.909723	-1.064406	0.199920
C	-4.085295	-0.393771	-2.015576
H	-4.731553	0.395469	-2.410666
H	-4.597097	-1.353853	-2.139773
H	-3.169882	-0.394483	-2.612253
C	-3.037971	-1.643899	0.357995
H	-3.073217	-1.588761	1.453239
H	-3.681241	-2.480780	0.052440
C	-1.383419	-2.813061	-1.708922
H	-0.415135	-3.250230	-1.964576
H	-1.622094	-2.063661	-2.464658
H	-2.140530	-3.602651	-1.724511
C	-1.002853	-3.495734	1.018484
H	-0.043544	-3.959419	0.773997
H	-1.795797	-4.238419	0.888653
H	-0.973626	-3.186534	2.066422
N	0.064018	-0.309764	2.024206
N	0.067673	-0.369699	3.148705
H	-0.060938	-0.121746	-1.306298
H	2.542209	1.539133	0.799276

$[N_2H]^+$

N	0.000000	0.000000	-0.443242
N	0.000000	0.000000	0.654779
H	0.000000	0.000000	-1.480759

N_2

N	0.000000	0.000000	0.551945
N	0.000000	0.000000	-0.551945