Appendix C

Supplementary Information for Chapter 4

Adapted from:

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C.1 General procedures

General Considerations: All manipulations were carried out using standard Schlenk or glovebox techniques under an N_2 or Ar atmosphere. Unless otherwise noted, solvents were deoxygenated and dried by thoroughly sparging with N_2 gas followed by passage through an activated alumina column in a solvent purification system (SG Water, USA LLC). For electrochemical measurements under an Ar atmosphere, solvents were further degassed and then left under Ar. All solvents were stored over activated 3 or 4 Å molecular sieves prior to use. Anhydrous ammonia gas was dried by passage through a calcium oxide drying tube. All reagents were purchased from commercial vendors and used without further purification unless otherwise stated. Tris(2-pyridylmethyl)amine (TPA),[1] tris(2-pyridylmethylamine) iron(II) triflate bis-acetonitrile ($[(TPA)Fe(MeCN)_2]OTf_2$),[2] 6-(1,1-di(pyridin-2-yl)ethyl)-2,2'-bipyridine ($bpyPy_2Me$),[3] and 6-(1,1-di(pyridin-2-yl)ethyl)-2,2'-bipyridine iron(II) triflate bis-acetonitrile ($[(bpyPy_2Me)Fe(MeCN)_2]OTf_2$)[4] $^{15}NH_4OTf$ was prepared from $^{15}NH_4Cl$ (Cambridge Isotope Laboratories) by anion exchange with silver triflate or metathesis with triflic acid, followed by repeated recrystallization from boiling acetonitrile. ^1H NMR chemical shifts are reported in ppm relative to tetramethylsilane, using residual solvent resonances as internal standards.

Electrochemistry: Voltammetry experiments were carried out with a Biologic VSP-300 or CH Instruments 600B potentiostat using a one-compartment three-electrode cell, and coulometry experiments were carried out with a Biologic VSP-300 potentiostat using a one-compartment three-electrode cell with a septum capped 14/20 joint for headspace analysis. For voltammetry, a boron-doped diamond (BDD) working electrode (3 mm diameter), a Pt

wire counter electrode, and a Ag/AgOTf reference electrode (5 mM AgOTf and 0.1 M $TBAPF_6$ in MeCN) were employed. For CPC, the same reference electrode was used, but a BDD plate (geometric area: 4 cm^2) and a Pt mesh were used respectively as working and counter electrode. All redox potentials in the present work are reported versus the Fc/Fc^+ couple, measured before each experiment to be approximately +0.12 V versus our Ag/AgOTf reference electrode.

CVs were collected at 100 $mV \cdot s^{-1}$ unless specified otherwise. $E_{1/2}$ values for the reversible waves were obtained from the half potential between the oxidative and reductive peaks. CV measurements were performed applying IR compensation, compensating 85% of the resistance measured at one high frequency value (100 kHz). Potential values for waves that are not fully reversible were obtained as the apparent standard potential from differential pulse voltammetry measurements

Gas Chromatography: Gas chromatography was performed in the Environmental Analysis Center using HP 5890 Series II instruments. Gas quantification was performed using a molecular sieve column attached to a thermal conductivity detector. Argon was the carrier gas. Standard curves were generated by direct injection of hydrogen or nitrogen gas. Quantification of background nitrogen was determined using the background oxygen signal. Isotopic measurements were performed with a separate HP 5890 Series II equipped with a GasPro column using helium as the carrier gas.

NMR: NMR spectroscopy was performed using Varian and Bruker 400 MHz NMR spectrometers equipped with broadband auto-tune probes. ^1H NMR chemical shifts are

reported in ppm relative to tetramethylsilane, using residual solvent resonances as internal standards.

UV-vis: Spectra were collected using a Cary 60 instrument with Cary WinUV software.

X-ray Crystallography: XRD studies were carried out at the Beckman Institute Crystallography Facility on a Bruker D8 Venture diffractometer (Cu Kα radiation). Structures were solved using direct methods with SHELXS or SHELXT and refined against F^2 on all data by full-matrix least squares with SHELXL.[5] All of the solutions were performed in the Olex2 program.[6] The crystals were mounted on a glass fiber under Paratone N oil.

X-ray Photoelectron Spectroscopy: XPS measurements were carried out in the Caltech Molecular Materials Resource Center using a Surface Science Instruments M-Probe ESCA spectrometer with the sample held at ultra-high vacuum (< 2 x 10^{-9} Torr), using the Al K α line at 1486.6 eV as a monochromatic X-ray source. XPS measurements were checked for surface charging effects, and the diamond carbon (sp3) 1s peak was verified to be within ±0.3 eV of 285 eV. A full scan from 0–1000 eV was acquired, and then scans at the binding energies typical for carbon (274-294 eV), boron (176-196 eV), nitrogen (389-409 eV), oxygen (522-542 eV), and iron (690-730 eV) were measured. For measurements of the BDD plate electrode after catalysis, the electrode was rinsed with acetonitrile and air dried prior to data collection.

C.2 NMR spectra for electronic structure elucidation

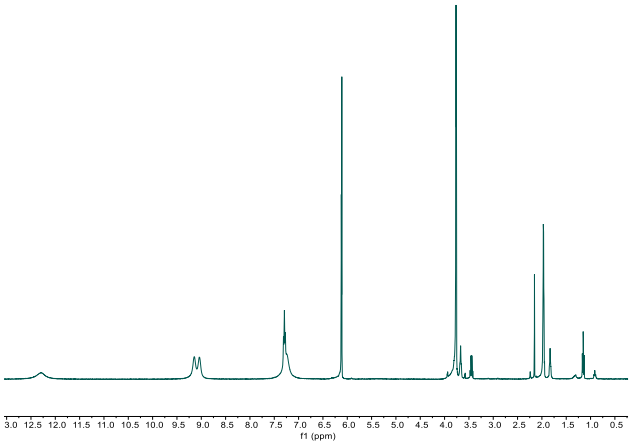

Figure C1. ^{1}H NMR spectrum of [(TPA)Fe(MeCN)$_2$]OTf$_2$ in CD_3CN at 25 °C. Spectrum also shows 1,3,5-trimethoxybenzene used for Evan's method.

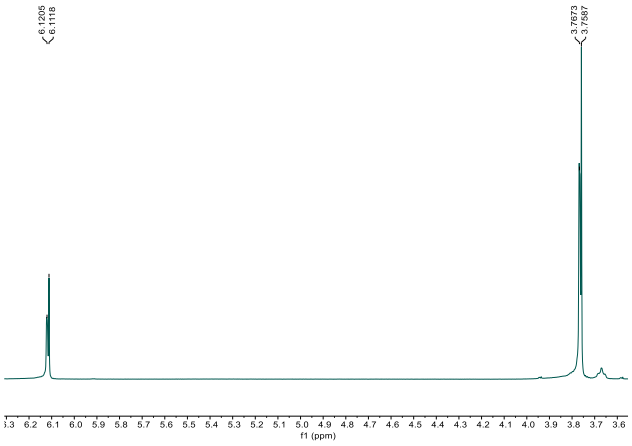

Figure C2. 1,3,5-trimethoxybenzene signals used for Evan's method for [(TPA)Fe(MeCN)$_2$]OTf$_2$ in CD_3CN at 25 °C. [Fe] = 0.011 M, $\Delta f = 3.46$ Hz, f = 400.15 MHz, $\mu = 0.68\mu_B$.

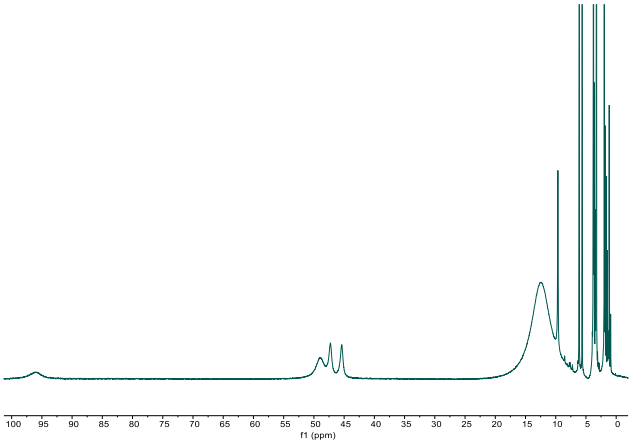

Figure C3. ^{1}H NMR spectrum of $[(TPA)Fe(L)_2]OTf_2$ (L = MeCN, NH_3) formed by mixing $[(TPA)Fe(MeCN)_2]OTf_2$ with 75 equivalents of NH_3 in CD_3CN at 25 °C. Spectrum also shows 1,3,5-trimethoxybenzene used for Evan's method.

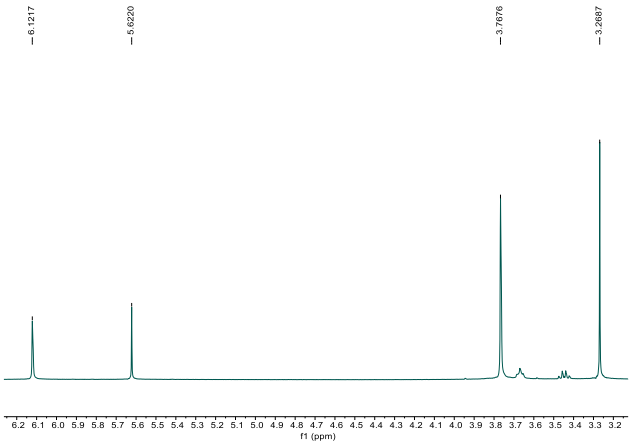

Figure C4. 1,3,5-trimethoxybenzene signals used for Evan's method for $[(TPA)Fe(L)_2]OTf_2$ (L = MeCN, NH_3), formed by mixing $[(TPA)Fe(MeCN)_2]OTf_2$ with 75 equivalents of NH_3 in CD_3CN at 25 °C. [Fe] = 0.011 M, $\Delta f = 200$ Hz, $f = 400.15$ MHz, $\mu = 5.2\mu_B$.

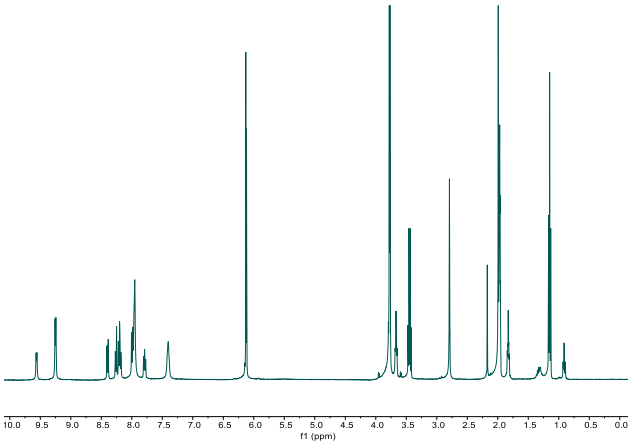

Figure C5. ^{1}H NMR spectrum of [(bpyPy$_2$Me)Fe(MeCN)$_2$]OTf$_2$ in CD$_3$CN at 25 °C. Spectrum also shows 1,3,5-trimethoxybenzene used for Evan's method.

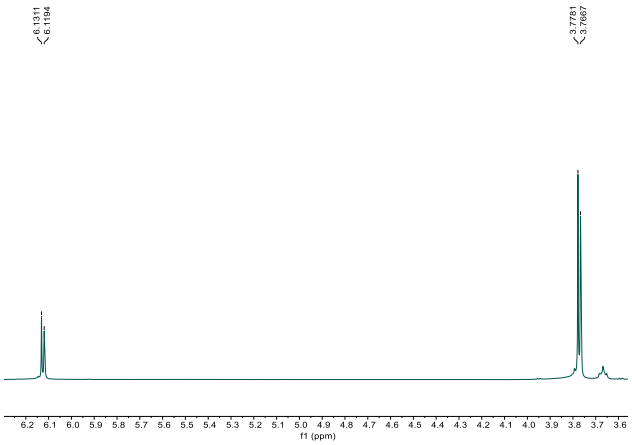

Figure C6. 1,3,5-trimethoxybenzene signals used for Evan's method for [(bpyPy$_2$Me)Fe(MeCN)$_2$]OTf$_2$ in CD$_3$CN at 25 °C. [Fe] = 0.011 M, $\Delta f = 4.62$ Hz, $f = 400.15$ MHz, $\mu = 0.79\mu_B$.

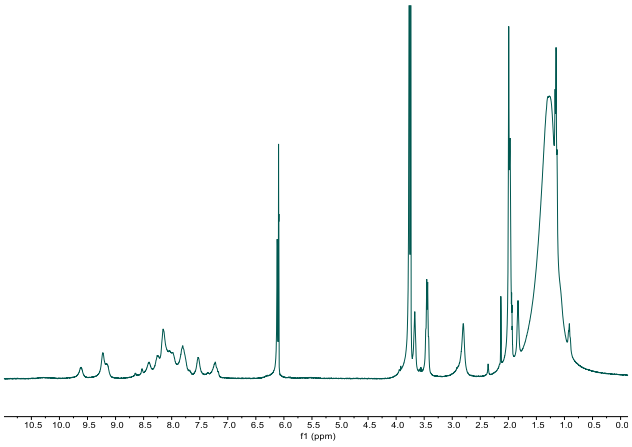

Figure C7. ^{1}H NMR spectrum of [(bpyPy$_2$Me)Fe(L)$_2$]OTf$_2$ (L = MeCN, NH$_3$) formed by mixing [(bpyPy$_2$Me)Fe(MeCN)$_2$]OTf$_2$ with 75 equivalents of NH$_3$ in CD$_3$CN at 25 °C. Spectrum also shows 1,3,5-trimethoxybenzene used for Evan's method.

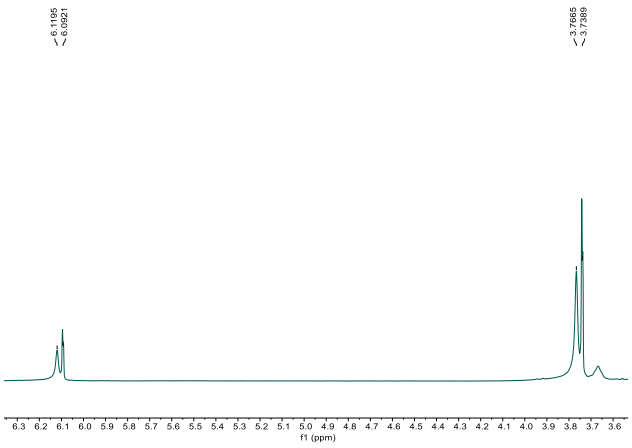

Figure C8. 1,3,5-trimethoxybenzene signals used for Evan's method for [(bpyPy$_2$Me)Fe(L)$_2$]OTf$_2$ (L = MeCN, NH$_3$), formed by mixing [(bpyPy$_2$Me)Fe(MeCN)$_2$]OTf$_2$ with 75 equivalents of NH$_3$ in CD$_3$CN at 25 °C. [Fe] = 0.011 M, Δf = 11.0 Hz, f = 400.15 MHz, μ = 1.2μ_B.

C.3 UV-vis spectra

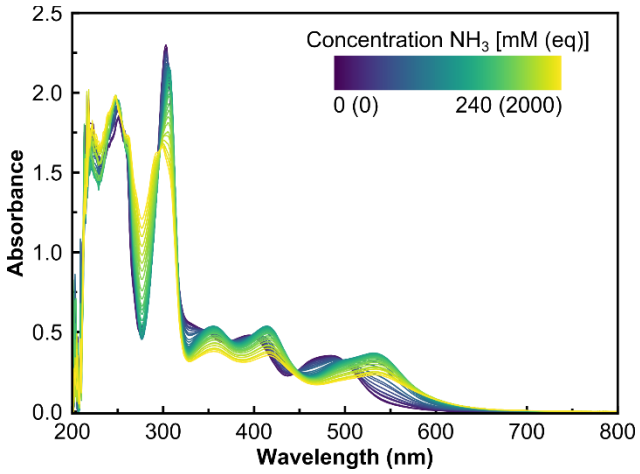

Figure C9. UV-vis spectra of acetonitrile solutions containing 0.12 mM [(bpyPy$_2$Me)Fe(MeCN)$_2$]OTf$_2$ and varying equivalents NH_3 in a 1 cm cuvette.

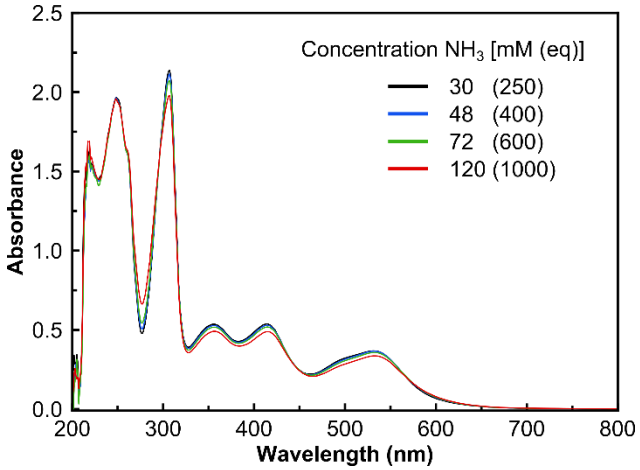

Figure C10. UV-vis spectra of acetonitrile solutions containing 0.12 mM [(bpyPy$_2$Me)Fe(MeCN)$_2$]OTf$_2$ with 250 (black), 400 (blue), 600 (green), or 1000 (red) equivalents NH_3 in a 1 cm cuvette. This shows the onset of demetallation around 600 equivalents NH_3.

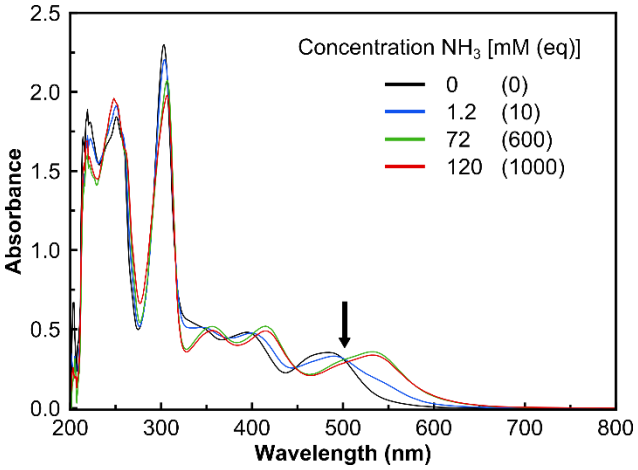

Figure C11. UV-vis spectra of acetonitrile solutions containing 0.12 mM $[(bpyPy_2Me)Fe(MeCN)_2]OTf_2$ with 0 (black), 10 (blue), 600 (green), or 1000 (red) equivalents NH_3 in a 1 cm cuvette. An arrow highlights an isosbestic point ~500 nm which is maintained for 0, 10, and 600 equivalents but has begun to show deviations assigned to demetallation at 1000 equivalents.

C.4 Catalytic controlled potential coulometry experiments

Procedures for controlled potential coulometry:

Preparation of the BDD electrode: A 10 cm^2 boron-doped diamond (BDD) plate electrode (IKA) was physically attached to standard electrical wire coated with chemical-resistant insulation, and the connection was covered with Teflon tape. The surface area of the electrode submerged in solution was around 4 cm^2.

BDD has a surface that exists in various states of reduction (H-terminated) and oxidation (O-terminated).[7] In order to remove attached nitrogen and iron generated during controlled potential coulometry experiments and to ensure a reliable electrode surface prior to CPC measurements, the BDD plate electrode was oxidatively treated prior to use. First, the electrode was soaked in concentrated nitric acid for 5 minutes. Then, a potential of 3.0 V vs Ag/AgCl was applied to the BDD electrode in a 0.5 M H_2SO_4 solution for 10 minutes. The electrode was then thoroughly rinsed with water prior to use.

Preparation of the platinum counter electrode: In order to ensure a highly active Pt surface for hydrogen evolution prior to CPC experiments, the Pt mesh counter electrode was soaked in concentrated hydrochloric acid for at least 5 minutes prior to usage.

Preparation of the custom Ag/AgOTf reference electrode: To ensure reliable potential measurements, the custom Ag/AgOTf reference electrode was prepared prior to each CPC experiment and then a CV of ferrocene was measured. In a glass tube fitted with a Vycor porous glass frit attached by Teflon heatshrink tubing, an acetonitrile solution containing 5

mM AgOTf and 0.1 M $TBAPF_6$ was added. A silver wire was placed inside and the electrode was sealed.

Preparation of ammonia solutions. For experiments with natural abundance ammonia, saturated 2 M solutions[8] in acetonitrile were prepared by bubbling anhydrous ammonia through acetonitrile in a Schlenk tube under an argon/ammonia atmosphere. For experiments with labeled $^{15}NH_3$, ammonia was liberated from $^{15}NH_4OTf$ by addition of 1.1 equivalents of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) to ^{15}N labeled ammonium triflate dissolved in acetonitrile in a Schlenk tube inside of an argon glovebox. This solution was then vacuum transferred to a separate, clean Schlenk tube.

CPC: Inside an argon glovebox, a gas-tight electrochemical cell equipped with a 24/40 cap containing three tungsten rods for electrical contacts and a valved 14/20 joint carefully sealed with a Suba-Seal septum was prepared. A BDD plate electrode (A = 4 cm^2), high surface area platinum mesh electrode, and custom Ag/AgOTf reference electrode were connected to the 24/40 cap. All chemical reagents were then rapidly added to the cell to prevent evaporation of ammonia, and then, the cell was sealed with the 24/40 cap. Prior to each CPC experiment, a ZIR and CV were taken. No IR compensation was applied for CPC measurements. The CPC experiment was then conducted for 24 h. The cell was then removed from the glovebox for analysis by gas chromatography. For headspace analysis, 100 μL of the headspace was injected into a GC-TCD for quantification using a lockable Hamilton syringe with a 26S gauge needle. For GC-MS, only 50 μL of the headspace was injected.

For each experiment, a 10 mL solution containing 0.05 mM [Fe], 20 mM NH_3 (1.0 mL of 0.2 M solution), and 50 mM NH_4OTf (84 mg) was prepared in acetonitrile.

Reload experiments: After a completed CPC experiment, the valved 14/20 joint on the electrochemical cell was sealed, the septum was removed, and a 14/20 joint-to-tubing adapter was connected. This joint was connected to a double-manifold Schlenk line and put under an argon atmosphere. Under a positive counter-flow of argon, the 24/40 electrode cap was removed and replaced with a ground-glass stopper. The cell was then carefully evaporated to dryness under vacuum and brought into an argon glovebox. To this cell containing ammonium triflate electrolyte and used catalyst was added 9 mL acetonitrile and 1.0 mL of a 0.2 M NH_3 solution to reset the ammonia concentration to the initial value. Then, the CPC experiment was performed following our standard procedures.

Table B1. Results of catalytic CPC experiments performed at 0.85 V vs Fc/Fc^+ for 24 h with 0.05 mM [Fe] and 20 mM NH_3 (400 equivalents). For entries where reload experiments were conducted, the entries are listed as x.1 and x.2 for the initial and subsequent reload experiment, respectively. LOQ indicates that the amount of gas produced was below the limit of quantification.

Entry	Fe Source	Eq. N_2	Charge (C)	FE N_2 (%)	FE H_2 (%)
1.1	$[(bpyPy_2Me)Fe(MeCN)_2]OTf_2$	89	29.9	86	77
2.1	$[(bpyPy_2Me)Fe(MeCN)_2]OTf_2$	83	26.5	91	80
3	$[(bpyPy_2Me)Fe(MeCN)_2]OTf_2$	97	31.1	91	93
4*	$[(bpyPy_2Me)Fe(MeCN)_2]OTf_2$	102	36.5	81	84
Avg. 1.1–4	$[(bpyPy_2Me)Fe(MeCN)_2]OTf_2$	93	–	87	84
1.2	$[(bpyPy_2Me)Fe(MeCN)_2]OTf_2$	55	21.1	77	78
2.2	$[(bpyPy_2Me)Fe(MeCN)_2]OTf_2$	57	19.7	84	67
Avg. Reload	$[(bpyPy_2Me)Fe(MeCN)_2]OTf_2$	56	–	81	73
3	None (NH_3 only)	LOQ	0.86	LOQ	73
4.1	$FeOTf_2 \cdot 2$ MeCN	7.7	8.2	27	74
5	$FeOTf_2 \cdot 2$ MeCN	7.1	7.5	28	33
Avg. 4.1–5	$FeOTf_2 \cdot 2$ MeCN	7.4	–	28	54
4.2	$FeOTf_2 \cdot 2$ MeCN	LOQ	1.2	LOQ	65

* Experiment performed with $^{15}NH_3$ and $^{15}NH_4OTf$

NMR spectra showing active catalyst after CPC:

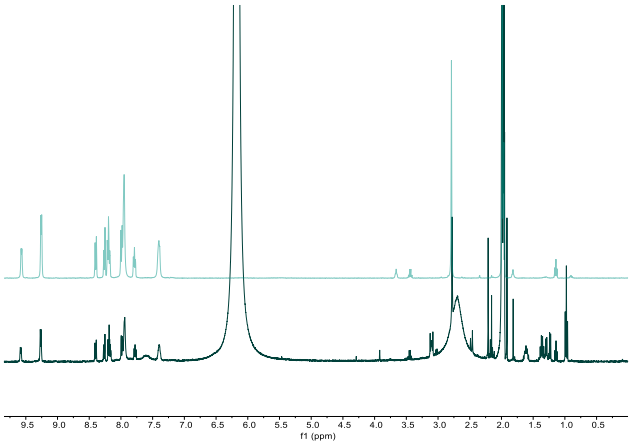

Figure C12. ^{1}H NMR spectra of [(bpyPy$_2$Me)Fe(MeCN)$_2$]OTf$_2$ precatalyst (top) and a sample extracted after a CPC experiment (bottom) in CD_3CN. The bottom spectrum shows that active catalyst remains after CPC experiments, as corroborated by reload experiments.

C.5 Electrode rinse test after CPC

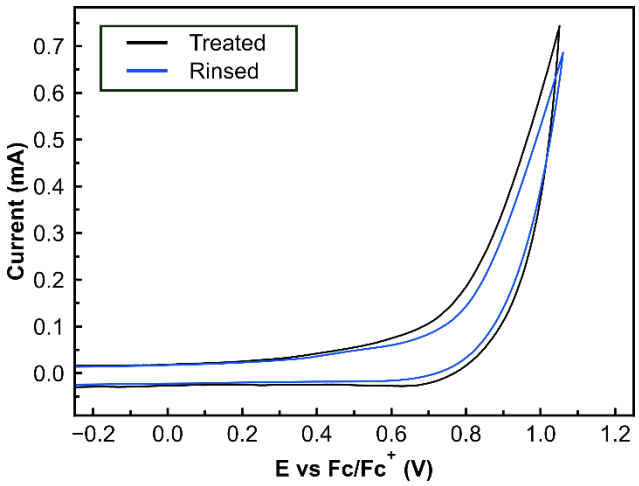

Figure C13. CVs of treated BDD plate electrode and the same electrode after CPC and rinsing with MeCN, recorded in MeCN with 0.05 M NH_4OTf and 20 mM NH_3; Pt counter and Ag/AgOTf reference electrodes. The rinsed electrode corresponds to the electrode after a 2 hour CPC experiment containing the new $[(bpyPy_2Me)Fe(MeCN)_2]OTf_2$ electrocatalyst under the optimized conditions detailed in Table C1. These measurements do not support the possibility of deposition of catalytically active material onto the electrode. This is in agreement with our previous investigation of the electrode after CPC with $[(TPA)Fe(MeCN)_2]OTf_2$.[9]

C.6 GC-MS data for $^{15}NH_3$ experiment

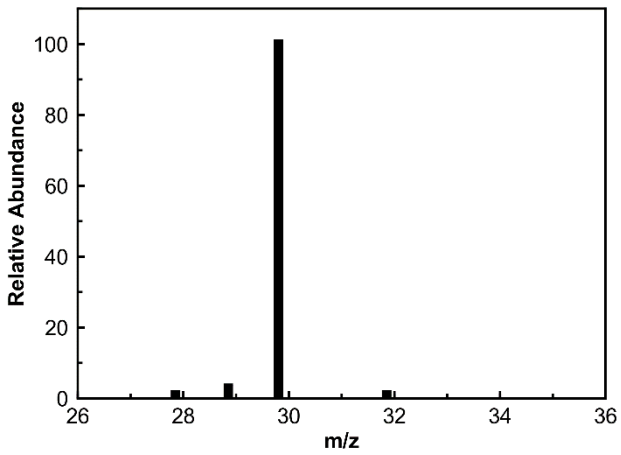

Figure C14. GC mass spectrum of headspace after CPC experiment using $^{15}NH_3$, showing $^{30}N_2$ as the major product.

C.7 XPS spectra of BDD plate electrode

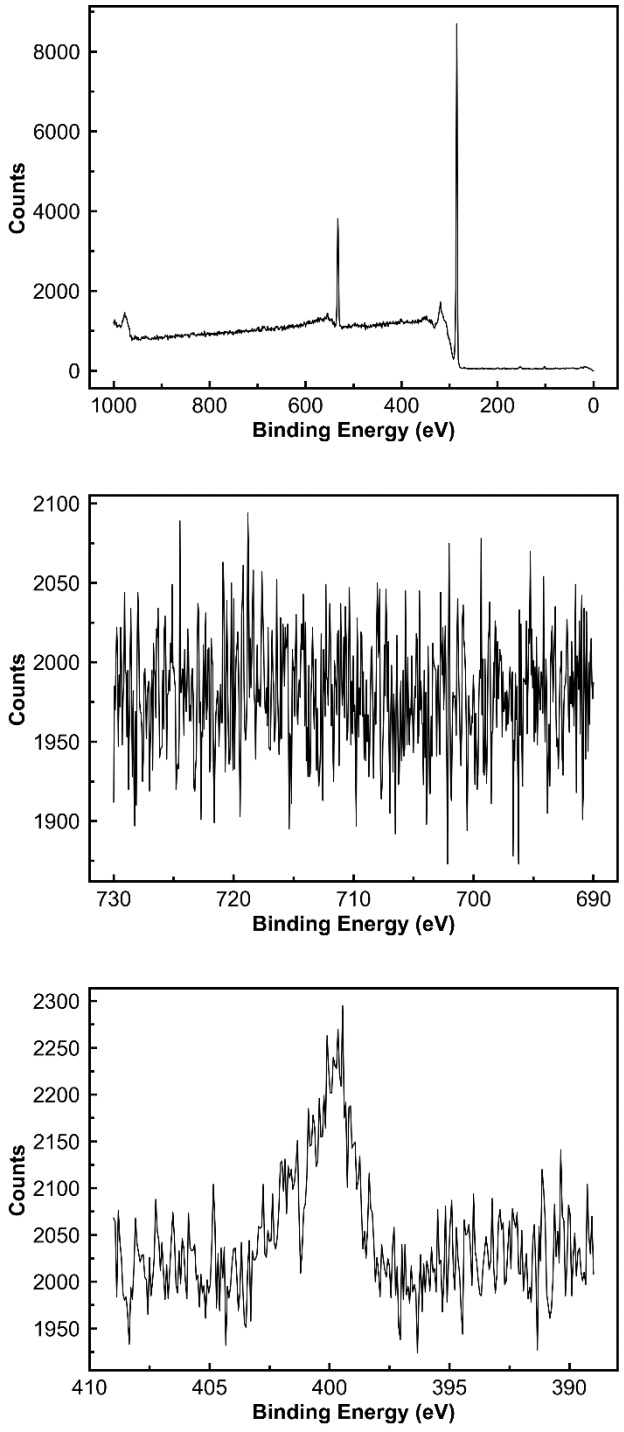

Figure C15. Full XPS spectrum of clean, treated BDD plate electrode and higher resolution spectra centered on the regions characteristic for Fe 2p and N 1s.

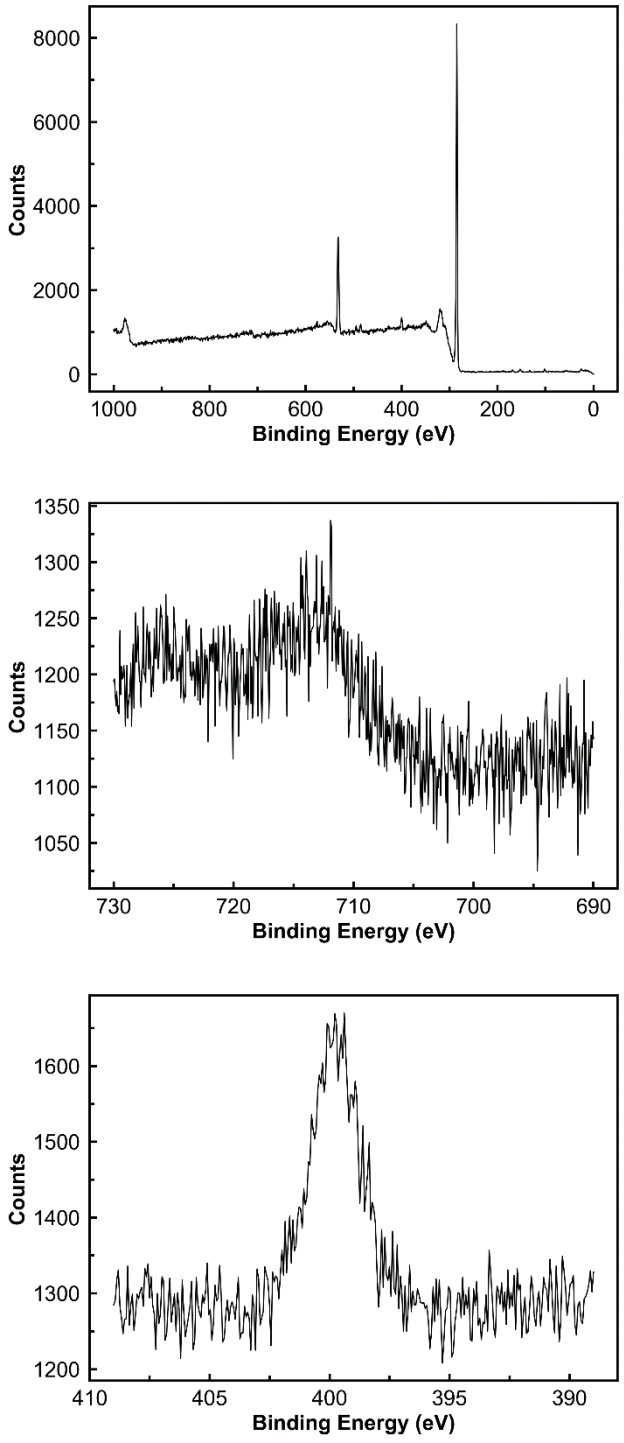

Figure C16. Full XPS spectrum of rinsed BDD plate electrode after 24 h CPC with 0.05 mM $[(bpyPy_2Me)Fe(MeCN)_2]OTf_2$ and 20 mM NH_3 solution and higher resolution spectra centered on the regions characteristic for Fe 2p and N 1s.

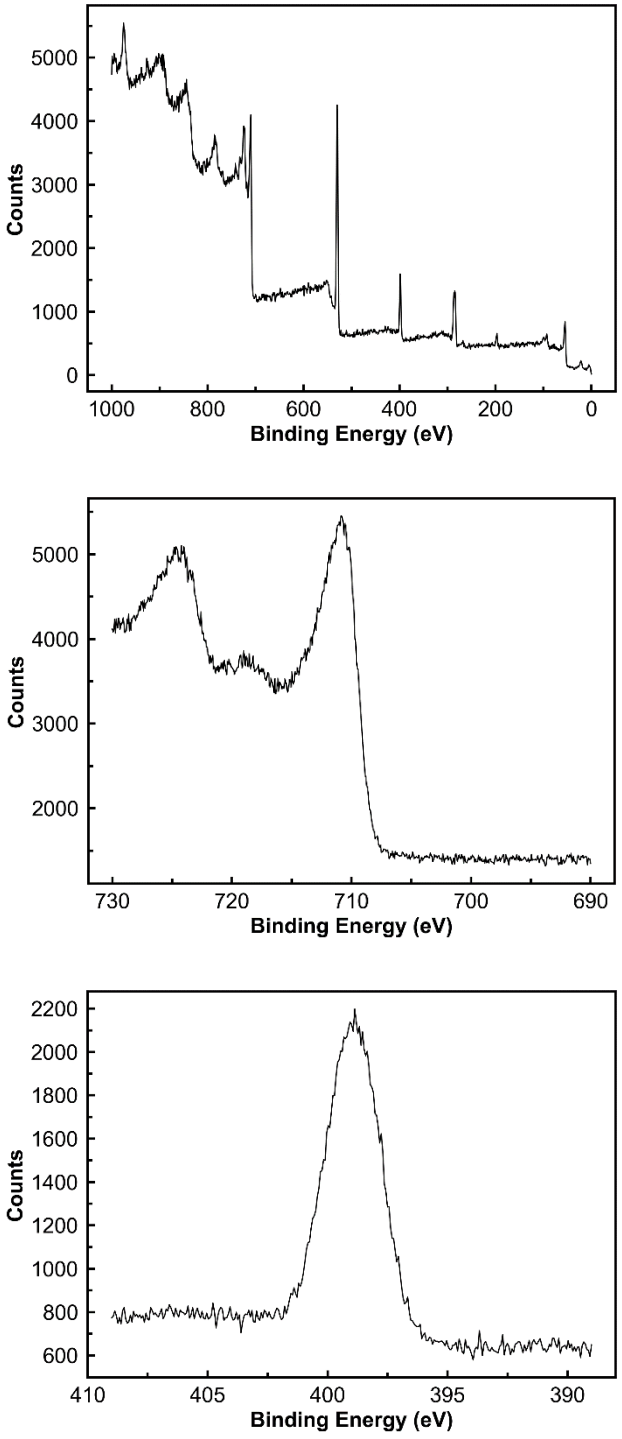

Figure C17. Full XPS spectrum of rinsed BDD plate electrode after 24 h CPC with 0.05 mM $FeOTf_2 \cdot 2$ MeCN and 20 mM NH_3 solution and higher resolution spectra centered on the regions characteristic for Fe 2p and N 1s.

C.8 DPV data for E_1 analysis

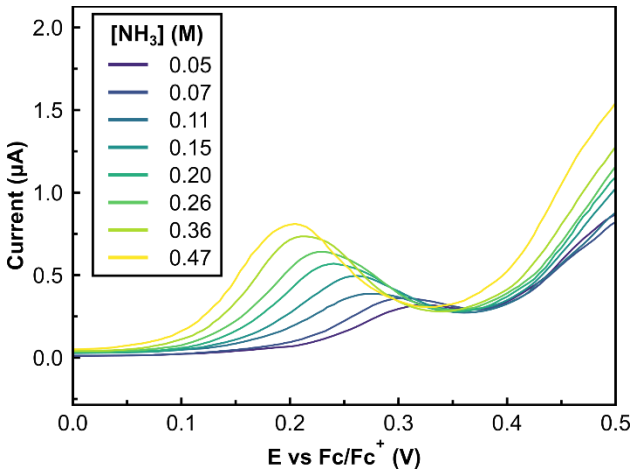

Figure C18. DPVs of 0.5 mM $[(bpyPy_2Me)Fe(MeCN)_2]OTf_2$ with varying NH_3 concentration in order to study the EC process at E_1. Recorded in MeCN with 0.05 M NH_4OTf using BDD working, Pt counter, and Ag/AgOTf reference electrodes.

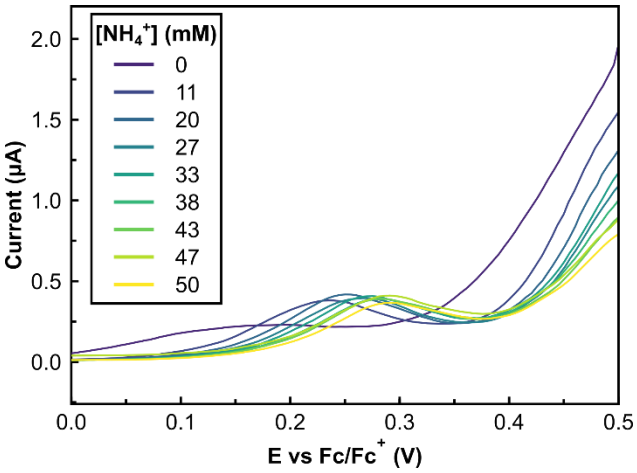

Figure C19. DPVs of 0.5 mM $[(bpyPy_2Me)Fe(MeCN)_2]OTf_2$ with varying NH_4^+ concentration in order to study the EC process at E_1. Recorded in MeCN with 0.2 M NH_3 and 0.1 M $TBAPF_6$ using BDD working, Pt counter, and Ag/AgOTf reference electrodes.

C.9 Further analysis of speciation related to E_1

In addition to the electrochemical and crystallographic data presented in the main text, we provide additional support for the assignment of the E_1 process here. We first further address the speciation at Fe(II), prior to E_1. The predominance of $[(bpyPy_2Me)Fe(MeCN)(NH_3)]OTf_2$ prior to E_1 in MeCN containing NH_3 is corroborated by SC-XRD (Fig. C20). From MeCN/NH_3 mixtures, $[(bpyPy_2Me)Fe(MeCN)(NH_3)]OTf_2$ can be isolated; alternatively, only $[(bpyPy_2Me)Fe(NH_3)_2]OTf_2$ has been crystallized in DCM/NH_3 mixtures containing 2 equivalents MeCN from the $[(bpyPy_2Me)Fe(MeCN)_2]OTf_2$ starting material. Isolation of the bis-ammine in DCM is compatible with DFT calculations which indicate a slight (3 kcal/mol) thermodynamic preference versus the mono-ammine; however, in MeCN solvent the large excess of MeCN relative to NH_3 likely favors the mono-acetonitrile adduct. Thus, $[(bpyPy_2Me)Fe(MeCN)(NH_3)]OTf_2$ is likely the primary iron species in bulk solution under our catalytic conditions.

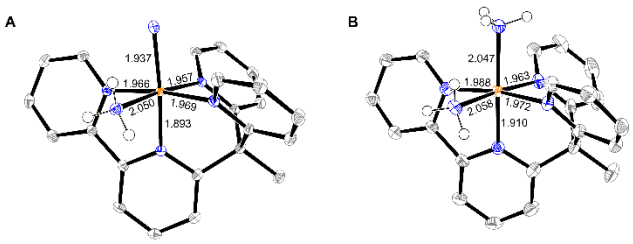

Figure C20. Solid-state crystal structure of **(A)** $[(bpyPy_2Me)Fe(MeCN)(NH_3)]OTf_2$ and **(B)** $[(bpyPy_2Me)Fe(NH_3)_2]OTf_2$ at 100 K, with select bond lengths labeled in angstroms. Thermal ellipsoids are shown at 50% probability. Triflate counterions and L_{aux} hydrogen atoms are omitted for clarity. The acetonitrile in **(A)** is truncated at nitrogen.

As mentioned in the main text, we have assigned the E_1 process to the proton-coupled oxidation of $[(bpyPy_2Me)Fe(MeCN)(NH_3)]^{2+}$ to $[(bpyPy_2Me)Fe(NH_2)(NH_3)]^{2+}$. This conclusion is in excellent agreement with our DFT results (Fig. C21) which show identical experimental and predicted potentials. However, two other likely pathways from $[(bpyPy_2Me)Fe(MeCN)(NH_3)]^{2+}$ are proton-coupled oxidation without additional ammonia substitution (Scheme 4.2a in main text) or oxidation without proton transfer. Based on our DFT results, oxidation without proton transfer is the next lowest energy process, generating $[(bpyPy_2Me)Fe(MeCN)(NH_3)]^{3+}$. The computed oxidation potential is 0.61 V, and we label this process E_1*.

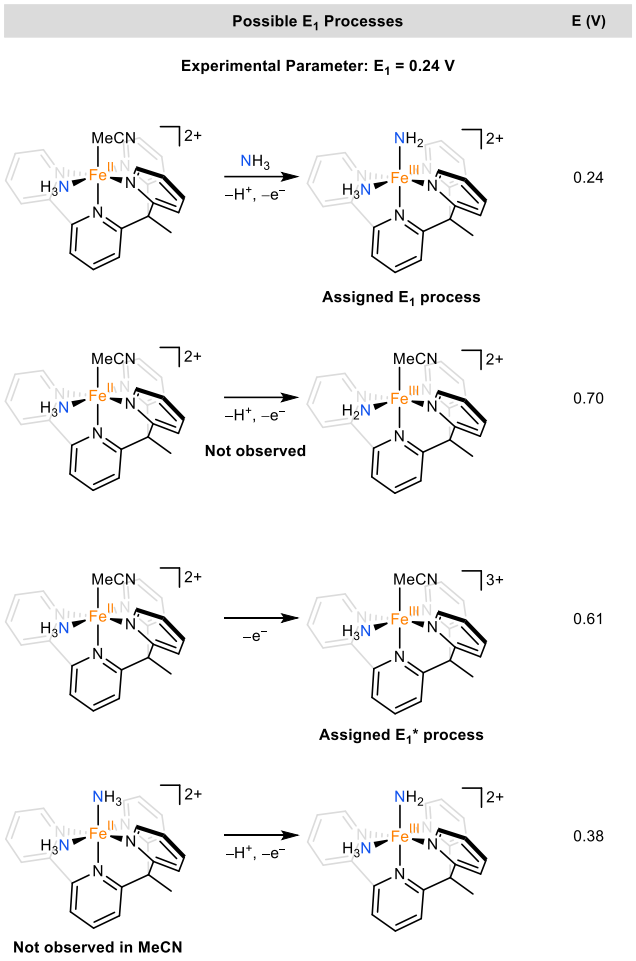

Figure C21. Possible E_1 processes and their calculated E (V) values.

When $[(bpyPy_2Me)Fe(MeCN)(NH_3)]^{2+}$ is investigated by CV at high scan rates under certain concentration regimes, an additional feature appears in the cyclic voltammogram as a shoulder in the catalytic E_2 wave at about 0.55 V (Fig. C22). This shoulder is minor at 200 mV/s but becomes clear at higher scan rates, e.g., 10000 mV/s. By DPV, this shoulder is more easily identified (Fig. C23). Given that the E_1 process, a proton-coupled oxidation associated with an additional ammonia substitution, could be slow due to

the second order dependence on NH_3, it is unsurprising that this second feature can be observed. Interestingly, this shoulder does not move with varying NH_3 concentration as would be expected if it were also coupled to proton transfer. Furthermore, an increase in current at E1* (Fig. C21, 2000 mV/s) results in an increase in return current at E_1, indicating that they are linked via a square mechanism, i.e., E_1 and E_1* generate the same product upon reduction. All of these data points agree with our assignment of E_1* as oxidation without proton transfer to generate $[(bpyPy_2Me)Fe(MeCN)(NH_3)]^{3+}$.

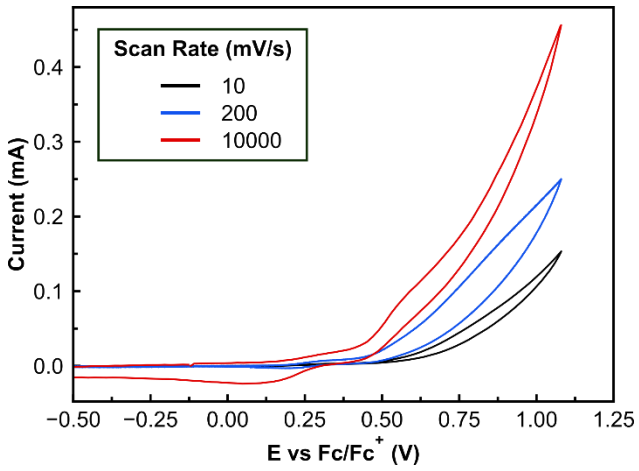

Figure C22. CVs of 0.5 mM $[(bpyPy_2Me)Fe(MeCN)_2]OTf_2$ with 0.2 M NH_3 at varying scan rates. Recorded in MeCN with 0.05 M NH_4OTf using BDD working, Pt counter, and Ag/AgOTf reference electrodes. The shoulder that appears at ~0.55 V is discussed above.

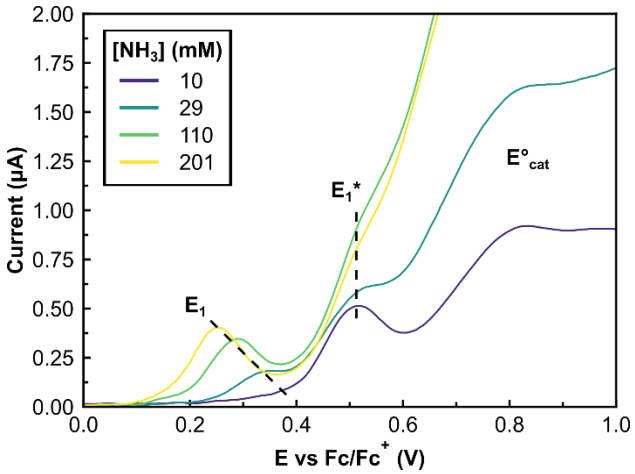

Figure C23. DPVs of 0.5 mM [(bpyPy$_2$Me)Fe(MeCN)$_2$]OTf$_2$ with varying NH_3 concentration in order to study the EC process at E_1. Recorded in MeCN with 0.05 M NH_4OTf using BDD working, Pt counter, and Ag/AgOTf reference electrodes. Labels highlight the E_1* and $E°_{cat}$ processes discussed above.

C.10 Catalytic rate versus iron and NH_3 concentrations (E_2)

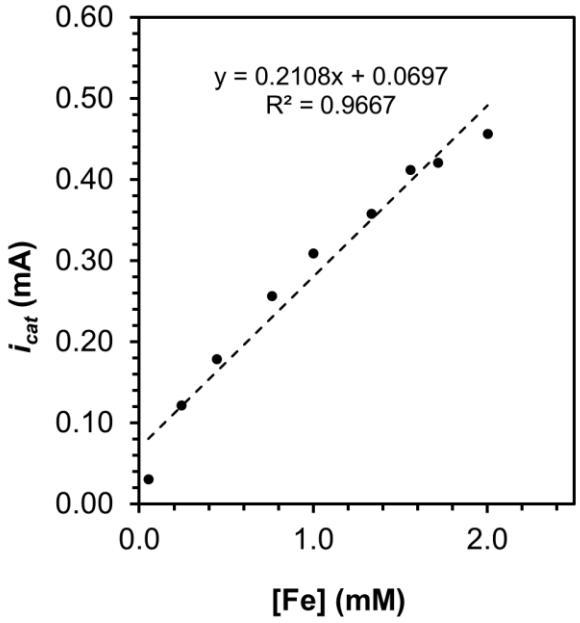

Figure C24. Rate dependence as measured by catalytic current at 1.08 V with varying concentrations of $[(bpyPy_2Me)Fe(MeCN)_2]OTf_2$ in MeCN with 0.05 M NH_4OTf and 0.2 M NH_3 with BDD working, Pt counter, and Ag/AgOTf reference electrodes.

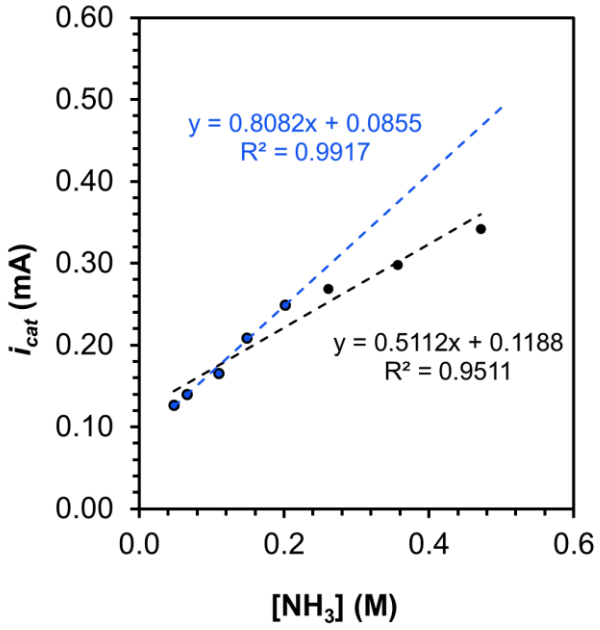

Figure C25. Rate dependence as measured by catalytic current at 1.08 V with varying concentrations of NH_3 and 0.5 mM $[(bpyPy_2Me)Fe(MeCN)_2]OTf_2$ in MeCN with 0.05 M NH_4OTf with BDD working, Pt counter, and Ag/AgOTf reference electrodes. The linear regression lines indicate a first-order dependence on $[NH_3]$. The low $[NH_3]$ regime is perfectly linear (R^2 = 0.99), but at higher concentrations the higher rate likely results in substrate depletion manifested by the mild concave behavior for the overall fit (R^2 = 0.95).

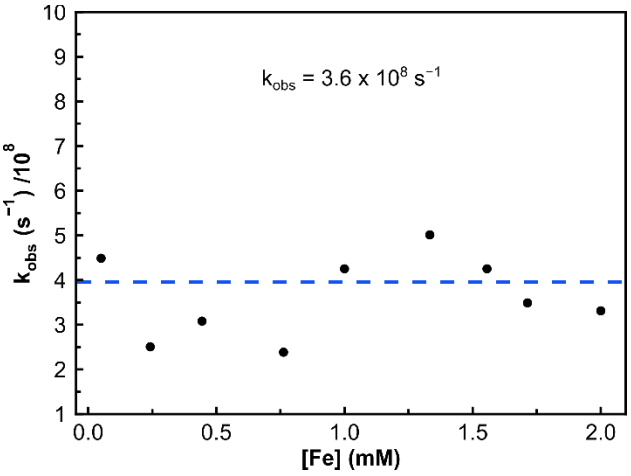

Figure C26. FOWA calculated k_{obs} for AO using varying concentrations of $[(bpyPy_2Me)Fe(MeCN)_2]OTf_2$ in MeCN with 0.05 M NH_4OTf and 0.2 M NH_3 with BDD working, Pt counter, and Ag/AgOTf reference electrodes. A first-order dependence on [Fe] is incorporated into k_{obs}, thus the zero-order dependence of k_{obs} on [Fe] in this plot indicates an overall first-order dependence on [Fe].

C.11 Procedure for FOWA

Foot of the wave analysis was performed by using the equations deducted for EC_{cat}:

$$\frac{i}{i_p} = \frac{n \cdot 2.24 \cdot \sqrt{\frac{R \cdot T}{F \cdot \nu} \cdot k_{obs}}}{1 + \exp\left[\frac{F}{R \cdot T}(E°_{cat} - E)\right]}$$

F is Faraday's constant, R is the gas constant, and T is the temperature. In this case, n = 6 due to the 6 electrons involved in ammonia oxidation to dinitrogen. The intensity of the one-electron wave (i_p) has been estimated from the one-electron oxidation precatalytic wave at E_1 for each condition. $E°_{cat}$ was determined via differential pulse voltammetry. For each condition, the FOWA was performed in similar regions of the potential range in order to ensure a fair comparison. This region was selected as the foot-of-the-wave region where the plot of i/i_p versus $1/(1+\exp[F/(RT)(E°_{cat}–E)])$ behaves linearly ($R^2 > 0.85$). Then, from the slope of that plot, the apparent pseudo-first order rate constant k_{obs} can be obtained and thus the value of the apparent second-order rate constant k'_{obs}. A representative example of this methodology is shown below for one condition.

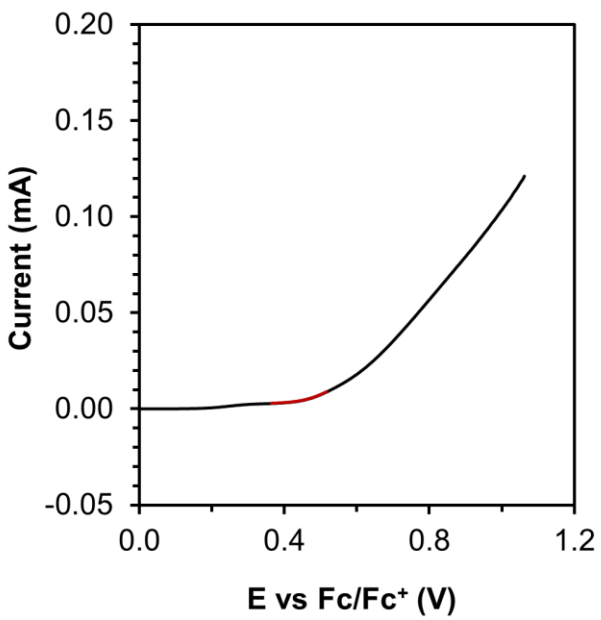

Figure C27. Linear sweep voltammogram with red trace showing the data range employed for performing the FOWA.

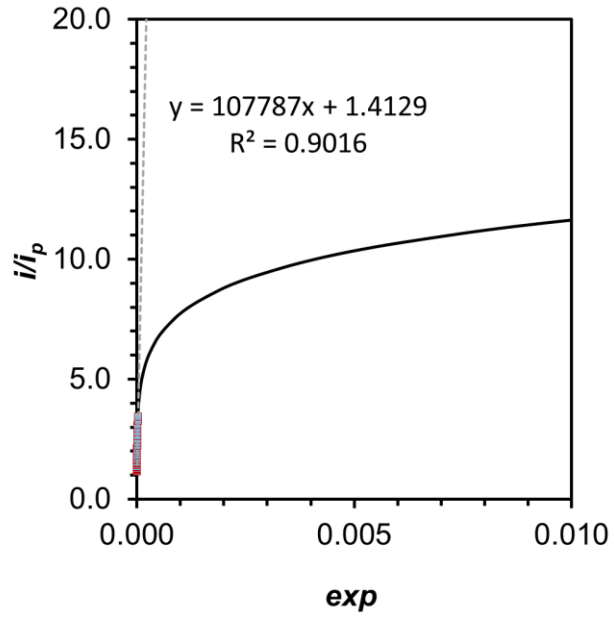

Figure C28. FOWA for an EC_{cat} mechanism calculated from the above linear sweep voltammogram showing strong concavity. The highlighted section and dotted line show the data employed for FOWA.

C.12 Further reactivity considered at E_2

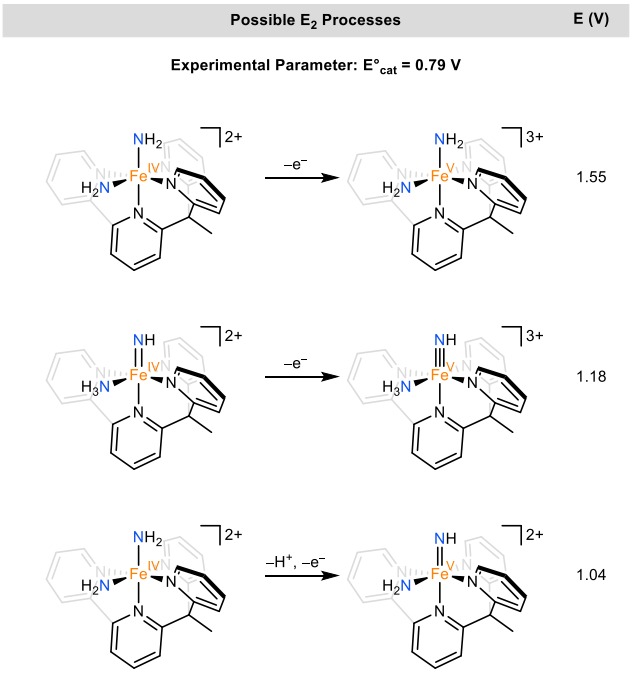

Figure C29. Further E_2 processes considered and their calculated E (V) values. All estimated E values are above the experimental $E°_{cat}$ value. This data supports the hypothesis that N–N bond formation occurs after formation of the species presented in the main text, prior to further removal of protons and electrons.

C.13 Computational methodology

All computations were performed using the ORCA software package, version 4.0 or above.[10] The DFT functional used was TPSS with the def2-SVP basis set for all atoms except iron, for which an augmented def2-TZVP basis set was used. An acetonitrile solvation model (conductor-like polarizable continuum model, CPCM) was used as implemented in ORCA. The RI-J approximation was used to speed up Coulomb integrals (as default). The convergence criteria employed were “tightscf” and “veryslowconv” as defined by ORCA. The Gibbs free energy at 298.15 K was computed in ORCA using harmonic vibrational frequencies computed numerically via “NumFreq”.

Sample input header:

```
! RI TPSS def2-SVP def2/J Opt NumFreq PAL8 tightscf veryslowconv
! CPCM(acetonitrile)
%basis
newgto Fe "def2-TZVP" end
end
```

To determine thermochemical values, oxidations are referenced to ferrocene/ferrocenium (Fc/Fc^+), and reactions involving net hydrogen atom transfer are computed using TEMPO as a reference value (BDFE = 66.5 kcal/mol) and the acetonitrile C_G value of 54.9 kcal/mol.[11]

For oxidations:

$Ox^- + Fc \rightarrow Ox + Fc^+ \quad \Delta G_{ox}$

E (V) = ΔG_{ox} / F, where F (Faraday's constant) is in units of Hartree. 1 Hartree = 27.211 eV.

For reactions involving net hydrogen atom transfer:

Reactants + TEMPO $\rightarrow$ Products + TEMPOH $\quad \Delta G_{BDFE}$

E (V) = [ΔG_{BDFE} – 54.9 + 66.5 – 1.37 pK_a] / 23.06, where ΔG_{BDFE} is in units of kcal/mol (1 Hartree = 627.51 kcal/mol). The pK_a is derived from that of NH_3, 16.5 in MeCN,[8] and adjusted by the Henderson–Hasselbalch equation to match the standard experimental CV conditions of 0.2 M NH_3 and 0.05 M NH_4^+, resulting in pK_a = 17.1.

C.14 DFT spin-state ordering

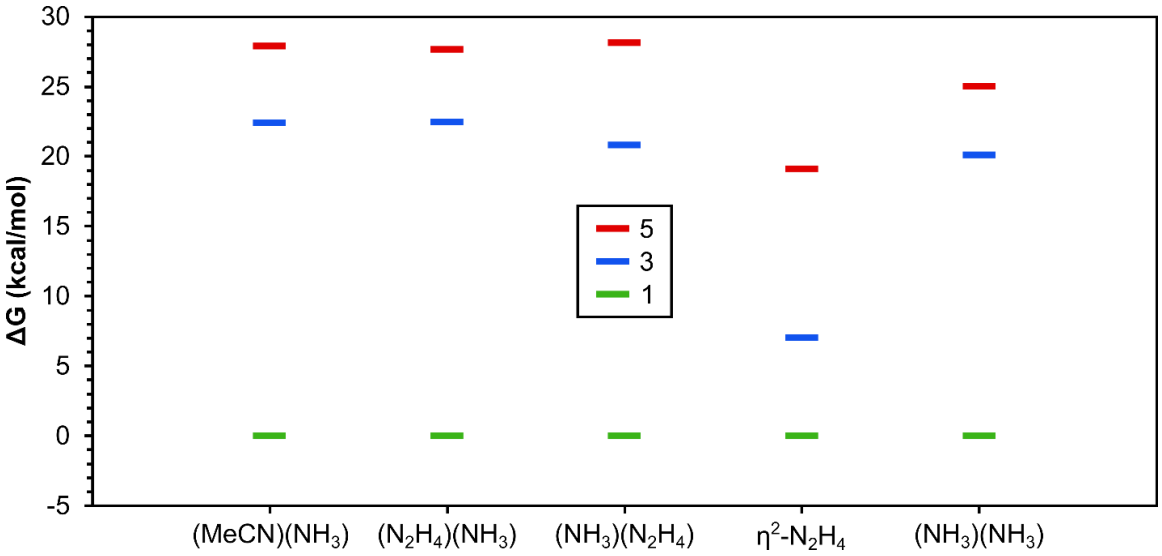

Figure C30. Relative energies for multiplicities of $[(bpyPy_2Me)Fe(L_{ax})(L_{eq})]^{n+}$ complexes with formal oxidation states of +2. L_{ax} and L_{eq} represent ligands axial/*trans* to bipyridine and equatorial/*trans* to pyridine, respectively, in accordance with the orientation defined in the main-text. The lowest energy multiplicity is defined as 0.

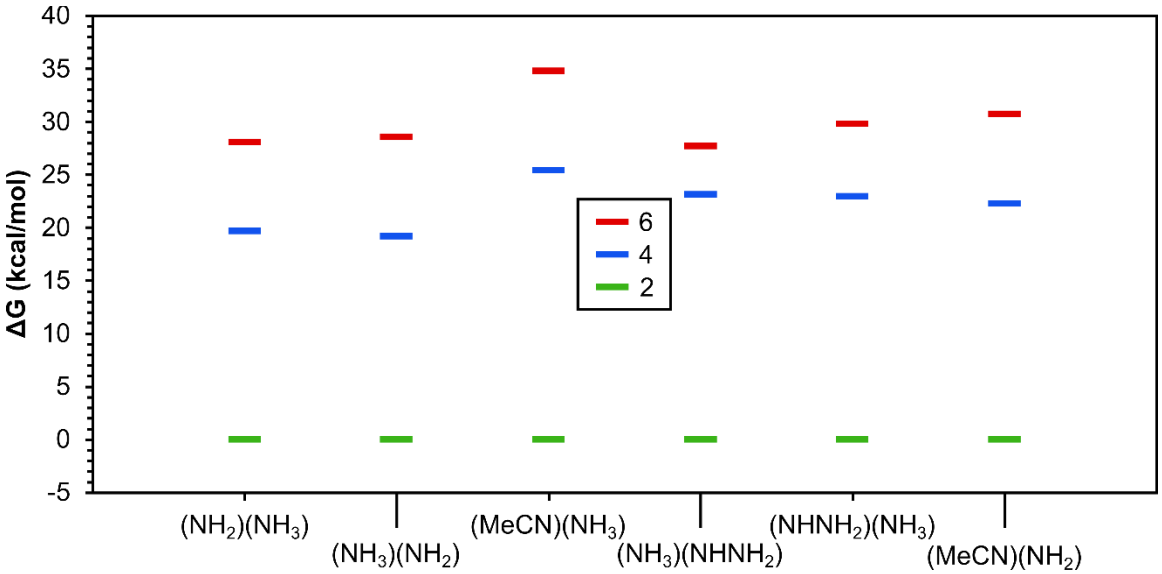

Figure C31. Relative energies for multiplicities of $[(bpyPy_2Me)Fe(L_{ax})(L_{eq})]^{n+}$ complexes with formal oxidation states of +3. L_{ax} and L_{eq} represent ligands axial/*trans* to bipyridine and equatorial/*trans* to pyridine, respectively, in accordance with the orientation defined in the main-text. The lowest energy multiplicity is defined as 0.

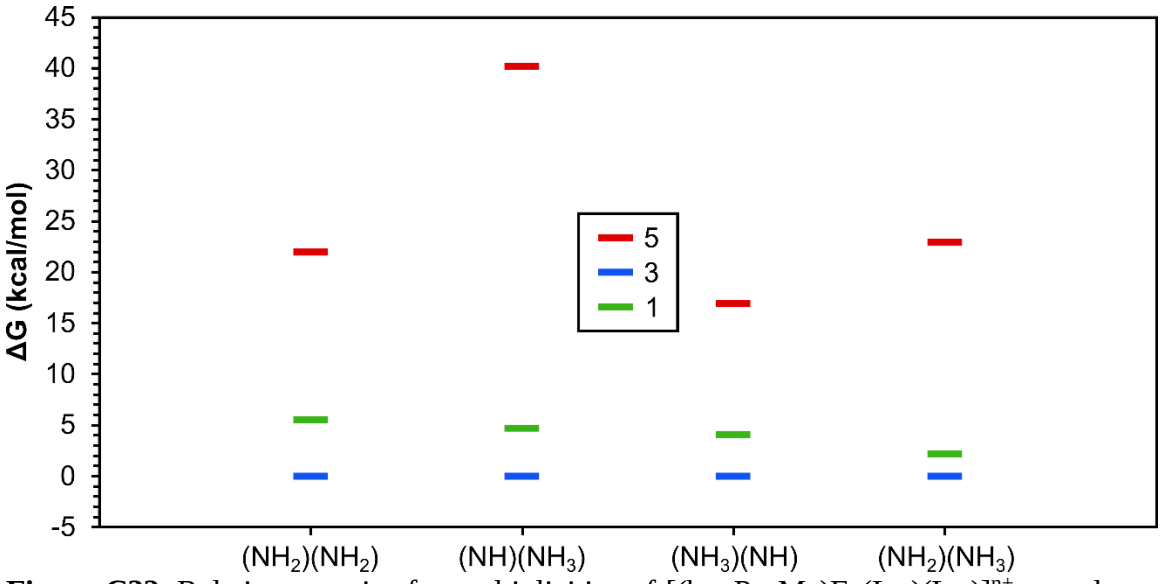

Figure C32. Relative energies for multiplicities of $[(bpyPy_2Me)Fe(L_{ax})(L_{eq})]^{n+}$ complexes with formal oxidation states of +4. L_{ax} and L_{eq} represent ligands axial/*trans* to bipyridine and equatorial/*trans* to pyridine, respectively, in accordance with the orientation defined in the main-text. The lowest energy multiplicity is defined as 0.

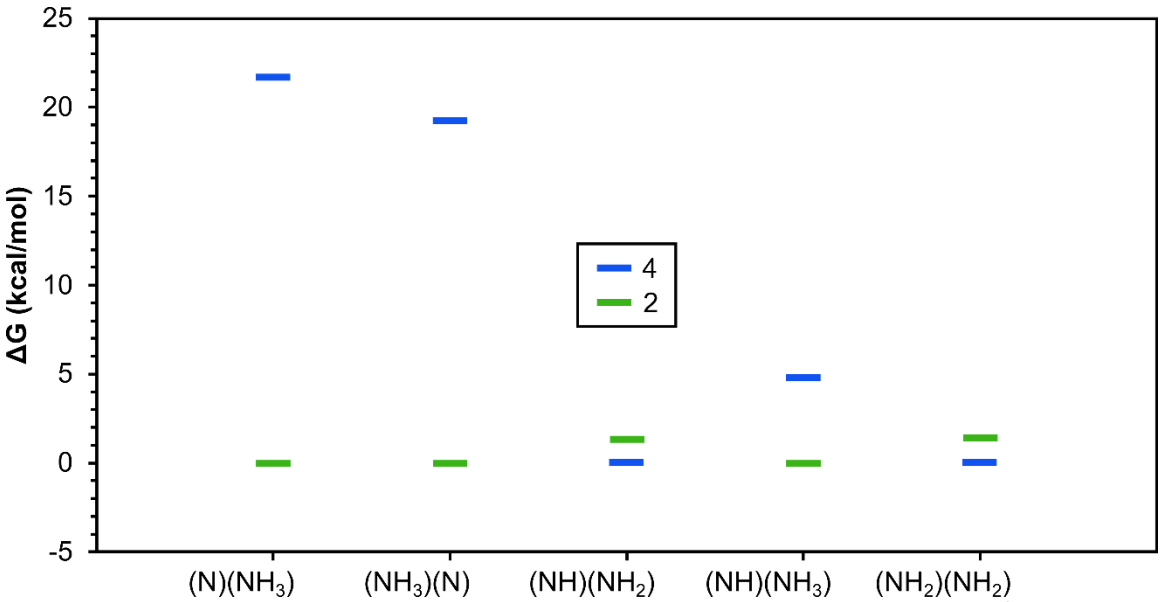

Figure C33. Relative energies for multiplicities of $[(bpyPy_2Me)Fe(L_{ax})(L_{eq})]^{n+}$ complexes with formal oxidation states of +5. L_{ax} and L_{eq} represent ligands axial/*trans* to bipyridine and equatorial/*trans* to pyridine, respectively, in accordance with the orientation defined in the main-text. The lowest energy multiplicity is defined as 0.

C.15 DFT tabulated energies

Table C2. Gibbs free energy, oxidation state (O.S.), charge, and multiplicity for each compound studied in this work. The naming convention for $[(bpyPy_2Me)Fe(L_{ax})(L_{eq})]^{n+}$, where L_{ax} and L_{eq} represent ligands axial/*trans* to bipyridine and equatorial/*trans* to pyridine, respectively, in accordance with the orientation defined in the main-text, is $Fe(L_{ax})(L_{eq})$.

Compound	O.S.	Charge	Multiplicity	Gibbs Free Energy (E_h)
$Fe(MeCN)(NH_3)$	2	2	1	−2520.170506
$Fe(MeCN)(NH_3)$	2	2	3	−2520.134781
$Fe(MeCN)(NH_3)$	2	2	5	−2520.126099
$Fe(N_2H_4)(NH_3)$	2	2	1	−2499.275282
$Fe(N_2H_4)(NH_3)$	2	2	3	−2499.239539
$Fe(N_2H_4)(NH_3)$	2	2	5	−2499.231216
$Fe(NH_3)(N_2H_4)$	2	2	1	−2499.280876
$Fe(NH_3)(N_2H_4)$	2	2	3	−2499.247766
$Fe(NH_3)(N_2H_4)$	2	2	5	−2499.236084
$Fe(\eta^2\text{-}N_2H_4)$	2	2	1	−2442.758364
$Fe(\eta^1\text{-}N_2H_4)$*	2	2	3	−2442.747149
$Fe(\eta^1\text{-}N_2H_4)$*	2	2	5	−2442.727913
$Fe(NH_3)_2$	2	2	1	−2444.013227
$Fe(NH_3)_2$	2	2	3	−2443.981207
$Fe(NH_3)_2$	2	2	5	−2443.973412
$Fe(NH_2)(NH_3)$	3	2	2	−2443.388803
$Fe(NH_2)(NH_3)$	3	2	4	−2443.357443
$Fe(NH_2)(NH_3)$	3	2	6	−2443.34405
$Fe(NH_3)(NH_2)$	3	2	2	−2443.383476
$Fe(NH_3)(NH_2)$	3	2	4	−2443.352874
$Fe(NH_3)(NH_2)$	3	2	6	−2443.337927
$Fe(MeCN)(NH_3)$	3	3	2	−2519.973567
$Fe(MeCN)(NH_3)$	3	3	4	−2519.933032
$Fe(MeCN)(NH_3)$	3	3	6	−2519.918134
$Fe(NH_3)(NHNH_2)$	3	2	2	−2498.67244
$Fe(NH_3)(NHNH_2)$	3	2	4	−2498.635561
$Fe(NH_3)(NHNH_2)$	3	2	6	−2498.628327
$Fe(NHNH_2)(NH_3)$	3	2	2	−2498.676109
$Fe(NHNH_2)(NH_3)$	3	2	4	−2498.639554
$Fe(NHNH_2)(NH_3)$	3	2	6	−2498.628596
$Fe(MeCN)(NH_2)$	3	2	2	−2519.534136
$Fe(MeCN)(NH_2)$	3	2	4	−2519.498649
$Fe(MeCN)(NH_2)$	3	2	6	−2519.48518
$Fe(NH_2)(NH_2)$	4	2	3	−2442.748256
$Fe(NH_2)(NH_2)$	4	2	1	−2442.739497

Compound	O.S.	Charge	Multiplicity	Gibbs Free Energy (E_h)
$Fe(NH_2)(NH_2)$	4	2	5	−2442.713299
$Fe(NH)(NH_3)$	4	2	3	−2442.74475
$Fe(NH)(NH_3)$	4	2	1	−2442.737322
$Fe(NH)(NH_3)$	4	2	5	−2442.680746
$Fe(NH_3)(NH)$	4	2	3	−2442.734741
$Fe(NH_3)(NH)$	4	2	1	−2442.72829
$Fe(NH_3)(NH)$	4	2	5	−2442.707865
$Fe(NH_2)(NH_3)$	4	3	3	−2443.173804
$Fe(NH_2)(NH_3)$	4	3	1	−2443.170371
$Fe(NH_2)(NH_3)$	4	3	5	−2443.137346
$Fe(N)(NH_3)$	5	2	2	−2442.125412
$Fe(N)(NH_3)$	5	2	4	−2442.090902
$Fe(NH_3)(N)$	5	2	2	−2442.11944
$Fe(NH_3)(N)$	5	2	4	−2442.088784
$Fe(NH)(NH_2)$	5	2	4	−2442.099408
$Fe(NH)(NH_2)$	5	2	2	−2442.097272
$Fe(NH)(NH_3)$	5	3	2	−2442.526792
$Fe(NH)(NH_3)$	5	3	4	−2442.519145
$Fe(NH_2)(NH_2)$	5	3	4	−2442.516784
$Fe(NH_2)(NH_2)$	5	3	2	−2442.514531
MeCN	–	0	1	−132.6671601
NH_3	–	0	1	−56.50501517
N_2H_4	–	0	1	−111.7692421
Ferrocene	2	0	1	−1650.613945
Ferrocenium	3	1	2	−1650.439308
TEMPO	–	0	2	−483.24406649
TEMPOH	–	0	1	−483.83585272

* For $Fe(N_2H_4)$, calculations with multiplicities of 3 or 5 resulted in optimized geometries containing η^1-N_2H_4 moieities; η^2-N_2H_4 coordination was only observed for the lowest energy singlet state.

C.16 DFT structures

Cartesian coordinates in angstrom units are provided. The naming convention is $[(bpyPy_2Me)Fe(L_{ax})(L_{eq})]^{n+}$, where L_{ax} and L_{eq} represent ligands axial/*trans* to bipyridine and equatorial/*trans* to pyridine, respectively, in accordance with the orientation defined in the main-text.

$[(bpyPy_2Me)Fe(MeCN)(NH_3)]^{2+}$, multiplicity = 1
C -2.5812420000 2.1854410000 -0.9943090000
C -3.0217660000 0.8802290000 -0.7505960000
C -2.0629920000 -0.1136280000 -0.5108580000
N -0.7289330000 0.1718060000 -0.5950930000
C -0.2977210000 1.4502580000 -0.6623920000
C -1.2134820000 2.4865760000 -0.8951380000
C -3.5780150000 -2.0225160000 0.2320770000
C -2.3105100000 -1.4688140000 -0.0023780000
C -3.6734330000 -3.2780260000 0.8408120000
C -2.4942460000 -3.9450220000 1.2012940000
C -1.2610950000 -3.3495070000 0.9214680000
N -1.1564730000 -2.1402770000 0.3264780000
C 1.1970940000 1.6469490000 -0.3363680000
C 1.5351780000 3.1453320000 -0.2748940000
C 2.0661280000 0.9212210000 -1.3777610000
C 1.4461390000 0.9552330000 1.0342530000
N 1.1544700000 -0.3733690000 1.1334160000
C 1.3453510000 -1.0144660000 2.3113780000
C 1.8462000000 -0.3726350000 3.4428090000
C 2.1614110000 0.9876660000 3.3544860000
C 1.9557160000 1.6528890000 2.1400560000
C 3.0282510000 1.5819880000 -2.1571800000
C 3.8083240000 0.8578870000 -3.0658040000
C 3.6113300000 -0.5236210000 -3.1683230000
C 2.6406570000 -1.1208780000 -2.3661030000
N 1.8728370000 -0.4188090000 -1.4921070000
H -3.3027470000 2.9809780000 -1.2012290000
H -4.6524710000 -3.7255750000 1.0338840000
H -2.5173130000 -4.9241040000 1.6862270000
H -0.3246170000 -3.8545620000 1.1679380000
H 0.9171690000 3.6524760000 0.4812650000
H 2.5936540000 3.2996290000 -0.0173040000

H 1.3459720000 3.6226960000 -1.2486520000
H 1.0817780000 -2.0748540000 2.3319930000
H 1.9826380000 -0.9378570000 4.3688070000
H 2.5602980000 1.5301510000 4.2168980000
H 2.1956700000 2.7136940000 2.0594060000
H 3.1720610000 2.6584090000 -2.0561060000
H 4.5587950000 1.3686600000 -3.6767970000
H 4.1975990000 -1.1415180000 -3.8541250000
H 2.4634050000 -2.1979560000 -2.4119290000
Fe 0.4571770000 -1.3049970000 -0.4451370000
H -0.8754380000 3.5195090000 -0.9871880000
N 1.5623420000 -2.8147330000 -0.1573420000
N -0.2218100000 -2.1161660000 -2.1835550000
H -1.2230990000 -1.9408650000 -2.3488320000
H -0.1113430000 -3.1381050000 -2.2216850000
H 0.2538100000 -1.7453880000 -3.0160680000
H -4.4765270000 -1.4701800000 -0.0537390000
H -4.0881310000 0.6442440000 -0.7153050000
C 2.2675500000 -3.7299440000 0.0181330000
C 3.1447560000 -4.8685140000 0.2448010000
H 3.1314360000 -5.1387990000 1.3141690000
H 4.1753420000 -4.6094880000 -0.0521240000
H 2.7994910000 -5.7290660000 -0.3521540000

[(bpyPy$_2$Me)Fe(MeCN)(NH$_3$)]$^{2+}$, multiplicity = 3
C -2.5824880000 2.1460730000 -0.9169440000
C -3.0324110000 0.8471120000 -0.6690650000
C -2.0863310000 -0.1507490000 -0.4025140000
N -0.7419370000 0.1224020000 -0.4351310000
C -0.2987770000 1.3998360000 -0.5541770000
C -1.2130030000 2.4311930000 -0.8206540000
C -3.6840890000 -2.0375660000 0.2040690000
C -2.3912740000 -1.5215580000 0.0178920000
C -3.8329320000 -3.3374540000 0.6962860000
C -2.6873640000 -4.0923620000 0.9901690000
C -1.4298680000 -3.5283890000 0.7635690000
N -1.2784660000 -2.2736220000 0.2866340000
C 1.2048740000 1.6561840000 -0.2965590000
C 1.4938760000 3.1680460000 -0.3206260000
C 2.0742640000 0.9209440000 -1.3429870000
C 1.5452160000 1.0604650000 1.1006020000
N 1.3213110000 -0.2634900000 1.2705060000
C 1.5973720000 -0.8505890000 2.4549890000
C 2.1115330000 -0.1391160000 3.5401800000
C 2.3527340000 1.2299800000 3.3791580000
C 2.0692190000 1.8356970000 2.1481130000

C 3.0576920000 1.5814380000 -2.0991920000
C 3.8362550000 0.8555720000 -3.0083490000
C 3.6196040000 -0.5201190000 -3.1430230000
C 2.6286700000 -1.1116540000 -2.3596260000
N 1.8740470000 -0.4100370000 -1.4838040000
H -3.2933810000 2.9449010000 -1.1459380000
H -4.8316850000 -3.7555380000 0.8521190000
H -2.7595320000 -5.1099590000 1.3819800000
H -0.5130760000 -4.0895170000 0.9598960000
H 0.8790410000 3.6941750000 0.4246930000
H 2.5513980000 3.3657480000 -0.0912070000
H 1.2743590000 3.5913770000 -1.3128660000
H 1.3942420000 -1.9244530000 2.5259210000
H 2.3179800000 -0.6534600000 4.4828190000
H 2.7596440000 1.8274590000 4.2008150000
H 2.2604540000 2.9013370000 2.0160400000
H 3.2236110000 2.6527970000 -1.9828400000
H 4.6031200000 1.3648320000 -3.6003170000
H 4.2019380000 -1.1309680000 -3.8384200000
H 2.4203800000 -2.1822780000 -2.4291840000
Fe 0.4314340000 -1.3768780000 -0.3002340000
H -0.8670940000 3.4568510000 -0.9488960000
N 1.5536280000 -2.8964380000 -0.0980340000
N -0.2953420000 -2.1685180000 -2.3912990000
H -1.3200360000 -2.2127780000 -2.4611410000
H 0.0300950000 -3.1215040000 -2.5954550000
H 0.0048990000 -1.5914940000 -3.1861440000
H -4.5597620000 -1.4262630000 -0.0263830000
H -4.0992050000 0.6115320000 -0.6679220000
C 2.2564570000 -3.8127910000 0.0770920000
C 3.1340060000 -4.9499100000 0.2983210000
H 3.1015970000 -5.2351960000 1.3633560000
H 4.1678670000 -4.6795440000 0.0247890000
H 2.8018600000 -5.8020760000 -0.3176030000

[(bpyPy$_2$Me)Fe(MeCN)(NH$_3$)]$^{2+}$, multiplicity = 5
C -2.5913420000 2.1732430000 -0.9514330000
C -3.0444050000 0.8798530000 -0.6775890000
C -2.0961820000 -0.1107950000 -0.3766080000
N -0.7665160000 0.1721160000 -0.3849780000
C -0.3203310000 1.4345020000 -0.5466250000
C -1.2233960000 2.4662420000 -0.8555790000
C -3.7585250000 -1.9490980000 0.2003710000
C -2.4386660000 -1.4910890000 0.0435500000
C -3.9810450000 -3.2470860000 0.6720410000
C -2.8822570000 -4.0624810000 0.9766090000

C -1.5965210000 -3.5496450000 0.7807710000
N -1.3776460000 -2.2993740000 0.3275740000
C 1.1949840000 1.6837070000 -0.2930150000
C 1.4682350000 3.2004550000 -0.2816540000
C 2.0595490000 0.9972930000 -1.3824250000
C 1.5627530000 1.0638920000 1.0897630000
N 1.4487890000 -0.2801680000 1.2376680000
C 1.7644720000 -0.8621850000 2.4147980000
C 2.2057320000 -0.1338270000 3.5208370000
C 2.3253150000 1.2532990000 3.3879390000
C 2.0032010000 1.8553060000 2.1642040000
C 2.9624920000 1.7169350000 -2.1857690000
C 3.7566890000 1.0369030000 -3.1174860000
C 3.6419020000 -0.3531080000 -3.2296610000
C 2.7187840000 -1.0021370000 -2.4083180000
N 1.9448120000 -0.3440370000 -1.5182120000
H -3.3029320000 2.9640690000 -1.2059870000
H -5.0029410000 -3.6156390000 0.8024300000
H -3.0117400000 -5.0808990000 1.3517550000
H -0.7077980000 -4.1552780000 0.9847850000
H 0.8445620000 3.7036890000 0.4721460000
H 2.5239650000 3.4062520000 -0.0501460000
H 1.2406700000 3.6447870000 -1.2624190000
H 1.6563810000 -1.9517240000 2.4612080000
H 2.4508390000 -0.6479160000 4.4542570000
H 2.6698910000 1.8691410000 4.2244400000
H 2.1017700000 2.9363690000 2.0601310000
H 3.0589270000 2.7988620000 -2.0894260000
H 4.4622250000 1.5939950000 -3.7421260000
H 4.2487460000 -0.9281170000 -3.9346370000
H 2.5855770000 -2.0881270000 -2.4546760000
Fe 0.5269130000 -1.4856610000 -0.3052620000
H -0.8803890000 3.4885080000 -1.0158050000
N 1.7136470000 -3.1823430000 -0.0153630000
N -0.1855920000 -2.2733400000 -2.2998310000
H -1.2044920000 -2.2068480000 -2.4235270000
H 0.0396140000 -3.2663820000 -2.4431900000
H 0.2133460000 -1.7778280000 -3.1063020000
H -4.6034930000 -1.2982370000 -0.0356300000
H -4.1128770000 0.6528260000 -0.6889350000
C 2.3960080000 -4.1115610000 0.1642010000
C 3.2508080000 -5.2641530000 0.3855240000
H 3.2304940000 -5.5401030000 1.4528750000
H 4.2831960000 -5.0132540000 0.0890140000
H 2.8904250000 -6.1101210000 -0.2228040000

[(bpyPy$_2$Me)Fe(N$_2$H$_4$)(NH$_3$)]$^{2+}$, multiplicity = 1
C -2.5311680000 2.2158950000 -0.9662520000
C -2.9964880000 0.9156060000 -0.7445590000
C -2.0568180000 -0.1008550000 -0.5200790000
N -0.7172990000 0.1572450000 -0.6052750000
C -0.2621780000 1.4298830000 -0.6511140000
C -1.1570080000 2.4881510000 -0.8622560000
C -3.6124250000 -1.9680340000 0.2236470000
C -2.3292670000 -1.4520730000 -0.0146090000
C -3.7493290000 -3.2107110000 0.8487580000
C -2.5904050000 -3.9021860000 1.2272430000
C -1.3423420000 -3.3434040000 0.9400920000
N -1.1897470000 -2.1520470000 0.3187460000
C 1.2417600000 1.5864010000 -0.3402380000
C 1.6144190000 3.0755470000 -0.2551220000
C 2.0647750000 0.8648050000 -1.4188950000
C 1.4870000000 0.8669310000 1.0147370000
N 1.1608740000 -0.4567800000 1.0937370000
C 1.2998900000 -1.1044610000 2.2780470000
C 1.8022620000 -0.4884520000 3.4225820000
C 2.1719100000 0.8595230000 3.3464670000
C 2.0036860000 1.5381890000 2.1339000000
C 3.0100580000 1.5268920000 -2.2175570000
C 3.7276760000 0.8215280000 -3.1895080000
C 3.4796980000 -0.5473370000 -3.3398880000
C 2.5307550000 -1.1467500000 -2.5149760000
N 1.8280490000 -0.4678390000 -1.5668570000
H -3.2372110000 3.0288160000 -1.1585290000
H -4.7417710000 -3.6270020000 1.0440400000
H -2.6392350000 -4.8697740000 1.7336750000
H -0.4348620000 -3.8845640000 1.2220750000
H 1.0171780000 3.5806620000 0.5192210000
H 2.6796750000 3.2025520000 -0.0099370000
H 1.4208390000 3.5757220000 -1.2163830000
H 0.9839610000 -2.1515960000 2.2975900000
H 1.8954770000 -1.0624030000 4.3483430000
H 2.5770010000 1.3827870000 4.2177290000
H 2.2740620000 2.5925370000 2.0655540000
H 3.1871020000 2.5948060000 -2.0852810000
H 4.4639720000 1.3350080000 -3.8147860000
H 4.0075670000 -1.1541090000 -4.0804360000
H 2.3184580000 -2.2146420000 -2.6166500000
Fe 0.4407880000 -1.3387660000 -0.4885150000
H -0.7989910000 3.5161960000 -0.9350340000
N 1.6166560000 -2.9986050000 -0.2531350000
H 1.6297220000 -3.5603360000 -1.1168580000

H 1.1999820000 -3.6570130000 0.4184420000
N -0.3047020000 -2.1396150000 -2.2083820000
H -1.2775510000 -1.8419740000 -2.3691680000
H -0.3382760000 -3.1685140000 -2.2324920000
H 0.1944130000 -1.8579710000 -3.0626450000
N 3.0270290000 -2.9312410000 0.1535600000
H -4.4933830000 -1.3916630000 -0.0698180000
H -4.0675550000 0.7013380000 -0.7121780000
H 3.4802590000 -2.3051930000 -0.5251420000
H 3.0343470000 -2.3935700000 1.0304540000

[(bpyPy$_2$Me)Fe(N$_2$H$_4$)(NH$_3$)]$^{2+}$, multiplicity = 3
C -2.5298590000 2.1912600000 -0.8523600000
C -3.0066840000 0.8996760000 -0.6233860000
C -2.0804990000 -0.1251500000 -0.3830640000
N -0.7313200000 0.1161450000 -0.4232790000
C -0.2609060000 1.3867640000 -0.5298410000
C -1.1516710000 2.4433370000 -0.7668370000
C -3.7169530000 -1.9825640000 0.1806700000
C -2.4096030000 -1.4949390000 0.0099410000
C -3.9075850000 -3.2891690000 0.6342430000
C -2.7813080000 -4.0818560000 0.9068790000
C -1.5111300000 -3.5437220000 0.7002060000
N -1.3100070000 -2.2800030000 0.2596710000
C 1.2529720000 1.5980190000 -0.2919360000
C 1.5843070000 3.1019130000 -0.3112410000
C 2.0768780000 0.8503860000 -1.3648030000
C 1.5822070000 0.9889940000 1.1015650000
N 1.3151760000 -0.3287420000 1.2743010000
C 1.5342050000 -0.9037510000 2.4792610000
C 2.0492270000 -0.2002430000 3.5681830000
C 2.3509610000 1.1558080000 3.3959850000
C 2.1125180000 1.7551340000 2.1530840000
C 3.0581160000 1.4954050000 -2.1383650000
C 3.7682310000 0.7742820000 -3.1041670000
C 3.4822400000 -0.5839420000 -3.2849330000
C 2.5017780000 -1.1605060000 -2.4794220000
N 1.8210270000 -0.4682200000 -1.5364310000
H -3.2247980000 3.0100320000 -1.0592430000
H -4.9180210000 -3.6837010000 0.7750890000
H -2.8779020000 -5.1093960000 1.2673330000
H -0.6239960000 -4.1544980000 0.8886290000
H 0.9924130000 3.6396810000 0.4446030000
H 2.6493890000 3.2704840000 -0.0938880000
H 1.3635340000 3.5360210000 -1.2981850000
H 1.2789250000 -1.9653280000 2.5714870000

H 2.2067290000 -0.7102090000 4.5223700000
H 2.7636330000 1.7477050000 4.2187010000
H 2.3400020000 2.8126590000 2.0144640000
H 3.2706650000 2.5551490000 -1.9964210000
H 4.5301870000 1.2735620000 -3.7105320000
H 3.9995820000 -1.1896530000 -4.0336810000
H 2.2312840000 -2.2139390000 -2.5994560000
Fe 0.4200680000 -1.4117840000 -0.3108980000
H -0.7841690000 3.4634630000 -0.8807960000
N 1.5711780000 -3.0641470000 -0.0564850000
H 1.4148000000 -3.7334140000 -0.8234460000
H 1.2399040000 -3.5850740000 0.7690220000
N -0.3680710000 -2.2503840000 -2.4324230000
H -1.3960100000 -2.2373610000 -2.4274440000
H -0.1244980000 -3.2081770000 -2.7174640000
H -0.1022850000 -1.6560710000 -3.2277480000
N 3.0250010000 -3.0124930000 0.1298570000
H -4.5734120000 -1.3393790000 -0.0354300000
H -4.0789250000 0.6905920000 -0.6169730000
H 3.4145540000 -2.6910410000 -0.7649480000
H 3.1922950000 -2.2297610000 0.7754710000

[(bpyPy$_2$Me)Fe(N$_2$H$_4$)(NH$_3$)]$^{2+}$, multiplicity = 5
C -2.5482370000 2.2118170000 -0.8660130000
C -3.0251570000 0.9251060000 -0.6068490000
C -2.0937800000 -0.0966560000 -0.3591690000
N -0.7586960000 0.1513340000 -0.4039240000
C -0.2862710000 1.4083310000 -0.5442900000
C -1.1712460000 2.4688220000 -0.8020160000
C -3.7921790000 -1.9055510000 0.1736860000
C -2.4601980000 -1.4741410000 0.0394540000
C -4.0529030000 -3.2068280000 0.6129930000
C -2.9731820000 -4.0499850000 0.9104200000
C -1.6755960000 -3.5578620000 0.7444540000
N -1.4126800000 -2.3038770000 0.3204060000
C 1.2370490000 1.6227490000 -0.3098900000
C 1.5418620000 3.1338850000 -0.2862040000
C 2.0760530000 0.9349000000 -1.4148400000
C 1.5931300000 0.9836710000 1.0674650000
N 1.4073100000 -0.3533940000 1.2212580000
C 1.6627960000 -0.9269670000 2.4190380000
C 2.1343450000 -0.2135900000 3.5210270000
C 2.3473130000 1.1607380000 3.3712620000
C 2.0703260000 1.7614040000 2.1371760000
C 3.0057340000 1.6427730000 -2.1978210000
C 3.7547200000 0.9676740000 -3.1688450000

C 3.5619880000 -0.4064470000 -3.3480620000
C 2.6164840000 -1.0428180000 -2.5442010000
N 1.8973070000 -0.3934700000 -1.6018200000
H -3.2468460000 3.0258520000 -1.0807420000
H -5.0841530000 -3.5552030000 0.7228620000
H -3.1250900000 -5.0739900000 1.2623210000
H -0.8140980000 -4.1973030000 0.9602440000
H 0.9369610000 3.6414820000 0.4801210000
H 2.6036240000 3.3161940000 -0.0637840000
H 1.3141980000 3.5911340000 -1.2606860000
H 1.4742620000 -2.0026150000 2.4962500000
H 2.3259980000 -0.7301550000 4.4653740000
H 2.7203890000 1.7664250000 4.2028610000
H 2.2276420000 2.8337620000 2.0203790000
H 3.1531670000 2.7138750000 -2.0595630000
H 4.4787800000 1.5166420000 -3.7789390000
H 4.1206670000 -0.9770260000 -4.0947370000
H 2.4141170000 -2.1127150000 -2.6601430000
Fe 0.5180970000 -1.5432720000 -0.3760180000
H -0.8077010000 3.4867210000 -0.9444220000
N 1.6235250000 -3.3676580000 0.1303610000
H 1.4332610000 -4.1268230000 -0.5379230000
H 1.3588850000 -3.7869510000 1.0330130000
N -0.2361700000 -2.3391660000 -2.3441890000
H -1.2551340000 -2.4759060000 -2.3357210000
H 0.1462760000 -3.2416450000 -2.6558170000
H -0.0626590000 -1.6893870000 -3.1218820000
N 3.0897250000 -3.2460880000 0.1873860000
H -4.6181890000 -1.2297160000 -0.0592890000
H -4.0988540000 0.7264980000 -0.5854740000
H 3.4028070000 -3.1885520000 -0.7894640000
H 3.2746050000 -2.3081820000 0.5684080000

[(bpyPy$_2$Me)Fe(NH$_3$)(N$_2$H$_4$)]$^{2+}$, multiplicity = 1
C -2.5696540000 2.2279200000 -0.9630660000
C -3.0387160000 0.9305160000 -0.7306690000
C -2.1017520000 -0.0874850000 -0.5034830000
N -0.7603950000 0.1663290000 -0.5928590000
C -0.3006750000 1.4382070000 -0.6474420000
C -1.1939210000 2.4963110000 -0.8653060000
C -3.6556790000 -1.9607600000 0.2383530000
C -2.3743910000 -1.4379400000 0.0025820000
C -3.7860230000 -3.2086950000 0.8541720000
C -2.6238600000 -3.9012930000 1.2237960000
C -1.3772960000 -3.3364040000 0.9432160000
N -1.2328610000 -2.1358700000 0.3347230000

C 1.2027660000 1.5977860000 -0.3318120000
C 1.5771190000 3.0874310000 -0.2687210000
C 2.0411260000 0.8570700000 -1.3866440000
C 1.4473470000 0.8962550000 1.0327290000
N 1.1184090000 -0.4253320000 1.1286250000
C 1.2860800000 -1.0671130000 2.3110180000
C 1.8128250000 -0.4433150000 3.4401910000
C 2.1759030000 0.9051740000 3.3499010000
C 1.9836790000 1.5765350000 2.1367720000
C 3.0084560000 1.4956610000 -2.1771270000
C 3.7407630000 0.7623130000 -3.1181730000
C 3.4843440000 -0.6071860000 -3.2473370000
C 2.5144210000 -1.1849930000 -2.4303860000
N 1.8006080000 -0.4764370000 -1.5126390000
H -3.2731420000 3.0420650000 -1.1592980000
H -4.7764590000 -3.6303230000 1.0473900000
H -2.6707600000 -4.8757900000 1.7160910000
H -0.4621090000 -3.8712430000 1.2078690000
H 0.9790160000 3.6064470000 0.4952870000
H 2.6414900000 3.2159840000 -0.0208490000
H 1.3892420000 3.5726500000 -1.2389650000
H 0.9761020000 -2.1144020000 2.3436670000
H 1.9300090000 -1.0124900000 4.3664030000
H 2.5974760000 1.4336630000 4.2101790000
H 2.2541600000 2.6299580000 2.0559040000
H 3.1923810000 2.5645270000 -2.0620330000
H 4.4952160000 1.2571450000 -3.7371520000
H 4.0221650000 -1.2308980000 -3.9667150000
H 2.2838070000 -2.2516190000 -2.5147350000
Fe 0.3926610000 -1.3226100000 -0.4454510000
H -0.8333400000 3.5225360000 -0.9477020000
N 1.5915010000 -2.9308940000 -0.1704920000
H 1.4552400000 -3.5640590000 -0.9794200000
H 1.4311660000 -3.4992860000 0.6701150000
N -0.2989200000 -2.1300320000 -2.1934380000
H -1.3101790000 -1.9466580000 -2.3139330000
N -0.0044360000 -3.5345430000 -2.4131440000
H 0.1473620000 -1.6185990000 -2.9660150000
H 2.5890590000 -2.6844270000 -0.1375390000
H -4.5391010000 -1.3867940000 -0.0521210000
H -4.1104260000 0.7191150000 -0.6938030000
H -0.2897230000 -3.7787080000 -3.3709880000
H -0.6362040000 -4.0640930000 -1.7991960000

[(bpyPy$_2$Me)Fe(NH$_3$)(N$_2$H$_4$)]$^{2+}$, multiplicity = 3
C -2.5712720000 2.2311610000 -0.8495330000

C -3.0551430000 0.9422950000 -0.6183810000
C -2.1353190000 -0.0843620000 -0.3638540000
N -0.7837850000 0.1530830000 -0.3917340000
C -0.3069380000 1.4207740000 -0.5061150000
C -1.1925780000 2.4787270000 -0.7557830000
C -3.7723720000 -1.9391780000 0.2178720000
C -2.4670140000 -1.4500610000 0.0384540000
C -3.9570200000 -3.2376290000 0.6970290000
C -2.8276310000 -4.0188290000 0.9918100000
C -1.5580460000 -3.4819360000 0.7756640000
N -1.3653430000 -2.2281880000 0.3000650000
C 1.2079730000 1.6239970000 -0.2734060000
C 1.5480950000 3.1257180000 -0.2982500000
C 2.0289690000 0.8647090000 -1.3416670000
C 1.5571610000 1.0129210000 1.1149900000
N 1.3006570000 -0.3064150000 1.2829550000
C 1.5792950000 -0.9021990000 2.4638490000
C 2.1304480000 -0.2091950000 3.5420190000
C 2.4060170000 1.1540450000 3.3813490000
C 2.1178320000 1.7702310000 2.1569930000
C 3.0161830000 1.4995800000 -2.1147870000
C 3.7461590000 0.7627410000 -3.0540450000
C 3.4766760000 -0.6018560000 -3.2038930000
C 2.4862100000 -1.1695870000 -2.4035350000
N 1.7780810000 -0.4584260000 -1.4938750000
H -3.2613050000 3.0514810000 -1.0664880000
H -4.9658300000 -3.6337940000 0.8450830000
H -2.9223880000 -5.0367720000 1.3791980000
H -0.6638980000 -4.0741550000 0.9879130000
H 0.9633100000 3.6681230000 0.4599910000
H 2.6151700000 3.2885730000 -0.0867750000
H 1.3251960000 3.5595620000 -1.2848370000
H 1.3453370000 -1.9693700000 2.5404670000
H 2.3363100000 -0.7322730000 4.4799060000
H 2.8422200000 1.7377850000 4.1978390000
H 2.3332240000 2.8312240000 2.0249900000
H 3.2200550000 2.5633570000 -1.9914360000
H 4.5133930000 1.2543570000 -3.6600480000
H 4.0146300000 -1.2221780000 -3.9257730000
H 2.2383510000 -2.2314130000 -2.4991460000
Fe 0.3542790000 -1.3706890000 -0.2665630000
H -0.8204110000 3.4965620000 -0.8747360000
N 1.5049420000 -3.0173240000 -0.1549970000
H 1.3031600000 -3.5760850000 -1.0131690000
H 1.3447640000 -3.6417900000 0.6459360000
N -0.3911300000 -2.3049290000 -2.4043630000

H -1.3917340000 -2.1969740000 -2.6312710000
N 0.0232850000 -3.6874690000 -2.5236300000
H 0.1057810000 -1.7807910000 -3.1332710000
H 2.5137850000 -2.8197630000 -0.1463560000
H -4.6313770000 -1.3027420000 -0.0085130000
H -4.1280970000 0.7363070000 -0.6214140000
H -0.1510470000 -4.0259830000 -3.4806430000
H -0.6153990000 -4.2336520000 -1.9317550000

[(bpyPy$_2$Me)Fe(NH$_3$)(N$_2$H$_4$)]$^{2+}$, multiplicity = 5
C -2.5819470000 2.2386670000 -0.8673160000
C -3.0693090000 0.9558290000 -0.6081790000
C -2.1474640000 -0.0699330000 -0.3417270000
N -0.8088790000 0.1701430000 -0.3713090000
C -0.3269520000 1.4230430000 -0.5202120000
C -1.2034190000 2.4868780000 -0.7913920000
C -3.8604330000 -1.8630410000 0.2127120000
C -2.5266230000 -1.4409890000 0.0666120000
C -4.1261150000 -3.1542310000 0.6774160000
C -3.0512170000 -3.9999590000 0.9883710000
C -1.7512080000 -3.5216620000 0.8064900000
N -1.4857350000 -2.2770440000 0.3554630000
C 1.1983720000 1.6263530000 -0.2908030000
C 1.5196040000 3.1337480000 -0.2888440000
C 2.0273340000 0.9103600000 -1.3882340000
C 1.5667800000 1.0000010000 1.0888120000
N 1.3861470000 -0.3348450000 1.2487410000
C 1.6957780000 -0.9214560000 2.4256860000
C 2.2023560000 -0.2103110000 3.5140120000
C 2.3924720000 1.1679190000 3.3667560000
C 2.0721170000 1.7762260000 2.1462650000
C 2.9701040000 1.5925140000 -2.1783340000
C 3.7202390000 0.8883190000 -3.1282890000
C 3.5186060000 -0.4881990000 -3.2758890000
C 2.5609930000 -1.0998360000 -2.4655490000
N 1.8351260000 -0.4192890000 -1.5499940000
H -3.2727320000 3.0560610000 -1.0936500000
H -5.1589520000 -3.4937980000 0.7993370000
H -3.2104580000 -5.0146870000 1.3621600000
H -0.8879770000 -4.1562580000 1.0310080000
H 0.9252180000 3.6582040000 0.4738160000
H 2.5844370000 3.3078220000 -0.0737960000
H 1.2915060000 3.5819270000 -1.2678520000
H 1.5253770000 -2.0019580000 2.4897190000
H 2.4400010000 -0.7299210000 4.4462820000
H 2.7883700000 1.7707180000 4.1899150000

H 2.2232970000 2.8499130000 2.0305490000
H 3.1298240000 2.6644410000 -2.0594750000
H 4.4553370000 1.4171260000 -3.7431950000
H 4.0818660000 -1.0807480000 -4.0019940000
H 2.3523510000 -2.1728490000 -2.5528160000
Fe 0.4356390000 -1.5296630000 -0.2829110000
H -0.8324730000 3.5012390000 -0.9384000000
N 1.6528660000 -3.2930540000 -0.0127230000
H 1.5604010000 -3.8277970000 -0.8944180000
H 1.4552520000 -3.9514370000 0.7517580000
N -0.2934890000 -2.3494780000 -2.2995610000
H -1.3086030000 -2.2749180000 -2.4738960000
N 0.1795150000 -3.6992450000 -2.5499660000
H 0.1378580000 -1.7496330000 -3.0127190000
H 2.6492460000 -3.0584770000 0.0846210000
H -4.6840450000 -1.1869490000 -0.0282010000
H -4.1447320000 0.7634940000 -0.6007900000
H -0.0806740000 -3.9727370000 -3.5081250000
H -0.3790740000 -4.3152390000 -1.9456070000

[(bpyPy$_2$Me)Fe(η^2-N$_2$H$_4$)]$^{2+}$, multiplicity = 1
C -2.6032110000 2.4256830000 -0.9365670000
C -3.1273900000 1.1389800000 -0.7644410000
C -2.2365520000 0.0745180000 -0.5796810000
N -0.8841760000 0.2730210000 -0.6621170000
C -0.3734000000 1.5243730000 -0.6500170000
C -1.2192780000 2.6303800000 -0.8189780000
C -3.8547750000 -1.7642010000 0.1249580000
C -2.5618790000 -1.2757110000 -0.1119160000
C -4.0153150000 -3.0127850000 0.7353950000
C -2.8737180000 -3.7344660000 1.1110170000
C -1.6118100000 -3.2043230000 0.8262430000
N -1.4438250000 -2.0132640000 0.2063350000
C 1.1340540000 1.5948170000 -0.3448110000
C 1.5693500000 3.0587770000 -0.1672330000
C 1.9059600000 0.9083120000 -1.4836150000
C 1.4061110000 0.7720130000 0.9449820000
N 1.0541110000 -0.5462160000 0.9356220000
C 1.3095230000 -1.3180620000 2.0211610000
C 1.9218520000 -0.8180820000 3.1680940000
C 2.2805970000 0.5351430000 3.1984110000
C 2.0205030000 1.3308250000 2.0764990000
C 2.8682180000 1.5911080000 -2.2432100000
C 3.5624210000 0.9313460000 -3.2615390000
C 3.2739150000 -0.4170000000 -3.4902040000
C 2.3067170000 -1.0353660000 -2.7016520000

N 1.6157040000 -0.4052360000 -1.7150510000
H -3.2715150000 3.2764970000 -1.0968520000
H -5.0166060000 -3.4097660000 0.9257520000
H -2.9473830000 -4.7024680000 1.6135890000
H -0.7051680000 -3.7510400000 1.1038190000
H 1.0059240000 3.5286660000 0.6534650000
H 2.6427310000 3.1279620000 0.0642720000
H 1.3782350000 3.6327470000 -1.0866140000
H 1.0098200000 -2.3666760000 1.9480010000
H 2.1076510000 -1.4836400000 4.0153640000
H 2.7597400000 0.9701970000 4.0806280000
H 2.2994790000 2.3850760000 2.0869280000
H 3.0778090000 2.6416660000 -2.0401780000
H 4.3119870000 1.4611920000 -3.8566020000
H 3.7830250000 -0.9974520000 -4.2641490000
H 2.0946130000 -2.0899760000 -2.8878160000
Fe 0.1855120000 -1.2727160000 -0.6272230000
H -0.8138000000 3.6430400000 -0.8454590000
N -0.1763700000 -2.5830510000 -2.0687110000
H -1.0278420000 -3.1592010000 -2.1038070000
N 0.7755820000 -3.1057860000 -1.1160200000
H 0.2102290000 -2.5261080000 -3.0211370000
H -4.7240960000 -1.1650970000 -0.1577710000
H -4.2069650000 0.9711520000 -0.7368650000
H 1.6788060000 -3.3364830000 -1.5522330000
H 0.4244720000 -3.9646270000 -0.6725540000

[(bpyPy$_2$Me)Fe(η^2-N$_2$H$_4$)]$^{2+}$, multiplicity = 3 (N$_2$H$_4$ becomes η^1)
C -2.5596350000 2.6162900000 -0.4511670000
C -3.1367980000 1.3449530000 -0.4503820000
C -2.2967180000 0.2249830000 -0.3991480000
N -0.9338270000 0.3607690000 -0.3776680000
C -0.3638640000 1.5906890000 -0.3416820000
C -1.1649290000 2.7411720000 -0.3805410000
C -4.0687780000 -1.5895320000 -0.2504110000
C -2.7317180000 -1.1658710000 -0.3025400000
C -4.3519250000 -2.9450540000 -0.0682810000
C -3.2854290000 -3.8471990000 0.0709060000
C -1.9788320000 -3.3675230000 -0.0057210000
N -1.6898220000 -2.0570340000 -0.2078840000
C 1.1751790000 1.6273540000 -0.2522360000
C 1.6751850000 3.0815150000 -0.1795900000
C 1.7286440000 0.9251590000 -1.5167770000
C 1.5948290000 0.8472120000 1.0234280000
N 1.1549760000 -0.4304950000 1.1445880000
C 1.4466940000 -1.1474010000 2.2554360000

C 2.2048610000 -0.6262550000 3.3028040000
C 2.6864340000 0.6826100000 3.1831090000
C 2.3783440000 1.4241510000 2.0359310000
C 2.6196890000 1.5566430000 -2.3979510000
C 3.0414810000 0.8908930000 -3.5556000000
C 2.5692050000 -0.4007840000 -3.8107420000
C 1.7029690000 -0.9860640000 -2.8874630000
N 1.2959170000 -0.3371760000 -1.7684580000
H -3.1886520000 3.5098980000 -0.4926130000
H -5.3881260000 -3.2922150000 -0.0239940000
H -3.4553710000 -4.9143600000 0.2358090000
H -1.1350920000 -4.0527350000 0.1063490000
H 1.2606480000 3.5895410000 0.7041540000
H 2.7726440000 3.1146210000 -0.1108430000
H 1.3709590000 3.6417530000 -1.0764430000
H 1.0498600000 -2.1671020000 2.2996700000
H 2.4103670000 -1.2389880000 4.1845330000
H 3.2950580000 1.1298590000 3.9749560000
H 2.7496710000 2.4448880000 1.9398260000
H 2.9867090000 2.5623150000 -2.1916810000
H 3.7328370000 1.3829750000 -4.2466580000
H 2.8668000000 -0.9579610000 -4.7031620000
H 1.3320100000 -2.0122340000 -3.0018980000
Fe 0.1051230000 -1.2516060000 -0.4022010000
H -0.7115440000 3.7324590000 -0.3569150000
N 0.9049120000 -3.7447820000 -1.6949400000
H -0.0798020000 -4.0342440000 -1.6790630000
N 1.1471220000 -2.9686490000 -0.4932190000
H 1.4565250000 -4.6113370000 -1.6349320000
H -4.8764690000 -0.8594730000 -0.3421750000
H -4.2217630000 1.2210450000 -0.4788470000
H 2.1466580000 -2.7223890000 -0.5102050000
H 1.0363600000 -3.5465940000 0.3580470000

[(bpyPy$_2$Me)Fe(η^2-N$_2$H$_4$)]$^{2+}$, multiplicity = 5 (N$_2$H$_4$ becomes $\eta^{\backslash 1}$)
C -2.5765780000 2.6266260000 -0.4069460000
C -3.1518020000 1.3532670000 -0.3886770000
C -2.3025170000 0.2379480000 -0.3297150000
N -0.9544830000 0.3866960000 -0.3016940000
C -0.3838380000 1.6077310000 -0.3029860000
C -1.1827760000 2.7625400000 -0.3565830000
C -4.1245000000 -1.5274930000 -0.2360700000
C -2.7682280000 -1.1642260000 -0.2672100000
C -4.4735580000 -2.8779690000 -0.1365400000
C -3.4570970000 -3.8395920000 -0.0639930000
C -2.1287810000 -3.4103470000 -0.1064440000

N -1.7837500000 -2.1087820000 -0.2132400000
C 1.1682790000 1.6505290000 -0.2395530000
C 1.6467040000 3.1146080000 -0.1948100000
C 1.7294770000 0.9482010000 -1.5084390000
C 1.6338400000 0.9025520000 1.0440770000
N 1.3196480000 -0.4130680000 1.1728090000
C 1.6841950000 -1.1007340000 2.2795030000
C 2.3841650000 -0.5092590000 3.3302600000
C 2.7238050000 0.8428770000 3.2141080000
C 2.3477350000 1.5510310000 2.0655600000
C 2.5366610000 1.6228020000 -2.4385940000
C 3.0002770000 0.9498100000 -3.5766390000
C 2.6557200000 -0.3918280000 -3.7689280000
C 1.8582150000 -1.0130520000 -2.8071570000
N 1.4070800000 -0.3548530000 -1.7125920000
H -3.2109300000 3.5164970000 -0.4541230000
H -5.5266260000 -3.1730700000 -0.1104300000
H -3.6796450000 -4.9061940000 0.0237370000
H -1.3119920000 -4.1352800000 -0.0501120000
H 1.2335360000 3.6313080000 0.6842510000
H 2.7444640000 3.1656990000 -0.1421890000
H 1.3199580000 3.6573580000 -1.0941250000
H 1.3984290000 -2.1575060000 2.3138110000
H 2.6562380000 -1.1008790000 4.2082860000
H 3.2793930000 1.3505820000 4.0085970000
H 2.6140670000 2.6043630000 1.9780600000
H 2.8091820000 2.6672830000 -2.2876880000
H 3.6293860000 1.4764810000 -4.3009900000
H 2.9987760000 -0.9566210000 -4.6399820000
H 1.5741600000 -2.0721660000 -2.8790320000
Fe 0.2139010000 -1.3658240000 -0.3137820000
H -0.7378260000 3.7578180000 -0.3592410000
N 0.9818440000 -3.9534090000 -1.7501540000
H -0.0257070000 -4.0932590000 -1.8896410000
N 1.1494280000 -3.3085690000 -0.4597670000
H 1.3897450000 -4.8967570000 -1.7020440000
H -4.9014280000 -0.7612870000 -0.2834930000
H -4.2370720000 1.2347460000 -0.4166160000
H 2.1533180000 -3.0969330000 -0.3744540000
H 0.9570860000 -3.9617010000 0.3171290000

[(bpyPy$_2$Me)Fe(NH$_3$)(NH$_3$)]$^{2+}$, multiplicity = 1
C -2.5605910000 2.2304990000 -0.9564740000
C -3.0243190000 0.9305810000 -0.7271440000
C -2.0832920000 -0.0853100000 -0.5077570000
N -0.7433390000 0.1745760000 -0.6010550000

C -0.2882560000 1.4476180000 -0.6506570000
C -1.1856630000 2.5036500000 -0.8619830000
C -3.6281480000 -1.9728010000 0.2220590000
C -2.3504910000 -1.4412330000 -0.0119890000
C -3.7489310000 -3.2313500000 0.8187950000
C -2.5820980000 -3.9258120000 1.1686050000
C -1.3391320000 -3.3514810000 0.8899890000
N -1.2057150000 -2.1390110000 0.3050230000
C 1.2146090000 1.6095200000 -0.3341580000
C 1.5829600000 3.1002130000 -0.2599530000
C 2.0590820000 0.8790610000 -1.3905290000
C 1.4551340000 0.8999370000 1.0272220000
N 1.1251670000 -0.4226930000 1.1164660000
C 1.2672930000 -1.0598360000 2.3045790000
C 1.7784770000 -0.4375240000 3.4416910000
C 2.1519790000 0.9080970000 3.3546970000
C 1.9788360000 1.5785350000 2.1382620000
C 3.0296610000 1.5279520000 -2.1687870000
C 3.7764780000 0.8045970000 -3.1060080000
C 3.5320400000 -0.5662340000 -3.2413560000
C 2.5561310000 -1.1522360000 -2.4375050000
N 1.8252150000 -0.4547180000 -1.5258500000
H -3.2676520000 3.0426550000 -1.1480380000
H -4.7364240000 -3.6603230000 1.0110820000
H -2.6224710000 -4.9089670000 1.6440060000
H -0.4195110000 -3.8877750000 1.1364890000
H 0.9800640000 3.6119840000 0.5051220000
H 2.6458700000 3.2316970000 -0.0076150000
H 1.3962150000 3.5906420000 -1.2277830000
H 0.9454570000 -2.1040180000 2.3408990000
H 1.8745750000 -1.0054940000 4.3710510000
H 2.5634290000 1.4359050000 4.2202300000
H 2.2523700000 2.6313930000 2.0607840000
H 3.2059310000 2.5972040000 -2.0458950000
H 4.5338760000 1.3072230000 -3.7149800000
H 4.0835870000 -1.1849920000 -3.9546090000
H 2.3423190000 -2.2204590000 -2.5262350000
Fe 0.4112640000 -1.3127480000 -0.4728970000
H -0.8288220000 3.5313600000 -0.9422450000
N 1.5938680000 -2.9432600000 -0.1827150000
H 1.3335010000 -3.7789830000 -0.7233570000
H 1.6287350000 -3.2633740000 0.7940230000
N -0.2921230000 -2.1139980000 -2.2082680000
H -1.2854990000 -1.8878050000 -2.3613920000
H -0.2427590000 -3.1406630000 -2.2664040000
H 0.1867800000 -1.7606280000 -3.0467610000

H 2.5798910000 -2.7637880000 -0.4178540000
H -4.5158600000 -1.3990850000 -0.0555210000
H -4.0951250000 0.7151480000 -0.6875390000

[(bpyPy$_2$Me)Fe(NH$_3$)(NH$_3$)]$^{2+}$, multiplicity = 3
C -2.5665730000 2.2053190000 -0.8308930000
C -3.0405530000 0.9112750000 -0.6103240000
C -2.1113650000 -0.1131910000 -0.3810760000
N -0.7621890000 0.1323050000 -0.4247150000
C -0.2933920000 1.4040580000 -0.5250320000
C -1.1882940000 2.4599400000 -0.7492390000
C -3.7318990000 -1.9930870000 0.1669680000
C -2.4310750000 -1.4872500000 0.0021660000
C -3.9047040000 -3.3053860000 0.6116540000
C -2.7682570000 -4.0848450000 0.8822770000
C -1.5037450000 -3.5309580000 0.6825080000
N -1.3221930000 -2.2607400000 0.2491540000
C 1.2207390000 1.6179420000 -0.2899590000
C 1.5515450000 3.1214790000 -0.3247460000
C 2.0579960000 0.8556710000 -1.3419770000
C 1.5577290000 1.0204220000 1.1074960000
N 1.2913410000 -0.2949240000 1.2881550000
C 1.5425340000 -0.8702000000 2.4842200000
C 2.0844460000 -0.1663160000 3.5604080000
C 2.3772720000 1.1909070000 3.3824130000
C 2.1098140000 1.7902200000 2.1452360000
C 3.0352350000 1.4941910000 -2.1248570000
C 3.7809000000 0.7541070000 -3.0490930000
C 3.5357930000 -0.6175170000 -3.1761590000
C 2.5515940000 -1.1873190000 -2.3700510000
N 1.8320210000 -0.4742940000 -1.4719610000
H -3.2637300000 3.0244290000 -1.0288090000
H -4.9097430000 -3.7151990000 0.7474590000
H -2.8536420000 -5.1155160000 1.2367950000
H -0.6055280000 -4.1247300000 0.8688850000
H 0.9646280000 3.6654640000 0.4305510000
H 2.6178740000 3.2919210000 -0.1153270000
H 1.3238940000 3.5473340000 -1.3138200000
H 1.2915620000 -1.9317830000 2.5819560000
H 2.2684690000 -0.6762660000 4.5099970000
H 2.8074400000 1.7834120000 4.1957990000
H 2.3335540000 2.8477950000 2.0002790000
H 3.2185540000 2.5637660000 -2.0212590000
H 4.5403090000 1.2489120000 -3.6623480000
H 4.0864240000 -1.2404320000 -3.8861500000
H 2.3151010000 -2.2515960000 -2.4503720000

Fe 0.3823190000 -1.3917140000 -0.3140810000
H -0.8237890000 3.4818330000 -0.8564450000
N 1.5479250000 -3.0334640000 -0.0762520000
H 1.3168750000 -3.8047180000 -0.7168920000
H 1.4895000000 -3.4437640000 0.8665300000
N -0.3761560000 -2.1779020000 -2.4599190000
H -1.4035020000 -2.1821780000 -2.4975740000
H -0.1003600000 -3.1331570000 -2.7218550000
H -0.0845040000 -1.5835550000 -3.2458620000
H 2.5503190000 -2.8453790000 -0.2119970000
H -4.5963880000 -1.3600500000 -0.0474960000
H -4.1122600000 0.6992150000 -0.6017360000

[(bpyPy$_2$Me)Fe(NH$_3$)(NH$_3$)]$^{2+}$, multiplicity = 5
C -2.5715020000 2.2063130000 -0.8765320000
C -3.0462050000 0.9181580000 -0.6210170000
C -2.1135290000 -0.1002490000 -0.3634260000
N -0.7782320000 0.1535790000 -0.3963280000
C -0.3085500000 1.4111740000 -0.5386770000
C -1.1955250000 2.4681550000 -0.8031660000
C -3.8073840000 -1.9192760000 0.1637910000
C -2.4777020000 -1.4794820000 0.0322250000
C -4.0596670000 -3.2223030000 0.6027760000
C -2.9755840000 -4.0598730000 0.9035130000
C -1.6804090000 -3.5617730000 0.7392510000
N -1.4278980000 -2.3059250000 0.3142300000
C 1.2136040000 1.6278290000 -0.3041290000
C 1.5192800000 3.1385850000 -0.2891210000
C 2.0588570000 0.9299960000 -1.3998280000
C 1.5779300000 0.9941500000 1.0740550000
N 1.3971610000 -0.3421540000 1.2300930000
C 1.6911310000 -0.9234150000 2.4138560000
C 2.1851100000 -0.2116130000 3.5075240000
C 2.3802830000 1.1657560000 3.3609050000
C 2.0728690000 1.7712850000 2.1360820000
C 2.9855310000 1.6315350000 -2.1920430000
C 3.7591640000 0.9400360000 -3.1321150000
C 3.5971370000 -0.4430710000 -3.2681520000
C 2.6482490000 -1.0717450000 -2.4613840000
N 1.8999910000 -0.4041940000 -1.5561500000
H -3.2711020000 3.0177640000 -1.0977180000
H -5.0889310000 -3.5773430000 0.7101680000
H -3.1240230000 -5.0845390000 1.2550970000
H -0.8100430000 -4.1904080000 0.9528650000
H 0.9174640000 3.6501860000 0.4770580000
H 2.5820390000 3.3214000000 -0.0714520000

H 1.2885680000 3.5915900000 -1.2649500000
H 1.5169270000 -2.0019340000 2.4844770000
H 2.4071120000 -0.7311630000 4.4436580000
H 2.7669000000 1.7699800000 4.1874570000
H 2.2227160000 2.8449150000 2.0202650000
H 3.1140120000 2.7085740000 -2.0830810000
H 4.4823870000 1.4828520000 -3.7487710000
H 4.1827080000 -1.0262700000 -3.9839730000
H 2.4707040000 -2.1497890000 -2.5392450000
Fe 0.4878270000 -1.5418700000 -0.3461820000
H -0.8342210000 3.4868870000 -0.9455430000
N 1.6672160000 -3.3234890000 0.0366680000
H 1.4604420000 -4.1079410000 -0.5955050000
H 1.6036710000 -3.7207190000 0.9836180000
N -0.2979630000 -2.2658960000 -2.3391490000
H -1.3215760000 -2.1908300000 -2.4038780000
H -0.0921220000 -3.2509190000 -2.5523630000
H 0.0585790000 -1.7346160000 -3.1434140000
H 2.6684760000 -3.1253440000 -0.0950730000
H -4.6374810000 -1.2487350000 -0.0703160000
H -4.1193030000 0.7151220000 -0.6103440000

[(bpyPy$_2$Me)Fe(NH$_2$)(NH$_3$)]$^{2+}$, multiplicity = 2
C -2.5866610000 2.2410720000 -0.9393080000
C -3.0604590000 0.9461500000 -0.6999430000
C -2.1233790000 -0.0712290000 -0.4763760000
N -0.7886810000 0.1869430000 -0.5573040000
C -0.3222320000 1.4472890000 -0.6367280000
C -1.2115570000 2.5094810000 -0.8601030000
C -3.6793800000 -1.9571610000 0.2417580000
C -2.4012080000 -1.4342840000 -0.0010500000
C -3.7990520000 -3.2293930000 0.8112560000
C -2.6344620000 -3.9416990000 1.1273510000
C -1.3890910000 -3.3738320000 0.8417460000
N -1.2663880000 -2.1502710000 0.2837550000
C 1.1826540000 1.6026970000 -0.3320610000
C 1.5568070000 3.0923720000 -0.2615780000
C 2.0304920000 0.8664140000 -1.3852610000
C 1.4383790000 0.8906990000 1.0283630000
N 1.1356470000 -0.4348410000 1.1173860000
C 1.3357740000 -1.0960630000 2.2819680000
C 1.8578660000 -0.4721970000 3.4143640000
C 2.1838930000 0.8856980000 3.3382730000
C 1.9700840000 1.5691590000 2.1350290000
C 2.9868990000 1.5183350000 -2.1797990000
C 3.7668680000 0.7808730000 -3.0769890000

C 3.5864940000 -0.6051650000 -3.1478700000
C 2.6209400000 -1.1935260000 -2.3337870000
N 1.8450550000 -0.4737190000 -1.4836710000
H -3.2903890000 3.0555960000 -1.1333100000
H -4.7870760000 -3.6534400000 1.0114220000
H -2.6779790000 -4.9327350000 1.5857580000
H -0.4535790000 -3.8979090000 1.0538360000
H 0.9604600000 3.6057800000 0.5074170000
H 2.6218930000 3.2190150000 -0.0165730000
H 1.3652020000 3.5834330000 -1.2279080000
H 1.0709740000 -2.1563260000 2.2781150000
H 2.0035640000 -1.0503940000 4.3308000000
H 2.5997170000 1.4134970000 4.2017880000
H 2.2210610000 2.6279940000 2.0646910000
H 3.1275080000 2.5967020000 -2.0981130000
H 4.5112240000 1.2852690000 -3.7006490000
H 4.1828820000 -1.2321920000 -3.8162530000
H 2.4552400000 -2.2740980000 -2.3308700000
Fe 0.4003340000 -1.3606740000 -0.4579400000
H -0.8496150000 3.5334000000 -0.9584970000
N 1.4033200000 -2.8583810000 -0.1596780000
H 1.1872010000 -3.7993390000 -0.5086290000
H 2.3645020000 -2.8353040000 0.1989430000
N -0.3064670000 -2.1257460000 -2.1981600000
H -1.1755260000 -1.6773560000 -2.5190240000
H -0.5158670000 -3.1300910000 -2.1325900000
H 0.3523700000 -2.0265350000 -2.9816170000
H -4.5667990000 -1.3694870000 -0.0050720000
H -4.1323920000 0.7382690000 -0.6607490000

[(bpyPy$_2$Me)Fe(NH$_2$)(NH$_3$)]$^{2+}$, multiplicity = 4
C -2.5608920000 2.1769040000 -0.9764550000
C -3.0538030000 0.9007430000 -0.6905690000
C -2.1418430000 -0.1203830000 -0.3962420000
N -0.7964660000 0.1147630000 -0.4256000000
C -0.3115440000 1.3687390000 -0.5720720000
C -1.1866020000 2.4241590000 -0.8822760000
C -3.8460600000 -1.9421020000 0.1423640000
C -2.5240650000 -1.4783290000 0.0485330000
C -4.0743870000 -3.2324940000 0.6367610000
C -2.9844950000 -4.0255830000 1.0209980000
C -1.6933160000 -3.5017030000 0.8848590000
N -1.4750680000 -2.2606540000 0.4160000000
C 1.1982740000 1.5896850000 -0.2994130000
C 1.4971260000 3.0995050000 -0.2302470000
C 2.0566000000 0.9263160000 -1.4038210000

C 1.5506790000 0.9084450000 1.0569990000
N 1.2986230000 -0.4211470000 1.2015830000
C 1.5781080000 -1.0510730000 2.3662670000
C 2.1344320000 -0.3852070000 3.4579490000
C 2.4182600000 0.9771670000 3.3257420000
C 2.1251060000 1.6248090000 2.1183810000
C 2.9831870000 1.6381980000 -2.1846840000
C 3.7628490000 0.9472750000 -3.1206520000
C 3.6154690000 -0.4390170000 -3.2450700000
C 2.6734430000 -1.0763460000 -2.4356550000
N 1.9031800000 -0.4042370000 -1.5555370000
H -3.2475370000 2.9901020000 -1.2284110000
H -5.0966750000 -3.6137150000 0.7182470000
H -3.1247650000 -5.0363850000 1.4135990000
H -0.7998940000 -4.0792890000 1.1448500000
H 0.8906120000 3.5825240000 0.5508760000
H 2.5593520000 3.2753090000 -0.0055160000
H 1.2726450000 3.5824690000 -1.1927710000
H 1.3424480000 -2.1187650000 2.4043990000
H 2.3399530000 -0.9329870000 4.3812940000
H 2.8634900000 1.5403270000 4.1515540000
H 2.3461510000 2.6870770000 2.0143190000
H 3.1067230000 2.7156090000 -2.0698410000
H 4.4861250000 1.4909420000 -3.7364100000
H 4.2163900000 -1.0211820000 -3.9490680000
H 2.5324340000 -2.1615170000 -2.4745670000
Fe 0.4178050000 -1.4587330000 -0.2914660000
H -0.8080790000 3.4343000000 -1.0383610000
N 1.4345920000 -2.9436960000 -0.0205750000
H 1.4191700000 -3.7619780000 -0.6393250000
H 2.3145700000 -2.9251000000 0.5076220000
N -0.2731640000 -2.2850580000 -2.1120950000
H -1.0933430000 -1.7929410000 -2.4895020000
H -0.5518710000 -3.2696940000 -2.0130100000
H 0.4256300000 -2.2688430000 -2.8648860000
H -4.6840300000 -1.3113760000 -0.1637270000
H -4.1284630000 0.7069190000 -0.6788060000

[(bpyPy$_2$Me)Fe(NH$_2$)(NH$_3$)]$^{2+}$, multiplicity = 6
C -2.5632960000 2.1674540000 -0.9918460000
C -3.0512850000 0.8899760000 -0.6981140000
C -2.1278490000 -0.1141810000 -0.3714000000
N -0.7964970000 0.1426150000 -0.3682480000
C -0.3166620000 1.3852400000 -0.5522580000
C -1.1914110000 2.4329100000 -0.8929520000
C -3.8261340000 -1.9063300000 0.2552620000

C -2.5009950000 -1.4849400000 0.0629190000
C -4.0658730000 -3.1973330000 0.7423780000
C -2.9812160000 -4.0365700000 1.0264750000
C -1.6872870000 -3.5570470000 0.7955100000
N -1.4566750000 -2.3160990000 0.3261340000
C 1.1994180000 1.5995600000 -0.2848220000
C 1.5033410000 3.1099740000 -0.2479930000
C 2.0549380000 0.9083880000 -1.3784860000
C 1.5493420000 0.9477180000 1.0858390000
N 1.3633320000 -0.3884330000 1.2252520000
C 1.6490110000 -1.0029490000 2.3931720000
C 2.1432810000 -0.3109440000 3.5003730000
C 2.3453720000 1.0667630000 3.3763460000
C 2.0473370000 1.7001880000 2.1619000000
C 2.9701560000 1.6199670000 -2.1740780000
C 3.7647050000 0.9328630000 -3.1001710000
C 3.6424190000 -0.4566760000 -3.2090820000
C 2.7106110000 -1.0995630000 -2.3934970000
N 1.9291540000 -0.4313200000 -1.5157870000
H -3.2549910000 2.9691920000 -1.2663370000
H -5.0925630000 -3.5398520000 0.9023760000
H -3.1260670000 -5.0476280000 1.4154840000
H -0.8026820000 -4.1727610000 0.9857530000
H 0.8882570000 3.6106810000 0.5147140000
H 2.5629640000 3.2901390000 -0.0135990000
H 1.2865910000 3.5753090000 -1.2211330000
H 1.4728720000 -2.0835480000 2.4253130000
H 2.3633620000 -0.8463430000 4.4278750000
H 2.7333070000 1.6533570000 4.2148920000
H 2.2073570000 2.7745260000 2.0669910000
H 3.0759340000 2.7005840000 -2.0738130000
H 4.4800530000 1.4836100000 -3.7190850000
H 4.2544230000 -1.0381120000 -3.9041690000
H 2.5802050000 -2.1865590000 -2.4186810000
Fe 0.4907530000 -1.6062340000 -0.3587940000
H -0.8222850000 3.4427310000 -1.0718580000
N 1.5320150000 -3.1738610000 -0.0729930000
H 1.3049880000 -4.1190450000 -0.4065540000
H 2.4148690000 -3.2360040000 0.4487550000
N -0.3303210000 -2.1936330000 -2.3324250000
H -1.0982830000 -1.5933430000 -2.6597360000
H -0.7043010000 -3.1509740000 -2.3147500000
H 0.3685780000 -2.1815270000 -3.0858050000
H -4.6609010000 -1.2359360000 0.0386420000
H -4.1243080000 0.6867520000 -0.7173320000

[(bpyPy$_2$Me)Fe(NH$_3$)(NH$_2$)]$^{2+}$, multiplicity = 2
C -2.5814980000 2.2060830000 -0.8621380000
C -3.0507210000 0.9114080000 -0.6133070000
C -2.1109740000 -0.1078200000 -0.4099400000
N -0.7809720000 0.1567660000 -0.5162310000
C -0.3096100000 1.4144360000 -0.6059720000
C -1.2053890000 2.4749750000 -0.8120330000
C -3.6599670000 -1.9994760000 0.2887560000
C -2.3804620000 -1.4744320000 0.0570630000
C -3.7849200000 -3.2780730000 0.8417110000
C -2.6222730000 -3.9963810000 1.1501030000
C -1.3761790000 -3.4234320000 0.8778980000
N -1.2432900000 -2.1910340000 0.3436350000
C 1.2015030000 1.5747590000 -0.3284180000
C 1.5762860000 3.0653770000 -0.2910440000
C 2.0317370000 0.8170770000 -1.3810450000
C 1.4611930000 0.8944100000 1.0446620000
N 1.0995380000 -0.4109440000 1.1725980000
C 1.2394120000 -1.0288920000 2.3675600000
C 1.7884540000 -0.3956660000 3.4818880000
C 2.1988740000 0.9349510000 3.3548860000
C 2.0234620000 1.5856310000 2.1275310000
C 3.0001810000 1.4501010000 -2.1746170000
C 3.7439140000 0.7054590000 -3.0972950000
C 3.5001490000 -0.6671800000 -3.2072930000
C 2.5229160000 -1.2373830000 -2.3930200000
N 1.8019550000 -0.5170390000 -1.4954570000
H -3.2890290000 3.0205150000 -1.0421770000
H -4.7741700000 -3.7046780000 1.0296990000
H -2.6663210000 -4.9965460000 1.5877850000
H -0.4589020000 -3.9766280000 1.0903210000
H 0.9903980000 3.5920880000 0.4769150000
H 2.6442790000 3.1968210000 -0.0618650000
H 1.3724360000 3.5378510000 -1.2642010000
H 0.8870400000 -2.0618370000 2.4336350000
H 1.8828900000 -0.9432720000 4.4232850000
H 2.6395810000 1.4702280000 4.2011890000
H 2.3234110000 2.6285300000 2.0218600000
H 3.1773430000 2.5213030000 -2.0748350000
H 4.5005350000 1.1961530000 -3.7169620000
H 4.0505830000 -1.2982050000 -3.9103570000
H 2.2876420000 -2.3023590000 -2.4640920000
Fe 0.3748430000 -1.3769330000 -0.4458040000
H -0.8445770000 3.4982680000 -0.9196940000
N 1.6034550000 -2.9434660000 -0.0440470000
H 1.3813060000 -3.7345280000 -0.6607610000

H 1.5671050000 -3.3104720000 0.9154240000
N -0.2345790000 -2.0924510000 -2.0220480000
H 0.0938490000 -1.7567580000 -2.9346900000
H -1.1635580000 -2.5165560000 -2.1277170000
H -4.5454980000 -1.4095770000 0.0406690000
H -4.1217670000 0.7041560000 -0.5529750000
H 2.5957150000 -2.7210270000 -0.2008960000

[(bpyPy$_2$Me)Fe(NH$_3$)(NH$_2$)]$^{2+}$, multiplicity = 4
C -2.5749440000 2.2152240000 -0.9192620000
C -3.0598310000 0.9353710000 -0.6237580000
C -2.1279550000 -0.0804940000 -0.3615070000
N -0.8049290000 0.1796310000 -0.4267610000
C -0.3203010000 1.4177900000 -0.5901260000
C -1.1976500000 2.4789440000 -0.8719800000
C -3.7480960000 -1.9175690000 0.3248200000
C -2.4425590000 -1.4526770000 0.1014410000
C -3.9373710000 -3.2081880000 0.8314760000
C -2.8160960000 -4.0025620000 1.1022040000
C -1.5439320000 -3.4799230000 0.8430830000
N -1.3571800000 -2.2362720000 0.3617800000
C 1.2008030000 1.5714070000 -0.3241000000
C 1.5617090000 3.0670950000 -0.2633540000
C 2.0301790000 0.8588500000 -1.4176670000
C 1.4864640000 0.8774070000 1.0398560000
N 1.1827620000 -0.4440680000 1.1749620000
C 1.3435190000 -1.0528930000 2.3720840000
C 1.8517700000 -0.3942390000 3.4910310000
C 2.2038610000 0.9519560000 3.3607800000
C 2.0105270000 1.5900770000 2.1292940000
C 2.9389550000 1.5452560000 -2.2391900000
C 3.6994900000 0.8375910000 -3.1780180000
C 3.5373730000 -0.5476150000 -3.2864590000
C 2.6010250000 -1.1674130000 -2.4600660000
N 1.8704140000 -0.4803780000 -1.5507570000
H -3.2748050000 3.0250080000 -1.1458820000
H -4.9479240000 -3.5865160000 1.0114450000
H -2.9138030000 -5.0157100000 1.5011840000
H -0.6470810000 -4.0799490000 1.0220970000
H 0.9707840000 3.5752260000 0.5136330000
H 2.6297680000 3.2081470000 -0.0398960000
H 1.3462490000 3.5531000000 -1.2266360000
H 1.0463700000 -2.1027070000 2.4298400000
H 1.9636250000 -0.9351230000 4.4342380000
H 2.6154650000 1.5102050000 4.2070210000
H 2.2669630000 2.6446050000 2.0270850000

H 3.0620900000 2.6249360000 -2.1520400000
H 4.4121380000 1.3701840000 -3.8152180000
H 4.1132290000 -1.1433650000 -3.9994900000
H 2.4083390000 -2.2425860000 -2.5216510000
Fe 0.4835820000 -1.4949610000 -0.4227410000
H -0.8307770000 3.4928070000 -1.0378980000
N 1.7922760000 -3.1532340000 0.1209950000
H 1.7333250000 -3.8621370000 -0.6199790000
H 1.6242100000 -3.6568610000 1.0008510000
N -0.1037420000 -2.2798830000 -1.9677340000
H 0.0897030000 -1.8382650000 -2.8750330000
H -1.0087940000 -2.7611240000 -2.0132400000
H -4.6058650000 -1.2761160000 0.1091400000
H -4.1345980000 0.7439130000 -0.5832460000
H 2.7766890000 -2.8584840000 0.1644980000

[(bpyPy$_2$Me)Fe(NH$_3$)(NH$_2$)]$^{2+}$, multiplicity = 6
C -2.5751695026 2.1727958726 -0.9295395171
C -3.0615640728 0.8987442183 -0.6202083321
C -2.1359164992 -0.1106654020 -0.3163891703
N -0.8046592568 0.1408547671 -0.3442386318
C -0.3218313873 1.3811651786 -0.5370572059
C -1.2002710230 2.4312456921 -0.8617081414
C -3.8303073578 -1.9103913103 0.2766925453
C -2.5035948080 -1.4781599589 0.1224085996
C -4.0779561074 -3.2023672486 0.7555195776
C -2.9958705735 -4.0328286528 1.0711113210
C -1.6996215351 -3.5408108582 0.8822496946
N -1.4582961942 -2.2986971931 0.4223910234
C 1.1993151418 1.5960423158 -0.2925861610
C 1.5003661858 3.1073016305 -0.2613830559
C 2.0444138299 0.9093139538 -1.3924084518
C 1.5593118428 0.9435715342 1.0748865678
N 1.3830095488 -0.3949253637 1.2111758486
C 1.6551973822 -0.9878264863 2.3925125208
C 2.1323795999 -0.2879812656 3.5023003518
C 2.3348004328 1.0883777760 3.3714096743
C 2.0436942344 1.7081408825 2.1491852592
C 2.9838071585 1.6110697534 -2.1675595550
C 3.7536336443 0.9245771445 -3.1151034072
C 3.5736407459 -0.4532443158 -3.2758862428
C 2.6150437151 -1.0863444041 -2.4839827050
N 1.8735537817 -0.4205968176 -1.5702589709
H -3.2690749409 2.9773567655 -1.1898442564
H -5.1066769520 -3.5525584372 0.8822496123
H -3.1426277420 -5.0458248667 1.4541162465

H -0.8278274110 -4.1629351778 1.1056805892
H 0.8856436764 3.6107199616 0.4995920703
H 2.5595492701 3.2909637244 -0.0281630243
H 1.2818490821 3.5672205380 -1.2369211570
H 1.4778487437 -2.0652871910 2.4539167066
H 2.3382394990 -0.8177637019 4.4362549245
H 2.7123029960 1.6829548969 4.2089662091
H 2.1962292082 2.7827702291 2.0465356059
H 3.1255473431 2.6841784966 -2.0371807391
H 4.4871655241 1.4685468535 -3.7184235766
H 4.1530117401 -1.0318383001 -4.0004938881
H 2.4112832547 -2.1576900480 -2.5822595037
Fe 0.4457123925 -1.6071061491 -0.4149627384
H -0.8305545359 3.4391332478 -1.0499385229
N 1.6266342585 -3.3362101446 0.1533965932
H 1.4180436029 -4.1193578638 -0.4792077232
H 1.5622239939 -3.7212797572 1.1044434172
N -0.1456260359 -2.3178302108 -2.1073372628
H 0.0186494639 -1.9247140751 -3.0422326327
H -0.7372504561 -3.1519051792 -2.2173083241
H -4.6622128834 -1.2470183763 0.0297912067
H -4.1360033263 0.7022864025 -0.6093353794
H 2.6262343077 -3.1317550798 0.0162811114

[(bpyPy$_2$Me)Fe(MeCN)(NH$_3$)]$^{3+}$, multiplicity = 2
C -2.5752200000 2.1884830000 -0.9954320000
C -3.0279790000 0.8939750000 -0.7222740000
C -2.0773860000 -0.1008500000 -0.4668970000
N -0.7450320000 0.1823460000 -0.5532910000
C -0.2949970000 1.4496970000 -0.6602260000
C -1.2061550000 2.4835500000 -0.9165180000
C -3.5954380000 -1.9989320000 0.2898250000
C -2.3316060000 -1.4534700000 0.0328170000
C -3.6814860000 -3.2734270000 0.8602520000
C -2.5027230000 -3.9706330000 1.1561570000
C -1.2701180000 -3.3862680000 0.8535050000
N -1.1835430000 -2.1534770000 0.3091460000
C 1.1998170000 1.6526520000 -0.3447630000
C 1.5381250000 3.1510320000 -0.2942320000
C 2.0695060000 0.9152720000 -1.3763110000
C 1.4466540000 0.9720340000 1.0289840000
N 1.1519370000 -0.3510060000 1.1315870000
C 1.3265020000 -1.0091980000 2.3012640000
C 1.8180700000 -0.3680350000 3.4371480000
C 2.1409290000 0.9894050000 3.3507280000
C 1.9521350000 1.6628990000 2.1372590000

C 3.0409690000 1.5641920000 -2.1495350000
C 3.8235780000 0.8262810000 -3.0447990000
C 3.6213470000 -0.5540730000 -3.1483430000
C 2.6393510000 -1.1435870000 -2.3573930000
N 1.8798790000 -0.4237230000 -1.4925910000
H -3.2916890000 2.9846900000 -1.2156680000
H -4.6590700000 -3.7158460000 1.0711510000
H -2.5233390000 -4.9647980000 1.6094110000
H -0.3335590000 -3.9120480000 1.0482900000
H 0.9157830000 3.6605060000 0.4566980000
H 2.5953750000 3.3027860000 -0.0317800000
H 1.3546730000 3.6196010000 -1.2726660000
H 1.0633950000 -2.0694380000 2.3197640000
H 1.9421490000 -0.9362300000 4.3622890000
H 2.5356020000 1.5274590000 4.2175090000
H 2.1980290000 2.7222890000 2.0596320000
H 3.1889470000 2.6401850000 -2.0568300000
H 4.5819860000 1.3292730000 -3.6518770000
H 4.2075870000 -1.1762000000 -3.8291310000
H 2.4472780000 -2.2167830000 -2.4125990000
Fe 0.4425640000 -1.3108620000 -0.4394630000
H -0.8603850000 3.5104700000 -1.0392620000
N 1.5818950000 -2.8424020000 -0.1667190000
N -0.2306230000 -2.0848560000 -2.1838530000
H -1.2566370000 -2.1241350000 -2.2547460000
H 0.1013940000 -3.0480870000 -2.3257180000
H 0.0839150000 -1.5380510000 -2.9964010000
H -4.4964430000 -1.4287700000 0.0524950000
H -4.0953180000 0.6665370000 -0.6811910000
C 2.2968210000 -3.7429520000 0.0213640000
C 3.1854390000 -4.8625520000 0.2515740000
H 3.2041990000 -5.0897370000 1.3309850000
H 4.2003000000 -4.5959910000 -0.0881480000
H 2.8192410000 -5.7395120000 -0.3077100000

[(bpyPy$_2$Me)Fe(MeCN)(NH$_3$)]$^{3+}$, multiplicity = 4
C -2.5652790000 2.1266200000 -1.0758820000
C -3.0267520000 0.8460270000 -0.7538270000
C -2.0902080000 -0.1388000000 -0.4188830000
N -0.7599790000 0.1530280000 -0.4473190000
C -0.2985850000 1.4100250000 -0.6266620000
C -1.2002910000 2.4256650000 -0.9795160000
C -3.7227240000 -1.9788100000 0.2363800000
C -2.4173960000 -1.4926800000 0.0780450000
C -3.9056340000 -3.2574960000 0.7801440000
C -2.7868990000 -4.0137560000 1.1502840000

C -1.5121160000 -3.4703060000 0.9503350000
N -1.3370730000 -2.2413560000 0.4316860000
C 1.2008780000 1.6592380000 -0.3317980000
C 1.4708110000 3.1733690000 -0.2608290000
C 2.0924430000 1.0013080000 -1.4130670000
C 1.5232140000 0.9840960000 1.0301160000
N 1.2811890000 -0.3491980000 1.1732550000
C 1.5248070000 -0.9895510000 2.3426540000
C 2.0379550000 -0.3165610000 3.4486350000
C 2.3164020000 1.0475660000 3.3242120000
C 2.0582310000 1.6978530000 2.1097020000
C 2.9853190000 1.7253760000 -2.2149810000
C 3.7981320000 1.0405160000 -3.1284300000
C 3.7116780000 -0.3530450000 -3.2175420000
C 2.7924260000 -1.0104500000 -2.4005370000
N 2.0007550000 -0.3428940000 -1.5326520000
H -3.2751470000 2.9091980000 -1.3580650000
H -4.9159300000 -3.6553690000 0.9121640000
H -2.8884920000 -5.0124120000 1.5828600000
H -0.6092160000 -4.0315970000 1.2088330000
H 0.8406080000 3.6432220000 0.5091430000
H 2.5263610000 3.3673560000 -0.0205070000
H 1.2504160000 3.6483940000 -1.2279240000
H 1.2960340000 -2.0569250000 2.3795240000
H 2.2159500000 -0.8647350000 4.3769250000
H 2.7310700000 1.6121570000 4.1644450000
H 2.2728700000 2.7619540000 2.0119150000
H 3.0573430000 2.8103020000 -2.1340780000
H 4.4985290000 1.5977940000 -3.7577060000
H 4.3383740000 -0.9281840000 -3.9038750000
H 2.6891730000 -2.0992140000 -2.4331770000
Fe 0.5245800000 -1.3504280000 -0.3336980000
H -0.8498190000 3.4413060000 -1.1641310000
N 1.6055050000 -2.9639880000 -0.0023580000
N -0.1009330000 -2.1346350000 -2.1081150000
H -1.0090850000 -2.6098120000 -2.0209790000
H 0.5441660000 -2.8421820000 -2.4843460000
H -0.2132240000 -1.4142900000 -2.8344290000
H -4.5837820000 -1.3728520000 -0.0541450000
H -4.0956690000 0.6234920000 -0.7438170000
C 2.2752690000 -3.9094520000 0.1254800000
C 3.1070320000 -5.0813190000 0.2868900000
H 3.1925590000 -5.3173900000 1.3610170000
H 4.1079370000 -4.8673020000 -0.1255290000
H 2.6528430000 -5.9291880000 -0.2523700000

[(bpyPy$_2$Me)Fe(MeCN)(NH$_3$)]$^{3+}$, multiplicity = 6
C -2.5959630000 2.1666360000 -0.9796670000
C -3.0549660000 0.8780640000 -0.6868670000
C -2.1100880000 -0.1080370000 -0.3783730000
N -0.7824690000 0.1847340000 -0.3981580000
C -0.3235220000 1.4410190000 -0.5733580000
C -1.2288610000 2.4643400000 -0.8957020000
C -3.7321670000 -1.9605360000 0.2550180000
C -2.4298460000 -1.4840880000 0.0567290000
C -3.9146180000 -3.2645000000 0.7348990000
C -2.7948710000 -4.0601600000 1.0056110000
C -1.5219050000 -3.5308880000 0.7721100000
N -1.3468270000 -2.2749680000 0.3121530000
C 1.1849260000 1.6863570000 -0.3108170000
C 1.4644770000 3.2008020000 -0.2902840000
C 2.0539440000 0.9929590000 -1.3877350000
C 1.5431610000 1.0493350000 1.0633460000
N 1.3701730000 -0.2899390000 1.2106210000
C 1.6576630000 -0.9018150000 2.3823490000
C 2.1436010000 -0.1974700000 3.4836710000
C 2.3364010000 1.1805530000 3.3516450000
C 2.0337670000 1.8080640000 2.1341700000
C 2.9872980000 1.6902110000 -2.1685760000
C 3.7946460000 0.9907310000 -3.0749660000
C 3.6633690000 -0.3976320000 -3.1846230000
C 2.7052030000 -1.0315320000 -2.3960030000
N 1.9207480000 -0.3483560000 -1.5292640000
H -3.3085290000 2.9551800000 -1.2377660000
H -4.9251400000 -3.6504510000 0.8967910000
H -2.8936350000 -5.0793100000 1.3876830000
H -0.6199940000 -4.1211910000 0.9540950000
H 0.8397870000 3.6979630000 0.4668810000
H 2.5205020000 3.3980060000 -0.0552650000
H 1.2423840000 3.6484900000 -1.2702020000
H 1.4928330000 -1.9822830000 2.4291020000
H 2.3647610000 -0.7278190000 4.4132550000
H 2.7200220000 1.7739570000 4.1870010000
H 2.1820730000 2.8832090000 2.0331860000
H 3.0963310000 2.7706210000 -2.0734450000
H 4.5235470000 1.5330650000 -3.6846410000
H 4.2802240000 -0.9860600000 -3.8684500000
H 2.5567360000 -2.1140340000 -2.4534120000
Fe 0.5143880000 -1.4522870000 -0.3579720000
H -0.8848320000 3.4843290000 -1.0672790000
N 1.6356250000 -3.1278410000 0.0690210000
N -0.1563390000 -2.1692850000 -2.3144570000

H -1.1739200000 -2.3175210000 -2.3450330000
H 0.2589980000 -3.0771340000 -2.5658290000
H 0.0570000000 -1.5259650000 -3.0881230000
H -4.5938720000 -1.3229370000 0.0462180000
H -4.1232040000 0.6522640000 -0.6883220000
C 2.3293490000 -4.0555630000 0.2101240000
C 3.1886610000 -5.2016340000 0.3873350000
H 3.2745530000 -5.4226590000 1.4648930000
H 4.1842150000 -4.9715180000 -0.0291500000
H 2.7508290000 -6.0657960000 -0.1406960000

[(bpyPy$_2$Me)Fe(NH$_3$)(NHNH$_2$)]$^{2+}$, multiplicity = 2
C -2.5496380000 2.1879910000 -1.0197640000
C -3.0083550000 0.8844470000 -0.7958490000
C -2.0641170000 -0.1218330000 -0.5501080000
N -0.7286550000 0.1558850000 -0.6089910000
C -0.2793910000 1.4270080000 -0.6612180000
C -1.1805060000 2.4759000000 -0.8983000000
C -3.6107860000 -2.0053310000 0.1794100000
C -2.3312090000 -1.4734320000 -0.0410100000
C -3.7405250000 -3.2464570000 0.8112220000
C -2.5813510000 -3.9217100000 1.2171330000
C -1.3343150000 -3.3477250000 0.9502350000
N -1.1938310000 -2.1579740000 0.3239560000
C 1.2196960000 1.5988920000 -0.3318300000
C 1.5783200000 3.0921770000 -0.2614460000
C 2.0732940000 0.8686850000 -1.3825780000
C 1.4600810000 0.8946490000 1.0322440000
N 1.1424450000 -0.4294090000 1.1226090000
C 1.2991550000 -1.0688270000 2.3066350000
C 1.8060440000 -0.4423680000 3.4437680000
C 2.1599140000 0.9084250000 3.3577890000
C 1.9773980000 1.5790080000 2.1424750000
C 3.0502220000 1.5198240000 -2.1516750000
C 3.8014000000 0.7978220000 -3.0860120000
C 3.5526820000 -0.5712440000 -3.2324700000
C 2.5689670000 -1.1598780000 -2.4399950000
N 1.8411470000 -0.4633860000 -1.5261100000
H -3.2601650000 2.9923390000 -1.2308240000
H -4.7307230000 -3.6751910000 0.9896780000
H -2.6284790000 -4.8886140000 1.7240240000
H -0.4179360000 -3.8688490000 1.2398190000
H 0.9655510000 3.6027060000 0.4966740000
H 2.6383540000 3.2316640000 -0.0017560000
H 1.3956090000 3.5770380000 -1.2327750000
H 0.9944210000 -2.1178870000 2.3384790000

H 1.9142880000 -1.0105830000 4.3715980000
H 2.5659190000 1.4403650000 4.2234090000
H 2.2390760000 2.6349230000 2.0659590000
H 3.2270890000 2.5882140000 -2.0230900000
H 4.5652080000 1.3010470000 -3.6865390000
H 4.1062400000 -1.1861410000 -3.9475040000
H 2.3402880000 -2.2235220000 -2.5390950000
Fe 0.4287240000 -1.3398260000 -0.4758980000
H -0.8304120000 3.5057940000 -0.9792350000
N 1.6302770000 -2.9514850000 -0.1790830000
H 1.4726290000 -3.6878540000 -0.8826940000
H 1.5411870000 -3.4239260000 0.7295640000
N -0.1879550000 -2.0947890000 -2.1219910000
N -0.4392110000 -3.4039800000 -2.3632170000
H -0.0550330000 -1.6020560000 -3.0141340000
H 2.6282840000 -2.7096300000 -0.2438150000
H -4.4951820000 -1.4456760000 -0.1349240000
H -4.0780700000 0.6610390000 -0.7822150000
H -0.8600010000 -3.6149960000 -3.2736490000
H -0.8992090000 -3.8921550000 -1.5880770000

[(bpyPy$_2$Me)Fe(NH$_3$)(NHNH$_2$)]$^{2+}$, multiplicity = 4
C -2.5264280000 2.1720960000 -1.0319420000
C -3.0142800000 0.8955150000 -0.7316900000
C -2.0951900000 -0.1174970000 -0.4232080000
N -0.7600420000 0.1343920000 -0.4441010000
C -0.2787540000 1.3838280000 -0.6034250000
C -1.1538490000 2.4333350000 -0.9355950000
C -3.7893350000 -1.9502020000 0.0666630000
C -2.4670770000 -1.4749170000 0.0442870000
C -4.0478530000 -3.2211900000 0.5937940000
C -2.9809050000 -3.9807580000 1.0904400000
C -1.6890590000 -3.4411170000 1.0245760000
N -1.4327070000 -2.2238420000 0.5131810000
C 1.2329750000 1.5921230000 -0.3201190000
C 1.5334640000 3.1008390000 -0.2292750000
C 2.0920560000 0.9447320000 -1.4357060000
C 1.5578710000 0.8916540000 1.0299240000
N 1.2706940000 -0.4349550000 1.1628920000
C 1.4931950000 -1.0540600000 2.3478830000
C 2.0379610000 -0.4018300000 3.4518210000
C 2.3658160000 0.9515460000 3.3237050000
C 2.1174920000 1.5979170000 2.1073460000
C 3.0079130000 1.6740420000 -2.2137440000
C 3.7636050000 1.0080720000 -3.1876760000
C 3.5874610000 -0.3684570000 -3.3695670000

C 2.6501680000 -1.0222610000 -2.5672230000
N 1.9282500000 -0.3802840000 -1.6251790000
H -3.2181910000 2.9765460000 -1.2983080000
H -5.0702450000 -3.6104600000 0.6157150000
H -3.1364260000 -4.9744280000 1.5187670000
H -0.8300360000 -4.0071120000 1.4024800000
H 0.9200340000 3.5745440000 0.5519660000
H 2.5935000000 3.2760940000 0.0060600000
H 1.3149000000 3.5963060000 -1.1870490000
H 1.2122780000 -2.1090010000 2.4060710000
H 2.1971720000 -0.9515380000 4.3832630000
H 2.8030260000 1.5062180000 4.1594250000
H 2.3619360000 2.6552640000 2.0056230000
H 3.1410330000 2.7469750000 -2.0698760000
H 4.4819850000 1.5660630000 -3.7966050000
H 4.1562970000 -0.9285290000 -4.1170100000
H 2.4604980000 -2.0951190000 -2.6786440000
Fe 0.5031360000 -1.4444210000 -0.3592320000
H -0.7808370000 3.4427340000 -1.1101270000
N 1.7307960000 -3.0762850000 -0.0747630000
H 1.6094890000 -3.7431760000 -0.8533460000
H 1.5557670000 -3.6171530000 0.7827930000
N -0.1485560000 -2.2681520000 -1.9392050000
N -0.2261200000 -3.6173340000 -2.1651760000
H -0.0432890000 -1.7819140000 -2.8389680000
H 2.7293620000 -2.8312370000 -0.0383930000
H -4.6070000000 -1.3392660000 -0.3233100000
H -4.0892680000 0.7008760000 -0.7178760000
H -0.5816120000 -3.8653360000 -3.0947310000
H -0.7442200000 -4.1107750000 -1.4287970000

[(bpyPy$_2$Me)Fe(NH$_3$)(NHNH$_2$)]$^{2+}$, multiplicity = 6
C -2.5552740000 2.1671830000 -0.9621470000
C -3.0265410000 0.8809750000 -0.6847880000
C -2.0915730000 -0.1236540000 -0.3894580000
N -0.7598510000 0.1395250000 -0.3999700000
C -0.2952440000 1.3942720000 -0.5622050000
C -1.1836460000 2.4397500000 -0.8714430000
C -3.7826740000 -1.9410910000 0.1497490000
C -2.4546310000 -1.4974860000 0.0292880000
C -4.0357330000 -3.2356970000 0.6161490000
C -2.9548850000 -4.0591860000 0.9568370000
C -1.6586760000 -3.5553260000 0.8042810000
N -1.4078180000 -2.3101830000 0.3510030000
C 1.2215810000 1.6276220000 -0.3062340000
C 1.5093870000 3.1417560000 -0.2873780000

C 2.0835530000 0.9389060000 -1.3934040000
C 1.5799740000 0.9953710000 1.0729900000
N 1.4323290000 -0.3456600000 1.2181310000
C 1.7253270000 -0.9270490000 2.4014280000
C 2.1859360000 -0.2102360000 3.5067440000
C 2.3473090000 1.1721220000 3.3710090000
C 2.0411610000 1.7779750000 2.1458020000
C 3.0343420000 1.6420640000 -2.1545580000
C 3.8158440000 0.9569220000 -3.0933610000
C 3.6360900000 -0.4205450000 -3.2590360000
C 2.6663190000 -1.0528140000 -2.4795130000
N 1.9125630000 -0.3905310000 -1.5741580000
H -3.2562140000 2.9683420000 -1.2141550000
H -5.0649840000 -3.5933160000 0.7151350000
H -3.1036360000 -5.0747670000 1.3325220000
H -0.7891730000 -4.1695530000 1.0585200000
H 0.8848140000 3.6481790000 0.4634840000
H 2.5647870000 3.3375390000 -0.0463450000
H 1.2948820000 3.5906280000 -1.2691570000
H 1.5794250000 -2.0104500000 2.4628330000
H 2.4110670000 -0.7299660000 4.4420580000
H 2.7079170000 1.7802550000 4.2063440000
H 2.1665950000 2.8558180000 2.0385280000
H 3.1753370000 2.7149590000 -2.0213590000
H 4.5579110000 1.5011850000 -3.6860270000
H 4.2246140000 -0.9981000000 -3.9772090000
H 2.4667600000 -2.1248020000 -2.5812360000
Fe 0.5191620000 -1.5668340000 -0.3568110000
H -0.8253190000 3.4562700000 -1.0340180000
N 1.6819680000 -3.3565960000 0.0745070000
H 1.5086930000 -4.1013290000 -0.6142540000
H 1.5940240000 -3.8098180000 0.9937100000
N -0.1061910000 -2.3116700000 -2.2060950000
N -0.5044880000 -3.5632680000 -2.5375830000
H -0.0030510000 -1.7639880000 -3.0702470000
H 2.6837380000 -3.1362170000 -0.0116640000
H -4.6126740000 -1.2818710000 -0.1142900000
H -4.0985210000 0.6707920000 -0.6887160000
H -1.0192110000 -3.6659050000 -3.4182080000
H -0.9245440000 -4.0913940000 -1.7672130000

[(bpyPy$_2$Me)Fe(NHNH$_2$)(NH$_3$)]$^{2+}$, multiplicity = 2
C -2.5622260000 2.2256970000 -0.9490980000
C -3.0164990000 0.9215810000 -0.7258320000
C -2.0673650000 -0.0878320000 -0.5115780000
N -0.7309750000 0.1838220000 -0.6036510000

C -0.2853410000 1.4579620000 -0.6533860000
C -1.1894560000 2.5098450000 -0.8573410000
C -3.5946040000 -1.9844080000 0.2387660000
C -2.3239230000 -1.4474970000 -0.0184720000
C -3.6967510000 -3.2417480000 0.8423330000
C -2.5206110000 -3.9270460000 1.1788540000
C -1.2849600000 -3.3480500000 0.8764270000
N -1.1737860000 -2.1404060000 0.2793400000
C 1.2179210000 1.6250530000 -0.3456890000
C 1.5794180000 3.1168630000 -0.2582810000
C 2.0585080000 0.9103650000 -1.4174260000
C 1.4709000000 0.9029320000 1.0087380000
N 1.1752270000 -0.4280070000 1.0813400000
C 1.3489590000 -1.0898330000 2.2518500000
C 1.8381440000 -0.4679290000 3.3994690000
C 2.1634370000 0.8915720000 3.3363590000
C 1.9743180000 1.5782570000 2.1310010000
C 2.9997540000 1.5781960000 -2.2157230000
C 3.7481920000 0.8650320000 -3.1590900000
C 3.5431660000 -0.5142430000 -3.2766240000
C 2.5952860000 -1.1209660000 -2.4551060000
N 1.8560780000 -0.4280660000 -1.5472540000
H -3.2763100000 3.0332560000 -1.1343580000
H -4.6785840000 -3.6754570000 1.0531730000
H -2.5486400000 -4.9061190000 1.6647180000
H -0.3490410000 -3.8632540000 1.1094510000
H 0.9776270000 3.6174610000 0.5154060000
H 2.6434950000 3.2507290000 -0.0115640000
H 1.3837350000 3.6162210000 -1.2195830000
H 1.0860270000 -2.1501280000 2.2451210000
H 1.9589640000 -1.0480600000 4.3182760000
H 2.5555070000 1.4180040000 4.2118130000
H 2.2177550000 2.6396380000 2.0713900000
H 3.1506940000 2.6526970000 -2.1059960000
H 4.4807410000 1.3820930000 -3.7861240000
H 4.1061000000 -1.1227550000 -3.9896000000
H 2.4092200000 -2.1972900000 -2.5033700000
Fe 0.4460430000 -1.3158680000 -0.5046280000
H -0.8406720000 3.5407950000 -0.9329080000
N 1.5114070000 -2.8759040000 -0.2944060000
H 1.1821890000 -3.8277210000 -0.4977500000
N -0.2911110000 -2.0701450000 -2.2476690000
H -1.2654410000 -1.7902160000 -2.4276510000
H -0.2892330000 -3.0976500000 -2.2940050000
H 0.2328520000 -1.7544420000 -3.0741420000
N 2.7663320000 -2.9448440000 0.2185500000

H -4.4907320000 -1.4159230000 -0.0225540000
H -4.0855110000 0.6987680000 -0.6860630000
H 3.3212070000 -3.7603270000 -0.0595280000
H 3.2824010000 -2.0621020000 0.1734480000

[(bpyPy$_2$Me)Fe(NHNH$_2$)(NH$_3$)]$^{2+}$, multiplicity = 4
C -2.5639220000 2.1565130000 -0.8642230000
C -3.0063490000 0.8566760000 -0.6062010000
C -2.0505400000 -0.1427210000 -0.3805060000
N -0.7125590000 0.1343180000 -0.4571080000
C -0.2718360000 1.4096560000 -0.5807530000
C -1.1926330000 2.4441850000 -0.8125870000
C -3.6332940000 -2.0311230000 0.2588590000
C -2.3432420000 -1.5195710000 0.0419920000
C -3.7762730000 -3.3309700000 0.7537300000
C -2.6273330000 -4.0884250000 1.0261000000
C -1.3737370000 -3.5287690000 0.7674170000
N -1.2286560000 -2.2781130000 0.2793080000
C 1.2397220000 1.6580820000 -0.3499740000
C 1.5212600000 3.1721270000 -0.3317780000
C 2.0933290000 0.9668500000 -1.4382100000
C 1.5974910000 1.0220210000 1.0280050000
N 1.3735670000 -0.3072940000 1.1834340000
C 1.6077590000 -0.8925160000 2.3792160000
C 2.1039440000 -0.1890260000 3.4777670000
C 2.3715470000 1.1753310000 3.3230530000
C 2.1132660000 1.7852010000 2.0889940000
C 3.0327570000 1.6643430000 -2.2176600000
C 3.7982550000 0.9698850000 -3.1617410000
C 3.6196160000 -0.4110900000 -3.3026170000
C 2.6725580000 -1.0389930000 -2.4935250000
N 1.9246140000 -0.3652210000 -1.5923420000
H -3.2835560000 2.9556120000 -1.0637110000
H -4.7732750000 -3.7452300000 0.9302660000
H -2.6937550000 -5.1039090000 1.4256970000
H -0.4537010000 -4.0900330000 0.9542510000
H 0.9172200000 3.6723770000 0.4402140000
H 2.5823520000 3.3687940000 -0.1188870000
H 1.2806170000 3.6231050000 -1.3063680000
H 1.3961110000 -1.9651940000 2.4435030000
H 2.2763000000 -0.7077880000 4.4247680000
H 2.7719460000 1.7670790000 4.1520230000
H 2.3125550000 2.8501310000 1.9654490000
H 3.1734560000 2.7387060000 -2.0960120000
H 4.5284730000 1.5068330000 -3.7752760000
H 4.1991910000 -0.9967790000 -4.0215320000

H 2.4962580000 -2.1175660000 -2.5452500000
Fe 0.4814360000 -1.3997230000 -0.4195650000
H -0.8528860000 3.4717800000 -0.9437170000
N 1.4944720000 -2.9873000000 -0.4513790000
H 1.0774400000 -3.7981900000 -0.9275030000
N -0.3354740000 -2.0309360000 -2.4843840000
H -1.3504360000 -2.1948010000 -2.4913580000
H 0.0745830000 -2.8818250000 -2.8906140000
H -0.1759370000 -1.2923540000 -3.1809820000
N 2.2638600000 -3.4380540000 0.5797660000
H -4.5125530000 -1.4167480000 0.0510490000
H -4.0731290000 0.6248530000 -0.5672800000
H 2.5950680000 -4.4025620000 0.4810110000
H 3.0138820000 -2.7890320000 0.8365400000

[(bpyPy$_2$Me)Fe(NHNH$_2$)(NH$_3$)]$^{2+}$, multiplicity = 6
C -2.5581420000 2.1780390000 -0.9619830000
C -3.0290380000 0.8925020000 -0.6793410000
C -2.0931010000 -0.1070110000 -0.3697740000
N -0.7628600000 0.1630350000 -0.3773820000
C -0.2989670000 1.4144300000 -0.5518860000
C -1.1873990000 2.4565310000 -0.8700810000
C -3.7786080000 -1.9092300000 0.2546080000
C -2.4535710000 -1.4844250000 0.0582790000
C -4.0169830000 -3.2031150000 0.7325630000
C -2.9299510000 -4.0436230000 1.0068230000
C -1.6384950000 -3.5599890000 0.7722190000
N -1.4060170000 -2.3176590000 0.3081700000
C 1.2213360000 1.6392230000 -0.3034910000
C 1.5115170000 3.1526840000 -0.2617180000
C 2.0635280000 0.9673360000 -1.4202120000
C 1.5861040000 0.9878930000 1.0647070000
N 1.4530600000 -0.3569530000 1.1908910000
C 1.7410380000 -0.9635250000 2.3626050000
C 2.1838960000 -0.2590150000 3.4841140000
C 2.3315340000 1.1267000000 3.3718810000
C 2.0306720000 1.7541490000 2.1550480000
C 2.9405440000 1.7016460000 -2.2386800000
C 3.7090930000 1.0378230000 -3.2028920000
C 3.5964080000 -0.3508550000 -3.3306520000
C 2.7028010000 -1.0154990000 -2.4895730000
N 1.9506070000 -0.3726840000 -1.5695370000
H -3.2606420000 2.9752650000 -1.2222630000
H -5.0430940000 -3.5476530000 0.8924050000
H -3.0725930000 -5.0585730000 1.3874960000
H -0.7562540000 -4.1826110000 0.9552590000

H 0.8972530000 3.6444610000 0.5075780000
H 2.5714350000 3.3414830000 -0.0339740000
H 1.2815890000 3.6206620000 -1.2303490000
H 1.6165060000 -2.0512550000 2.3866620000
H 2.4068730000 -0.7906000000 4.4131780000
H 2.6784850000 1.7240320000 4.2208480000
H 2.1444130000 2.8351070000 2.0703120000
H 3.0355910000 2.7824530000 -2.1317950000
H 4.3941090000 1.6059850000 -3.8400560000
H 4.1850480000 -0.9129640000 -4.0608770000
H 2.5749670000 -2.1025560000 -2.5357480000
Fe 0.5147480000 -1.5407750000 -0.3908030000
H -0.8311440000 3.4731480000 -1.0390270000
N 1.6994360000 -3.1615510000 -0.2246300000
H 1.3515410000 -4.1049350000 -0.4387920000
N -0.3129890000 -2.2075040000 -2.3629880000
H -1.2787790000 -1.9007950000 -2.5380590000
H -0.3291850000 -3.2307410000 -2.4636320000
H 0.2289650000 -1.8611660000 -3.1640020000
N 2.9245650000 -3.2850150000 0.3627900000
H -4.6150900000 -1.2377440000 0.0482790000
H -4.1002660000 0.6799740000 -0.6924290000
H 3.4727720000 -4.1016190000 0.0722140000
H 3.4725660000 -2.4203180000 0.3370670000

[(bpyPy$_2$Me)Fe(MeCN)(NH$_2$)]$^{2+}$, multiplicity = 2
C -2.5765020000 2.2143490000 -0.9239790000
C -3.0272850000 0.9114830000 -0.6848210000
C -2.0747130000 -0.0931660000 -0.4723320000
N -0.7465140000 0.1920660000 -0.5625180000
C -0.2958820000 1.4578790000 -0.6403340000
C -1.2063690000 2.5047410000 -0.8539930000
C -3.6005400000 -2.0093520000 0.2209930000
C -2.3296420000 -1.4630680000 -0.0070510000
C -3.7031990000 -3.2882290000 0.7789080000
C -2.5294630000 -3.9841920000 1.0964710000
C -1.2914360000 -3.3920280000 0.8267720000
N -1.1841750000 -2.1596540000 0.2871930000
C 1.2062370000 1.6416090000 -0.3426020000
C 1.5566080000 3.1375310000 -0.2868280000
C 2.0616200000 0.9063290000 -1.3913180000
C 1.4633520000 0.9509200000 1.0271770000
N 1.1349990000 -0.3643280000 1.1359600000
C 1.3071990000 -1.0076150000 2.3131890000
C 1.8372850000 -0.3767980000 3.4383580000
C 2.1983040000 0.9705930000 3.3382310000

C 2.0041610000 1.6390160000 2.1230250000
C 3.0270990000 1.5600930000 -2.1718940000
C 3.8012470000 0.8286430000 -3.0796980000
C 3.5955360000 -0.5507650000 -3.1842410000
C 2.6184590000 -1.1417750000 -2.3848040000
N 1.8623420000 -0.4308860000 -1.5107760000
H -3.2950480000 3.0175670000 -1.1107340000
H -4.6854960000 -3.7323070000 0.9638860000
H -2.5591800000 -4.9828550000 1.5401880000
H -0.3574310000 -3.9176230000 1.0376050000
H 0.9525730000 3.6478360000 0.4786860000
H 2.6195350000 3.2833260000 -0.0435810000
H 1.3571660000 3.6151170000 -1.2582350000
H 1.0079840000 -2.0582050000 2.3424880000
H 1.9579020000 -0.9399360000 4.3674760000
H 2.6213400000 1.5040210000 4.1947840000
H 2.2744800000 2.6918500000 2.0358860000
H 3.1784360000 2.6355730000 -2.0751150000
H 4.5545360000 1.3341120000 -3.6914380000
H 4.1765070000 -1.1709880000 -3.8720070000
H 2.4157260000 -2.2138390000 -2.4371040000
Fe 0.4301380000 -1.3244030000 -0.4859370000
H -0.8600670000 3.5343360000 -0.9512070000
N 1.5928580000 -2.8115780000 -0.1073600000
N -0.1713130000 -2.0192930000 -2.0757130000
H -1.0336820000 -2.5639780000 -2.1900920000
H 0.2025620000 -1.7475660000 -2.9919590000
H -4.4960880000 -1.4366110000 -0.0317930000
H -4.0952360000 0.6863730000 -0.6384280000
C 2.3266920000 -3.6913760000 0.1045080000
C 3.2375390000 -4.7935490000 0.3632680000
H 3.2654340000 -5.0016800000 1.4457980000
H 4.2486520000 -4.5254470000 0.0142850000
H 2.8879620000 -5.6907040000 -0.1742790000

[(bpyPy$_2$Me)Fe(MeCN)(NH$_2$)]$^{2+}$, multiplicity = 4
C -2.5867440000 2.2428960000 -0.9736560000
C -3.0517180000 0.9541650000 -0.6832550000
C -2.1025730000 -0.0434520000 -0.4124210000
N -0.7855650000 0.2437310000 -0.4650600000
C -0.3206840000 1.4886340000 -0.6254850000
C -1.2148100000 2.5334470000 -0.9147810000
C -3.6762830000 -1.9204380000 0.2785700000
C -2.3846660000 -1.4228490000 0.0473040000
C -3.8292830000 -3.2139560000 0.7905500000
C -2.6867830000 -3.9780380000 1.0594120000

C -1.4288460000 -3.4269570000 0.7909040000
N -1.2784530000 -2.1806650000 0.3025850000
C 1.1951350000 1.6597880000 -0.3419180000
C 1.5403780000 3.1590220000 -0.2865290000
C 2.0532900000 0.9441840000 -1.4115540000
C 1.4704590000 0.9742670000 1.0292470000
N 1.2110180000 -0.3570950000 1.1512220000
C 1.3904550000 -0.9763380000 2.3401420000
C 1.8581170000 -0.3066400000 3.4707640000
C 2.1502920000 1.0556030000 3.3594070000
C 1.9503070000 1.6981570000 2.1308670000
C 2.9714800000 1.6316190000 -2.2211020000
C 3.7714920000 0.9224950000 -3.1254800000
C 3.6409570000 -0.4677720000 -3.2122570000
C 2.6921970000 -1.0918930000 -2.4044290000
N 1.9217980000 -0.4009810000 -1.5306370000
H -3.2996580000 3.0393440000 -1.2067990000
H -4.8290910000 -3.6167940000 0.9772040000
H -2.7572040000 -4.9911500000 1.4642390000
H -0.5115880000 -3.9968150000 0.9652380000
H 0.9299320000 3.6667580000 0.4755050000
H 2.6025550000 3.3132220000 -0.0445780000
H 1.3365250000 3.6360640000 -1.2570510000
H 1.1529240000 -2.0427150000 2.3718820000
H 1.9876600000 -0.8520380000 4.4091800000
H 2.5259630000 1.6219610000 4.2169470000
H 2.1681330000 2.7624890000 2.0405550000
H 3.0723260000 2.7146980000 -2.1491940000
H 4.4916240000 1.4577080000 -3.7519200000
H 4.2509770000 -1.0641520000 -3.8956650000
H 2.5198580000 -2.1712290000 -2.4463300000
Fe 0.5299200000 -1.4051550000 -0.4577380000
H -0.8657620000 3.5541500000 -1.0775740000
N 1.7293690000 -3.0723950000 0.1497200000
N -0.0335300000 -2.1737980000 -2.0218030000
H -0.9022530000 -2.7154610000 -2.0847070000
H 0.1646730000 -1.7327470000 -2.9278700000
H -4.5509490000 -1.3009650000 0.0665170000
H -4.1229470000 0.7417780000 -0.6544210000
C 2.4771270000 -3.9638910000 0.2223490000
C 3.4050760000 -5.0772900000 0.3128030000
H 3.5599540000 -5.3418160000 1.3718830000
H 4.3683450000 -4.7853360000 -0.1378560000
H 2.9922810000 -5.9437930000 -0.2299620000

[(bpyPy$_2$Me)Fe(MeCN)(NH$_2$)]$^{2+}$, multiplicity = 6

C -2.5906420000 2.1900580000 -0.9586400000
C -3.0497220000 0.9026020000 -0.6629910000
C -2.1030000000 -0.0876860000 -0.3638940000
N -0.7774470000 0.1945180000 -0.3841120000
C -0.3212330000 1.4465420000 -0.5639920000
C -1.2224410000 2.4790960000 -0.8826080000
C -3.7521210000 -1.9401170000 0.2025530000
C -2.4379520000 -1.4676820000 0.0618210000
C -3.9636580000 -3.2433390000 0.6690660000
C -2.8595830000 -4.0438550000 0.9872220000
C -1.5767650000 -3.5128620000 0.8127000000
N -1.3719150000 -2.2598960000 0.3640950000
C 1.1928510000 1.6918780000 -0.3119400000
C 1.4643520000 3.2084490000 -0.2740650000
C 2.0596180000 1.0244840000 -1.4077890000
C 1.5610830000 1.0420130000 1.0557780000
N 1.4222140000 -0.3015020000 1.1817330000
C 1.7182730000 -0.9029000000 2.3531750000
C 2.1754970000 -0.1988340000 3.4689850000
C 2.3322620000 1.1850200000 3.3528170000
C 2.0224210000 1.8099220000 2.1373430000
C 2.9788980000 1.7482320000 -2.1862430000
C 3.7798180000 1.0757490000 -3.1177970000
C 3.6534830000 -0.3103950000 -3.2575980000
C 2.7096280000 -0.9660360000 -2.4666750000
N 1.9339580000 -0.3120640000 -1.5735010000
H -3.3016970000 2.9809880000 -1.2146250000
H -4.9823460000 -3.6255970000 0.7834840000
H -2.9797280000 -5.0642750000 1.3606090000
H -0.6834260000 -4.1046150000 1.0343730000
H 0.8373320000 3.6959100000 0.4876900000
H 2.5193380000 3.4109080000 -0.0370610000
H 1.2396920000 3.6677960000 -1.2482050000
H 1.5831820000 -1.9881950000 2.3899950000
H 2.4022880000 -0.7311640000 4.3966010000
H 2.6920280000 1.7822270000 4.1964000000
H 2.1424000000 2.8895750000 2.0462170000
H 3.0817030000 2.8274720000 -2.0715130000
H 4.4983460000 1.6364790000 -3.7236810000
H 4.2632440000 -0.8779420000 -3.9656240000
H 2.5506690000 -2.0464670000 -2.5444080000
Fe 0.5145860000 -1.5121740000 -0.4407300000
H -0.8746390000 3.4971380000 -1.0593150000
N 1.6674490000 -3.1783270000 0.1673340000
N -0.0484320000 -2.2365590000 -2.1400950000
H -0.7135310000 -3.0143920000 -2.2405550000

H 0.1966130000 -1.9072680000 -3.0820590000
H -4.6018260000 -1.2999630000 -0.0451050000
H -4.1192090000 0.6813450000 -0.6586400000
C 2.3698880000 -4.0998380000 0.2944780000
C 3.2424690000 -5.2476460000 0.4517300000
H 3.3365630000 -5.4924820000 1.5226840000
H 4.2361700000 -5.0053700000 0.0391250000
H 2.8162080000 -6.1073930000 -0.0915820000

[(bpyPy$_2$Me)Fe(NH$_2$)(NH$_2$)]$^{2+}$, multiplicity = 3
C -2.5791080000 2.2326740000 -0.9067130000
C -3.0495650000 0.9367380000 -0.6626990000
C -2.1102590000 -0.0808380000 -0.4543720000
N -0.7811760000 0.1871580000 -0.5469830000
C -0.3120270000 1.4424360000 -0.6287040000
C -1.2048010000 2.5044720000 -0.8444330000
C -3.6592740000 -1.9726580000 0.2642710000
C -2.3842220000 -1.4481030000 0.0139400000
C -3.7732700000 -3.2535580000 0.8177440000
C -2.6088670000 -3.9748660000 1.1092140000
C -1.3644470000 -3.4048050000 0.8192810000
N -1.2532220000 -2.1709360000 0.2874280000
C 1.1954110000 1.5970410000 -0.3313080000
C 1.5691740000 3.0870850000 -0.2628130000
C 2.0308280000 0.8621800000 -1.3954620000
C 1.4467440000 0.8896620000 1.0327250000
N 1.1173080000 -0.4261270000 1.1354070000
C 1.2724920000 -1.0735480000 2.3123750000
C 1.7911150000 -0.4472830000 3.4457640000
C 2.1576210000 0.8982700000 3.3518060000
C 1.9788300000 1.5712820000 2.1363470000
C 3.0028750000 1.5127220000 -2.1721880000
C 3.7606430000 0.7832770000 -3.0941360000
C 3.5352480000 -0.5918580000 -3.2197080000
C 2.5552060000 -1.1814330000 -2.4245300000
N 1.8155360000 -0.4690120000 -1.5379780000
H -3.2866130000 3.0461580000 -1.0910400000
H -4.7600910000 -3.6789500000 1.0208630000
H -2.6499520000 -4.9743120000 1.5489280000
H -0.4248700000 -3.9332480000 1.0016300000
H 0.9723090000 3.5999400000 0.5060070000
H 2.6337920000 3.2145070000 -0.0170470000
H 1.3774090000 3.5763170000 -1.2299330000
H 0.9716480000 -2.1245360000 2.3299330000
H 1.9002210000 -1.0128220000 4.3748820000
H 2.5736060000 1.4283420000 4.2138270000

H 2.2547380000 2.6230850000 2.0573750000
H 3.1733990000 2.5833000000 -2.0562650000
H 4.5206500000 1.2870450000 -3.6990350000
H 4.1068170000 -1.2101080000 -3.9170790000
H 2.3395650000 -2.2504650000 -2.4791130000
Fe 0.4051680000 -1.3912480000 -0.4887520000
H -0.8447100000 3.5285570000 -0.9468920000
N 1.4663140000 -2.8256860000 -0.0906540000
H 1.5040800000 -3.6638040000 -0.6795310000
H 2.3096720000 -2.7456660000 0.4894330000
N -0.2086520000 -2.1162880000 -2.0525070000
H 0.0373620000 -1.7582750000 -2.9823900000
H -0.9260070000 -2.8471920000 -2.1187870000
H -4.5492590000 -1.3830900000 0.0323490000
H -4.1207520000 0.7286160000 -0.6101900000

[(bpyPy$_2$Me)Fe(NH$_2$)(NH$_2$)]$^{2+}$, multiplicity = 1
C -2.5664860000 2.1928300000 -0.8183330000
C -3.0302110000 0.9036940000 -0.5347420000
C -2.0868690000 -0.1189150000 -0.3644780000
N -0.7646350000 0.1466710000 -0.5028520000
C -0.2903600000 1.3965290000 -0.6401520000
C -1.1891680000 2.4564800000 -0.8361760000
C -3.6363420000 -2.0072030000 0.3250190000
C -2.3572830000 -1.5042380000 0.0470500000
C -3.7702180000 -3.3208220000 0.7852600000
C -2.6175740000 -4.0979920000 0.9495700000
C -1.3730370000 -3.5416320000 0.6385490000
N -1.2322280000 -2.2732960000 0.2039560000
C 1.2244490000 1.5590440000 -0.3877290000
C 1.6004710000 3.0493670000 -0.3569770000
C 2.0723170000 0.7926800000 -1.4227590000
C 1.4611030000 0.8856920000 0.9898780000
N 1.0791880000 -0.4095500000 1.1160030000
C 1.1791600000 -1.0321650000 2.3117530000
C 1.6912740000 -0.3922730000 3.4404010000
C 2.1268590000 0.9307400000 3.3190140000
C 2.0062500000 1.5755170000 2.0824100000
C 3.0480200000 1.4198130000 -2.2118640000
C 3.8268690000 0.6605550000 -3.0934650000
C 3.6185750000 -0.7203170000 -3.1688740000
C 2.6300630000 -1.2881190000 -2.3661910000
N 1.8764380000 -0.5470090000 -1.5154660000
H -3.2781840000 3.0073400000 -0.9803770000
H -4.7593400000 -3.7292040000 1.0104090000
H -2.6669860000 -5.1295310000 1.3063020000

H -0.4674940000 -4.1435850000 0.7376360000
H 1.0120310000 3.5801860000 0.4060140000
H 2.6675900000 3.1798360000 -0.1233880000
H 1.4009310000 3.5165730000 -1.3335160000
H 0.8450010000 -2.0706180000 2.3515500000
H 1.7498740000 -0.9357170000 4.3871800000
H 2.5491650000 1.4640110000 4.1758480000
H 2.3288400000 2.6116000000 1.9758740000
H 3.2055120000 2.4962690000 -2.1392900000
H 4.5885650000 1.1490500000 -3.7087290000
H 4.2044490000 -1.3578180000 -3.8364250000
H 2.4123590000 -2.3598470000 -2.3849780000
Fe 0.4169210000 -1.4345620000 -0.5512190000
H -0.8281510000 3.4749500000 -0.9822380000
N 1.5260840000 -2.7445890000 -0.0479770000
H 1.2461280000 -3.5521530000 0.5193690000
H 2.5267480000 -2.5582000000 0.0921360000
N -0.2621560000 -1.8381460000 -2.1557200000
H -1.2330640000 -2.1394890000 -2.3002040000
H 0.1360120000 -1.4612550000 -3.0232590000
H -4.5148840000 -1.3730260000 0.1859440000
H -4.0989460000 0.7001550000 -0.4376240000

[(bpyPy$_2$Me)Fe(NH$_2$)(NH$_2$)]$^{2+}$, multiplicity = 5
C -2.5489870000 2.1628630000 -0.9993200000
C -3.0382900000 0.8892360000 -0.6925810000
C -2.1223310000 -0.1259330000 -0.3879190000
N -0.7852740000 0.1239680000 -0.4254750000
C -0.2994090000 1.3701080000 -0.5893930000
C -1.1758700000 2.4203370000 -0.9127730000
C -3.8179200000 -1.9471460000 0.1647900000
C -2.4976970000 -1.4778160000 0.0857720000
C -4.0497350000 -3.2239440000 0.6931760000
C -2.9649120000 -3.9970060000 1.1267030000
C -1.6739260000 -3.4677260000 1.0042140000
N -1.4529290000 -2.2404110000 0.5029540000
C 1.2101850000 1.5863590000 -0.3076220000
C 1.5068670000 3.0944370000 -0.2076520000
C 2.0691370000 0.9425480000 -1.4220740000
C 1.5399670000 0.8773640000 1.0367610000
N 1.2574390000 -0.4478310000 1.1687860000
C 1.4830080000 -1.0885400000 2.3396750000
C 2.0303410000 -0.4423650000 3.4467590000
C 2.3576440000 0.9106630000 3.3256700000
C 2.1075120000 1.5709540000 2.1160610000
C 2.9906010000 1.6675470000 -2.1959170000

C 3.7528150000 0.9933460000 -3.1587210000
C 3.5868810000 -0.3868510000 -3.3225250000
C 2.6526610000 -1.0400380000 -2.5160640000
N 1.9112290000 -0.3832440000 -1.5999480000
H -3.2401510000 2.9692550000 -1.2604630000
H -5.0711280000 -3.6101160000 0.7616420000
H -3.1070440000 -4.9964000000 1.5456920000
H -0.7874980000 -4.0357470000 1.3043120000
H 0.8938640000 3.5621380000 0.5773590000
H 2.5673190000 3.2672950000 0.0268770000
H 1.2877110000 3.5938230000 -1.1630300000
H 1.2110450000 -2.1474030000 2.3756640000
H 2.1936320000 -0.9988060000 4.3731980000
H 2.7988100000 1.4579970000 4.1640890000
H 2.3560940000 2.6279300000 2.0225620000
H 3.1226440000 2.7410720000 -2.0555650000
H 4.4738830000 1.5469180000 -3.7683270000
H 4.1681090000 -0.9537460000 -4.0550220000
H 2.4849000000 -2.1190380000 -2.5922790000
Fe 0.4360150000 -1.5042190000 -0.3666030000
H -0.8004210000 3.4288950000 -1.0847320000
N 1.5244440000 -2.9354710000 -0.0144550000
H 1.6055730000 -3.7417390000 -0.6403440000
H 2.3524580000 -2.8564010000 0.5876060000
N -0.1917640000 -2.2312640000 -1.9429090000
H 0.1499290000 -1.9771940000 -2.8764010000
H -0.7674970000 -3.0806550000 -1.9798430000
H -4.6523530000 -1.3329930000 -0.1814320000
H -4.1129450000 0.6951440000 -0.6706440000

[(bpyPy$_2$Me)Fe(NH)(NH$_3$)]$^{2+}$, multiplicity = 3
C -2.5865660000 2.2469210000 -0.8995420000
C -3.0541710000 0.9510590000 -0.6527740000
C -2.1116290000 -0.0673940000 -0.4544460000
N -0.7821740000 0.1981150000 -0.5663570000
C -0.3176970000 1.4562660000 -0.6471530000
C -1.2107730000 2.5193430000 -0.8483770000
C -3.6569860000 -1.9608530000 0.2775790000
C -2.3830390000 -1.4352800000 0.0191860000
C -3.7660780000 -3.2433920000 0.8272820000
C -2.5988210000 -3.9688200000 1.1006440000
C -1.3578510000 -3.3981610000 0.8009930000
N -1.2495760000 -2.1597200000 0.2772550000
C 1.1893250000 1.6024640000 -0.3463730000
C 1.5711830000 3.0900690000 -0.2752100000
C 2.0346990000 0.8610150000 -1.3990330000

C 1.4284650000 0.8908530000 1.0187090000
N 1.1034620000 -0.4279400000 1.1199440000
C 1.2719240000 -1.0821030000 2.2920120000
C 1.7850390000 -0.4551750000 3.4267550000
C 2.1392420000 0.8946280000 3.3398360000
C 1.9564920000 1.5696190000 2.1269850000
C 2.9960520000 1.5104240000 -2.1900630000
C 3.7793860000 0.7715530000 -3.0830210000
C 3.5967530000 -0.6138670000 -3.1579130000
C 2.6245390000 -1.2011790000 -2.3511620000
N 1.8485420000 -0.4785510000 -1.5041390000
H -3.2960950000 3.0607460000 -1.0745550000
H -4.7510560000 -3.6687680000 1.0393030000
H -2.6375650000 -4.9718540000 1.5324960000
H -0.4146260000 -3.9289490000 0.9605580000
H 0.9764110000 3.6051460000 0.4937420000
H 2.6367110000 3.2121830000 -0.0299630000
H 1.3799560000 3.5811270000 -1.2416090000
H 0.9895630000 -2.1376630000 2.2981970000
H 1.9040380000 -1.0259610000 4.3514990000
H 2.5524890000 1.4239160000 4.2036150000
H 2.2270430000 2.6230350000 2.0500470000
H 3.1394740000 2.5882310000 -2.1068850000
H 4.5292650000 1.2751770000 -3.7006150000
H 4.1963420000 -1.2409490000 -3.8232750000
H 2.4508530000 -2.2810290000 -2.3530630000
Fe 0.4165210000 -1.3793910000 -0.4797790000
H -0.8520090000 3.5442750000 -0.9482810000
N 1.4143690000 -2.7644200000 -0.1769490000
H 2.3329490000 -2.9275020000 0.2668180000
N -0.3116590000 -2.0946750000 -2.2324470000
H -1.2205630000 -1.6966010000 -2.5043740000
H -0.4390980000 -3.1130320000 -2.1808520000
H 0.3142730000 -1.9204610000 -3.0289600000
H -4.5491000000 -1.3707620000 0.0552150000
H -4.1248150000 0.7437340000 -0.5867010000

[(bpyPy$_2$Me)Fe(NH)(NH$_3$)]$^{2+}$, multiplicity = 1
C -2.5980530000 2.2382830000 -0.8837030000
C -3.0712430000 0.9490750000 -0.6114400000
C -2.1294680000 -0.0684800000 -0.4044030000
N -0.8034580000 0.1932800000 -0.5153670000
C -0.3310090000 1.4440940000 -0.6379090000
C -1.2203160000 2.5068800000 -0.8583630000
C -3.6731890000 -1.9618600000 0.3201280000
C -2.3984710000 -1.4440200000 0.0495570000

C -3.7870990000 -3.2577040000 0.8366220000
C -2.6226800000 -4.0034340000 1.0614940000
C -1.3819790000 -3.4385630000 0.7478710000
N -1.2686510000 -2.1867030000 0.2613440000
C 1.1821750000 1.5921640000 -0.3581800000
C 1.5619470000 3.0816430000 -0.3073740000
C 2.0405330000 0.8364090000 -1.3927750000
C 1.4349620000 0.8970900000 1.0090690000
N 1.1304390000 -0.4253960000 1.1126110000
C 1.3149180000 -1.0746940000 2.2873610000
C 1.8234980000 -0.4365000000 3.4173960000
C 2.1527990000 0.9193600000 3.3273130000
C 1.9547740000 1.5877800000 2.1132890000
C 2.9986060000 1.4810640000 -2.1905070000
C 3.8061830000 0.7342910000 -3.0554000000
C 3.6506960000 -0.6555260000 -3.0966410000
C 2.6781740000 -1.2388940000 -2.2876650000
N 1.8802320000 -0.5105260000 -1.4645020000
H -3.3056780000 3.0519900000 -1.0672780000
H -4.7723720000 -3.6764970000 1.0602900000
H -2.6635910000 -5.0169690000 1.4682360000
H -0.4376030000 -3.9806900000 0.8603500000
H 0.9666250000 3.6055970000 0.4551190000
H 2.6274350000 3.2093690000 -0.0647400000
H 1.3683760000 3.5602910000 -1.2795310000
H 1.0442220000 -2.1338850000 2.3009180000
H 1.9582700000 -1.0042400000 4.3418290000
H 2.5591080000 1.4574640000 4.1888620000
H 2.2053520000 2.6458430000 2.0318360000
H 3.1202740000 2.5633470000 -2.1360130000
H 4.5527090000 1.2361820000 -3.6783520000
H 4.2685700000 -1.2883920000 -3.7392710000
H 2.5184430000 -2.3214410000 -2.2862600000
Fe 0.4293030000 -1.3901060000 -0.4699790000
H -0.8602990000 3.5273430000 -0.9929850000
N 1.2909790000 -2.8207760000 -0.1097560000
H 2.3076000000 -2.6235140000 0.0613720000
N -0.3129240000 -2.0364620000 -2.2405220000
H -1.1151030000 -1.4846510000 -2.5717700000
H -0.6315500000 -3.0098810000 -2.1657110000
H 0.3761020000 -2.0166940000 -3.0039550000
H -4.5623430000 -1.3549210000 0.1340020000
H -4.1428170000 0.7480280000 -0.5417200000

[(bpyPy$_2$Me)Fe(NH)(NH$_3$)]$^{2+}$, multiplicity = 5
C -2.5930951701 2.2388102740 -0.9773191524

C -3.0677731407 0.9530798313 -0.6822881912
C -2.1227450836 -0.0406559036 -0.3838112707
N -0.8040995458 0.2377912160 -0.4146641419
C -0.3377154715 1.4755608051 -0.5970483039
C -1.2193767911 2.5241466153 -0.9095010533
C -3.6871798171 -1.9079161949 0.3641042371
C -2.4043089947 -1.4202573574 0.0767687082
C -3.8295888488 -3.2048053805 0.8725372179
C -2.6873252078 -3.9888881655 1.0786624377
C -1.4376045345 -3.4545594845 0.7509950529
N -1.2994528175 -2.2027664591 0.2684675855
C 1.1816764393 1.6238700173 -0.3151283269
C 1.5593289376 3.1146542184 -0.2660565566
C 2.0149655886 0.8801112875 -1.3846266202
C 1.4580807635 0.9332102262 1.0499534062
N 1.2877731739 -0.4125087928 1.1319741920
C 1.5255600002 -1.0738383092 2.2844253691
C 1.9330546914 -0.4124000391 3.4439957586
C 2.1122521078 0.9732740422 3.3864084333
C 1.8787454890 1.6489660588 2.1804599048
C 2.9155259829 1.5514746860 -2.2277245679
C 3.7221903654 0.8286279490 -3.1142311073
C 3.6366155382 -0.5678685300 -3.1322131985
C 2.7202050628 -1.1837972132 -2.2827360090
N 1.9150242683 -0.4736183412 -1.4550657102
H -3.2997339207 3.0355896964 -1.2273839000
H -4.8241254846 -3.5956243215 1.1064341165
H -2.7530048758 -5.0046663534 1.4757349012
H -0.5108129966 -4.0259505075 0.8555187786
H 0.9583104544 3.6365242336 0.4934435523
H 2.6242671413 3.2458570512 -0.0210670739
H 1.3636316695 3.5955449190 -1.2362832577
H 1.3929676338 -2.1598944406 2.2450991661
H 2.1169075140 -0.9815150905 4.3591602939
H 2.4406719822 1.5318162269 4.2681870624
H 2.0274566149 2.7284471878 2.1294070602
H 2.9962110982 2.6382315506 -2.1885939304
H 4.4225607888 1.3567673078 -3.7686647103
H 4.2665304314 -1.1794529014 -3.7836943350
H 2.6082970167 -2.2714142799 -2.2299891341
Fe 0.5016690633 -1.4738120049 -0.4513344025
H -0.8640986809 3.5410789059 -1.0817572610
N 1.4543920528 -3.0214115593 -0.1788123534
H 1.9594999684 -3.8725628600 0.1192186503
N -0.2570334438 -2.0619226160 -2.2754336082
H -0.9602226754 -1.4187596753 -2.6627960746

H -0.6955192786 -2.9871642757 -2.1960562468
H 0.4770127714 -2.1569777517 -2.9887719650
H -4.5631640074 -1.2752736239 0.2022575796
H -4.1399908229 0.7422941264 -0.6753620013

[(bpyPy$_2$Me)Fe(NH$_3$)(NH)]$^{2+}$, multiplicity = 3
C -2.5396260000 2.1898430000 -0.9808880000
C -3.0121980000 0.8945440000 -0.7409470000
C -2.0750150000 -0.1206580000 -0.5085400000
N -0.7442430000 0.1469790000 -0.5902160000
C -0.2735420000 1.4069910000 -0.6521990000
C -1.1672220000 2.4644260000 -0.8832480000
C -3.6371290000 -1.9783890000 0.2485790000
C -2.3540910000 -1.4706920000 0.0034720000
C -3.7733670000 -3.2232710000 0.8732080000
C -2.6201240000 -3.9238280000 1.2449910000
C -1.3684560000 -3.3706890000 0.9537600000
N -1.2285430000 -2.1780640000 0.3445380000
C 1.2262500000 1.5767900000 -0.3126720000
C 1.5831220000 3.0709110000 -0.2422960000
C 2.0902910000 0.8481690000 -1.3592940000
C 1.4490350000 0.8814400000 1.0601980000
N 1.1200270000 -0.4343710000 1.1580440000
C 1.2575870000 -1.0761920000 2.3398320000
C 1.7527760000 -0.4475640000 3.4822220000
C 2.1175340000 0.8990000000 3.3916650000
C 1.9601730000 1.5678570000 2.1712330000
C 3.0841980000 1.5022820000 -2.1045650000
C 3.8167370000 0.7927800000 -3.0622550000
C 3.5254500000 -0.5594850000 -3.2704410000
C 2.5280340000 -1.1508960000 -2.4981730000
N 1.8423610000 -0.4715480000 -1.5470960000
H -3.2440170000 3.0015890000 -1.1836720000
H -4.7669550000 -3.6352820000 1.0706820000
H -2.6732170000 -4.8938350000 1.7449530000
H -0.4565070000 -3.9133250000 1.2134490000
H 0.9620210000 3.5819260000 0.5084090000
H 2.6397020000 3.2095820000 0.0303780000
H 1.4125460000 3.5532310000 -1.2168440000
H 0.9570060000 -2.1272820000 2.3672030000
H 1.8456860000 -1.0108890000 4.4144380000
H 2.5160560000 1.4320650000 4.2600350000
H 2.2351720000 2.6200860000 2.0939510000
H 3.2853220000 2.5613600000 -1.9428540000
H 4.5941610000 1.2977290000 -3.6433950000
H 4.0512450000 -1.1560620000 -4.0206960000

H 2.2368880000 -2.1924570000 -2.6533940000
Fe 0.4105400000 -1.3929590000 -0.5085760000
H -0.8083910000 3.4902080000 -0.9729750000
N 1.6902740000 -2.9126160000 -0.1210920000
H 2.5114050000 -2.5954320000 0.4102220000
N -0.1613440000 -2.1984370000 -1.9466760000
H -0.4498750000 -3.1727910000 -2.1410500000
H -4.5181500000 -1.4009830000 -0.0413080000
H -4.0839560000 0.6855490000 -0.7045300000
H 1.2955670000 -3.6984520000 0.4104930000
H 2.0566400000 -3.3407320000 -0.9801060000

[(bpyPy$_2$Me)Fe(NH$_3$)(NH)]$^{2+}$, multiplicity = 1
C -2.5545170000 2.1810540000 -0.8727090000
C -3.0225240000 0.8863680000 -0.6268440000
C -2.0820850000 -0.1347450000 -0.4395700000
N -0.7517290000 0.1304610000 -0.5542460000
C -0.2763400000 1.3900410000 -0.6375870000
C -1.1780930000 2.4479380000 -0.8307000000
C -3.6266020000 -2.0202510000 0.2853790000
C -2.3513800000 -1.5057650000 0.0108590000
C -3.7426830000 -3.3082070000 0.8175850000
C -2.5779720000 -4.0475370000 1.0615960000
C -1.3367340000 -3.4844710000 0.7506150000
N -1.2140290000 -2.2401020000 0.2411040000
C 1.2311660000 1.5717040000 -0.3444950000
C 1.5820000000 3.0684400000 -0.3020150000
C 2.0975860000 0.8288650000 -1.3788590000
C 1.4683480000 0.9007700000 1.0378080000
N 1.1110570000 -0.4025440000 1.1564510000
C 1.2094160000 -1.0143520000 2.3558990000
C 1.7169980000 -0.3755860000 3.4878010000
C 2.1302560000 0.9546440000 3.3679430000
C 1.9940950000 1.6013790000 2.1331060000
C 3.0945200000 1.4731760000 -2.1284430000
C 3.8636720000 0.7398410000 -3.0392590000
C 3.6126850000 -0.6274370000 -3.1916770000
C 2.6008820000 -1.2061730000 -2.4264880000
N 1.8722920000 -0.4986050000 -1.5311330000
H -3.2621160000 2.9973010000 -1.0435500000
H -4.7283940000 -3.7266880000 1.0390820000
H -2.6172640000 -5.0566580000 1.4785010000
H -0.4181680000 -4.0534320000 0.9094550000
H 0.9745170000 3.5878570000 0.4538450000
H 2.6426420000 3.2135910000 -0.0495160000
H 1.3930380000 3.5370290000 -1.2800240000

H 0.8566020000 -2.0482500000 2.4158060000
H 1.7783980000 -0.9174960000 4.4352660000
H 2.5418560000 1.4940640000 4.2261980000
H 2.2946170000 2.6447410000 2.0333500000
H 3.2735540000 2.5414310000 -2.0047140000
H 4.6444100000 1.2376880000 -3.6222660000
H 4.1793430000 -1.2445250000 -3.8942040000
H 2.3319460000 -2.2587000000 -2.5427250000
Fe 0.3927440000 -1.4159150000 -0.5528110000
H -0.8189240000 3.4722580000 -0.9329690000
N 1.6661440000 -2.8973240000 -0.0419790000
H 2.6420610000 -2.6008590000 -0.1753150000
N -0.0540660000 -2.0556460000 -2.0722480000
H -1.0256370000 -2.4484330000 -2.0708060000
H -4.5147400000 -1.4153010000 0.0886370000
H -4.0927120000 0.6772430000 -0.5606380000
H 1.6075640000 -3.2015170000 0.9379860000
H 1.5401370000 -3.7432100000 -0.6105240000

[(bpyPy$_2$Me)Fe(NH$_3$)(NH)]$^{2+}$, multiplicity = 5
C -2.5125240000 2.1726860000 -1.0370240000
C -2.9992830000 0.8917110000 -0.7535490000
C -2.0734210000 -0.1180140000 -0.4517050000
N -0.7462850000 0.1407700000 -0.4784600000
C -0.2656360000 1.3880980000 -0.6137190000
C -1.1410170000 2.4417030000 -0.9284780000
C -3.7384530000 -1.9254880000 0.2046410000
C -2.4199090000 -1.4703420000 0.0452460000
C -3.9619110000 -3.1830400000 0.7771930000
C -2.8641800000 -3.9520650000 1.1817540000
C -1.5768520000 -3.4412600000 0.9785420000
N -1.3600860000 -2.2337640000 0.4278350000
C 1.2421640000 1.5807360000 -0.2961860000
C 1.5614860000 3.0837770000 -0.1984590000
C 2.0992260000 0.9195650000 -1.3991500000
C 1.5181470000 0.8700360000 1.0604150000
N 1.2392460000 -0.4574320000 1.1733120000
C 1.3973390000 -1.0842240000 2.3618000000
C 1.8722350000 -0.4329860000 3.4992090000
C 2.1991290000 0.9215700000 3.3931610000
C 2.0153960000 1.5743670000 2.1681730000
C 3.0354770000 1.6285920000 -2.1689170000
C 3.7545950000 0.9585390000 -3.1671480000
C 3.5159420000 -0.4022030000 -3.3900060000
C 2.5675010000 -1.0440440000 -2.5934960000
N 1.8956080000 -0.3976880000 -1.6157660000

H -3.2065410000 2.9779300000 -1.2948130000
H -4.9827470000 -3.5542180000 0.9073760000
H -2.9908060000 -4.9353100000 1.6416300000
H -0.6953480000 -4.0228510000 1.2647900000
H 0.9356400000 3.5653730000 0.5676690000
H 2.6179480000 3.2439420000 0.0622960000
H 1.3694280000 3.5807120000 -1.1611550000
H 1.1273730000 -2.1431980000 2.3987640000
H 1.9813120000 -0.9856190000 4.4359860000
H 2.5862480000 1.4749210000 4.2539530000
H 2.2574650000 2.6338640000 2.0856490000
H 3.2076290000 2.6920100000 -2.0004680000
H 4.4877480000 1.5040390000 -3.7693500000
H 4.0437810000 -0.9612620000 -4.1672360000
H 2.3101160000 -2.0978520000 -2.7363040000
Fe 0.5365150000 -1.5331530000 -0.4403800000
H -0.7725180000 3.4570420000 -1.0768500000
N 1.8506850000 -3.1061960000 0.0445700000
H 2.7192700000 -2.7798730000 0.4883350000
N -0.0215190000 -2.4146080000 -1.8135620000
H -0.4533830000 -3.3487280000 -1.9134360000
H -4.5802170000 -1.3045590000 -0.1103090000
H -4.0736250000 0.6940330000 -0.7455070000
H 1.4614820000 -3.8240500000 0.6695940000
H 2.1279660000 -3.6138350000 -0.8045110000

[(bpyPy$_2$Me)Fe(NH$_2$)(NH$_3$)]$^{3+}$, multiplicity = 3
C -2.5750700000 2.2362470000 -0.9707640000
C -3.0472160000 0.9405690000 -0.7237130000
C -2.1098880000 -0.0704970000 -0.4884120000
N -0.7777330000 0.1995890000 -0.5692140000
C -0.3118500000 1.4573580000 -0.6497320000
C -1.2035330000 2.5138960000 -0.8860840000
C -3.6565990000 -1.9516170000 0.2563520000
C -2.3838920000 -1.4280820000 0.0053510000
C -3.7695230000 -3.2169910000 0.8461260000
C -2.6071290000 -3.9258780000 1.1739680000
C -1.3623230000 -3.3670920000 0.8731610000
N -1.2531550000 -2.1476860000 0.3024820000
C 1.1873530000 1.6092510000 -0.3288790000
C 1.5677650000 3.0960940000 -0.2445810000
C 2.0202160000 0.8779530000 -1.3947690000
C 1.4313960000 0.8863740000 1.0279070000
N 1.1333830000 -0.4419880000 1.1181350000
C 1.3157690000 -1.1227970000 2.2745670000
C 1.8128440000 -0.5023530000 3.4184340000

C 2.1374650000 0.8555610000 3.3485900000
C 1.9459630000 1.5513220000 2.1454420000
C 2.9712070000 1.5276170000 -2.1925850000
C 3.7455230000 0.7891200000 -3.0944240000
C 3.5705970000 -0.5972840000 -3.1674630000
C 2.6088480000 -1.1892180000 -2.3547940000
N 1.8349980000 -0.4620590000 -1.5080700000
H -3.2824350000 3.0458310000 -1.1709210000
H -4.7570780000 -3.6399100000 1.0506560000
H -2.6487270000 -4.9089640000 1.6493760000
H -0.4323870000 -3.8976820000 1.0913000000
H 0.9674310000 3.6033480000 0.5254260000
H 2.6323590000 3.2141420000 0.0056000000
H 1.3813000000 3.5927990000 -1.2084300000
H 1.0607120000 -2.1854340000 2.2637190000
H 1.9440360000 -1.0845210000 4.3336830000
H 2.5401100000 1.3796150000 4.2203160000
H 2.1988600000 2.6101480000 2.0882410000
H 3.1160170000 2.6047030000 -2.1066370000
H 4.4884440000 1.2941490000 -3.7186140000
H 4.1671520000 -1.2232150000 -3.8356750000
H 2.4497220000 -2.2708390000 -2.3625740000
Fe 0.4073000000 -1.3524270000 -0.4601050000
H -0.8442530000 3.5389240000 -0.9840000000
N 1.4189240000 -2.8596560000 -0.2069750000
H 1.1783930000 -3.8001080000 -0.5482760000
H 2.3610330000 -2.8543200000 0.2067300000
N -0.2974570000 -2.1188030000 -2.1901170000
H -1.0959930000 -1.5798640000 -2.5538760000
H -0.6108860000 -3.0947210000 -2.1030400000
H 0.4039840000 -2.1065580000 -2.9422800000
H -4.5466210000 -1.3720580000 0.0012380000
H -4.1182880000 0.7307670000 -0.6852390000

[(bpyPy$_2$Me)Fe(NH$_2$)(NH$_3$)]$^{3+}$, multiplicity = 1
C -2.5600290000 2.1972380000 -0.9935870000
C -3.0362370000 0.9061110000 -0.7356780000
C -2.1027030000 -0.0994490000 -0.4671150000
N -0.7670780000 0.1696240000 -0.5208680000
C -0.2971490000 1.4278010000 -0.6250110000
C -1.1881870000 2.4750750000 -0.8956290000
C -3.6551700000 -1.9685480000 0.2883710000
C -2.3806360000 -1.4531960000 0.0185340000
C -3.7713100000 -3.2305230000 0.8810000000
C -2.6071900000 -3.9419450000 1.1946420000
C -1.3653430000 -3.3856350000 0.8741190000

N -1.2482550000 -2.1743570000 0.2941920000
C 1.1997250000 1.6079930000 -0.3150080000
C 1.5545830000 3.1071690000 -0.2494010000
C 2.0491500000 0.8657390000 -1.3616650000
C 1.4513150000 0.8946160000 1.0420220000
N 1.1141920000 -0.4153230000 1.1418270000
C 1.2334180000 -1.0739800000 2.3197120000
C 1.7390440000 -0.4527470000 3.4605820000
C 2.1349230000 0.8839300000 3.3711170000
C 1.9868980000 1.5567050000 2.1532560000
C 3.0117110000 1.5069470000 -2.1547360000
C 3.7739460000 0.7633400000 -3.0616500000
C 3.5696730000 -0.6184970000 -3.1506380000
C 2.6001960000 -1.2000750000 -2.3390530000
N 1.8533010000 -0.4712490000 -1.4696490000
H -3.2635060000 3.0035860000 -1.2191220000
H -4.7578520000 -3.6445350000 1.1068240000
H -2.6430080000 -4.9179060000 1.6840990000
H -0.4362150000 -3.9056010000 1.1050700000
H 0.9425750000 3.6098810000 0.5135980000
H 2.6158200000 3.2430630000 0.0031670000
H 1.3621390000 3.5874780000 -1.2203640000
H 0.9103480000 -2.1168440000 2.3404830000
H 1.8236750000 -1.0232270000 4.3890260000
H 2.5496590000 1.4080810000 4.2370250000
H 2.2861430000 2.5976220000 2.0735640000
H 3.1664520000 2.5829410000 -2.0673130000
H 4.5237600000 1.2608320000 -3.6835590000
H 4.1513320000 -1.2495450000 -3.8275450000
H 2.4182700000 -2.2779010000 -2.3648890000
Fe 0.4160580000 -1.3763490000 -0.4412920000
H -0.8251510000 3.4960500000 -1.0146880000
N 1.3860630000 -2.7772420000 -0.0961120000
H 1.0525940000 -3.7568440000 -0.0700990000
H 2.3892230000 -2.7683700000 0.1635500000
N -0.3283900000 -2.0596650000 -2.1855260000
H -1.1166380000 -1.4938540000 -2.5307690000
H -0.6603870000 -3.0311370000 -2.1239450000
H 0.3733420000 -2.0449610000 -2.9369180000
H -4.5434210000 -1.3793130000 0.0504570000
H -4.1075320000 0.6940420000 -0.7193130000

[(bpyPy$_2$Me)Fe(NH$_2$)(NH$_3$)]$^{3+}$, multiplicity = 5
C -2.5729800000 2.1755620000 -0.9182010000
C -3.0535180000 0.8895900000 -0.6485670000
C -2.1295070000 -0.1266100000 -0.3899420000

N -0.7875490000 0.1393480000 -0.4535670000
C -0.3047190000 1.3939410000 -0.5827270000
C -1.1993250000 2.4417590000 -0.8473420000
C -3.7466830000 -1.9802380000 0.2595120000
C -2.4538490000 -1.4920460000 0.0425270000
C -3.9064550000 -3.2793870000 0.7609440000
C -2.7745640000 -4.0579510000 1.0347050000
C -1.5083530000 -3.5254450000 0.7775840000
N -1.3572300000 -2.2738570000 0.2951260000
C 1.2013400000 1.6028680000 -0.3110400000
C 1.5281340000 3.1062570000 -0.2957490000
C 2.0465980000 0.8657790000 -1.3721200000
C 1.5164190000 0.9592580000 1.0709690000
N 1.2224050000 -0.3543800000 1.2326220000
C 1.4460230000 -0.9835980000 2.4074630000
C 2.0015260000 -0.3160970000 3.4992540000
C 2.3288450000 1.0352220000 3.3514740000
C 2.0832140000 1.6795320000 2.1297090000
C 3.0175030000 1.5209050000 -2.1442800000
C 3.8037560000 0.7873720000 -3.0396650000
C 3.6155350000 -0.5950950000 -3.1390460000
C 2.6327600000 -1.1882300000 -2.3501590000
N 1.8578420000 -0.4693970000 -1.5026040000
H -3.2731480000 2.9861650000 -1.1382870000
H -4.9101960000 -3.6761030000 0.9374720000
H -2.8587790000 -5.0715780000 1.4343670000
H -0.5943730000 -4.0997390000 0.9525670000
H 0.9267900000 3.6224050000 0.4675060000
H 2.5913470000 3.2683220000 -0.0667730000
H 1.3148990000 3.5584770000 -1.2755760000
H 1.1686250000 -2.0406240000 2.4675990000
H 2.1679130000 -0.8537880000 4.4360090000
H 2.7705180000 1.5958950000 4.1806690000
H 2.3340910000 2.7342570000 2.0146200000
H 3.1696580000 2.5956320000 -2.0450130000
H 4.5622190000 1.2950810000 -3.6428070000
H 4.2138530000 -1.2151450000 -3.8114300000
H 2.4552240000 -2.2656590000 -2.3919710000
Fe 0.3723990000 -1.4366510000 -0.3758730000
H -0.8345600000 3.4602110000 -0.9803280000
N 1.3974890000 -2.9240840000 -0.1459380000
H 1.3575550000 -3.7439020000 -0.7672640000
H 2.1714240000 -2.9962710000 0.5295180000
N -0.3829140000 -2.0880200000 -2.3584160000
H -1.1547500000 -1.4940010000 -2.6902480000
H -0.7461460000 -3.0504580000 -2.3407670000

H 0.3229740000 -2.0619840000 -3.1048310000
H -4.6165910000 -1.3546720000 0.0478300000
H -4.1256250000 0.6839210000 -0.6229590000

[(bpyPy$_2$Me)Fe(N)(NH$_3$)]$^{2+}$, multiplicity = 2
C -2.6071360000 2.2491750000 -0.8674970000
C -3.0690000000 0.9536270000 -0.6046050000
C -2.1167530000 -0.0589300000 -0.4161430000
N -0.7969130000 0.2154510000 -0.5397050000
C -0.3352590000 1.4680730000 -0.6520380000
C -1.2315680000 2.5297310000 -0.8503920000
C -3.6463400000 -1.9600610000 0.3133500000
C -2.3737460000 -1.4384450000 0.0413150000
C -3.7588270000 -3.2532530000 0.8367570000
C -2.5941460000 -3.9938380000 1.0735590000
C -1.3542320000 -3.4263820000 0.7623180000
N -1.2428440000 -2.1788440000 0.2628070000
C 1.1789030000 1.6074450000 -0.3747010000
C 1.5652280000 3.0950590000 -0.3149670000
C 2.0285490000 0.8573490000 -1.4223980000
C 1.4268460000 0.9050130000 0.9931110000
N 1.1210100000 -0.4171730000 1.1053990000
C 1.3023600000 -1.0673540000 2.2786370000
C 1.8057310000 -0.4263010000 3.4093860000
C 2.1346220000 0.9291220000 3.3160520000
C 1.9417740000 1.5955020000 2.0998420000
C 2.9541760000 1.5152400000 -2.2477540000
C 3.7660130000 0.7771270000 -3.1160640000
C 3.6549420000 -0.6172710000 -3.1297890000
C 2.7115600000 -1.2152110000 -2.2972910000
N 1.9033680000 -0.4931030000 -1.4826850000
H -3.3232720000 3.0590650000 -1.0345590000
H -4.7443500000 -3.6737270000 1.0567140000
H -2.6329800000 -5.0054340000 1.4861480000
H -0.4140270000 -3.9705300000 0.8960940000
H 0.9769200000 3.6142520000 0.4565750000
H 2.6335410000 3.2179570000 -0.0824610000
H 1.3619080000 3.5809730000 -1.2812710000
H 1.0395360000 -2.1279380000 2.2905990000
H 1.9375540000 -0.9924670000 4.3349960000
H 2.5378660000 1.4699700000 4.1773210000
H 2.1909760000 2.6538220000 2.0188070000
H 3.0482590000 2.6007690000 -2.2121220000
H 4.4852340000 1.2899830000 -3.7616210000
H 4.2837440000 -1.2418870000 -3.7695880000
H 2.5883610000 -2.3014700000 -2.2560860000

Fe 0.4636820000 -1.4162630000 -0.4866660000
H -0.8807390000 3.5554050000 -0.9719560000
N 1.3281760000 -2.7375360000 -0.1999760000
N -0.2834020000 -1.9953650000 -2.2638940000
H -0.9545850000 -1.3141590000 -2.6418530000
H -0.7705370000 -2.8980350000 -2.2049180000
H 0.4438150000 -2.1068930000 -2.9822260000
H -4.5369440000 -1.3567990000 0.1222290000
H -4.1386560000 0.7469910000 -0.5251080000

[(bpyPy$_2$Me)Fe(N)(NH$_3$)]$^{2+}$, multiplicity = 4
C -2.6148920000 2.2853280000 -0.8877650000
C -3.0828070000 0.9893210000 -0.6353870000
C -2.1355290000 -0.0256510000 -0.4418580000
N -0.8109360000 0.2406500000 -0.5528240000
C -0.3473990000 1.4936670000 -0.6486710000
C -1.2387380000 2.5592600000 -0.8522270000
C -3.6682440000 -1.9316960000 0.2870090000
C -2.3990470000 -1.4019820000 0.0207310000
C -3.7718530000 -3.2225590000 0.8198800000
C -2.6063550000 -3.9604430000 1.0687400000
C -1.3687310000 -3.3927050000 0.7559420000
N -1.2690580000 -2.1432050000 0.2553580000
C 1.1664770000 1.6308000000 -0.3603720000
C 1.5605630000 3.1158040000 -0.2990230000
C 2.0067090000 0.8765640000 -1.4113460000
C 1.4200800000 0.9248610000 1.0049070000
N 1.1727020000 -0.4116170000 1.0891750000
C 1.4075750000 -1.0954780000 2.2313260000
C 1.8789220000 -0.4612090000 3.3805210000
C 2.1341530000 0.9123670000 3.3233590000
C 1.9106250000 1.6066230000 2.1257420000
C 2.9417790000 1.5204680000 -2.2347030000
C 3.7488140000 0.7683140000 -3.0969030000
C 3.6269590000 -0.6255840000 -3.1057220000
C 2.6753150000 -1.2123920000 -2.2751290000
N 1.8695590000 -0.4739780000 -1.4728020000
H -3.3260510000 3.0983650000 -1.0598850000
H -4.7563670000 -3.6477670000 1.0356260000
H -2.6461230000 -4.9703140000 1.4848550000
H -0.4226760000 -3.9302180000 0.8823120000
H 0.9705320000 3.6380560000 0.4691140000
H 2.6281660000 3.2314600000 -0.0590730000
H 1.3657510000 3.6034860000 -1.2662110000
H 1.2215470000 -2.1728650000 2.1927430000
H 2.0510080000 -1.0444990000 4.2886220000

H 2.5158040000 1.4468120000 4.1984440000
H 2.1215070000 2.6750670000 2.0726660000
H 3.0493060000 2.6048960000 -2.2012010000
H 4.4762020000 1.2713050000 -3.7411340000
H 4.2544150000 -1.2574140000 -3.7395650000
H 2.5356150000 -2.2967820000 -2.2203410000
Fe 0.4151040000 -1.3634960000 -0.4673740000
H -0.8821030000 3.5841670000 -0.9636040000
N 1.3604800000 -2.8354280000 -0.2475220000
N -0.2617880000 -2.0994780000 -2.2266130000
H -1.1169580000 -1.6361260000 -2.5627610000
H -0.4634360000 -3.1043590000 -2.1512930000
H 0.4285290000 -2.0037660000 -2.9816870000
H -4.5630370000 -1.3382980000 0.0852790000
H -4.1536700000 0.7841080000 -0.5676740000

[(bpyPy$_2$Me)Fe(NH$_3$)(N)]$^{2+}$, multiplicity = 2
C -2.5642120000 2.2289620000 -0.8426820000
C -3.0420920000 0.9360100000 -0.6048370000
C -2.1106790000 -0.0946610000 -0.4288300000
N -0.7787040000 0.1619830000 -0.5505020000
C -0.2928040000 1.4164540000 -0.6266510000
C -1.1865560000 2.4846470000 -0.8047630000
C -3.6849330000 -1.9637010000 0.2759090000
C -2.4004860000 -1.4638680000 0.0237050000
C -3.8233320000 -3.2512580000 0.8071240000
C -2.6733260000 -4.0016330000 1.0784210000
C -1.4199420000 -3.4504540000 0.7887590000
N -1.2825990000 -2.2133850000 0.2767440000
C 1.2188620000 1.5841170000 -0.3539250000
C 1.5840810000 3.0782320000 -0.3209660000
C 2.0536690000 0.8353270000 -1.4089920000
C 1.4801950000 0.9157990000 1.0286560000
N 1.1153700000 -0.3822630000 1.1646490000
C 1.2443280000 -0.9900760000 2.3621960000
C 1.7831530000 -0.3487040000 3.4789920000
C 2.2005700000 0.9783110000 3.3405240000
C 2.0399540000 1.6195450000 2.1051380000
C 3.0432090000 1.4737380000 -2.1740580000
C 3.7834780000 0.7429960000 -3.1091900000
C 3.5134650000 -0.6196170000 -3.2721070000
C 2.5129470000 -1.1949410000 -2.4918250000
N 1.8104040000 -0.4879030000 -1.5730610000
H -3.2664140000 3.0518630000 -1.0036930000
H -4.8180430000 -3.6599750000 1.0065000000
H -2.7313830000 -5.0088920000 1.4987320000

H -0.5080550000 -4.0262780000 0.9648820000
H 0.9946200000 3.6028090000 0.4459670000
H 2.6502490000 3.2150900000 -0.0880600000
H 1.3811330000 3.5462140000 -1.2961940000
H 0.8928590000 -2.0243110000 2.4351730000
H 1.8657060000 -0.8852230000 4.4277910000
H 2.6366880000 1.5205470000 4.1849730000
H 2.3469110000 2.6598330000 1.9930130000
H 3.2378380000 2.5382620000 -2.0436250000
H 4.5561820000 1.2387130000 -3.7044090000
H 4.0555980000 -1.2352080000 -3.9945930000
H 2.2394960000 -2.2466730000 -2.6080520000
Fe 0.3450420000 -1.4115640000 -0.5815380000
H -0.8195020000 3.5070640000 -0.8982600000
N 1.6020970000 -2.8987290000 -0.0884220000
H 1.4578630000 -3.7514290000 -0.6423240000
H 1.5375640000 -3.1848910000 0.8968740000
N -0.1675210000 -2.0361960000 -1.9733660000
H 2.5831050000 -2.6211640000 -0.2270840000
H -4.5642680000 -1.3520350000 0.0611380000
H -4.1137720000 0.7370230000 -0.5352650000

[(bpyPy$_2$Me)Fe(NH$_3$)(N)]$^{2+}$, multiplicity = 4
C -2.5306310000 2.2084930000 -0.8929070000
C -3.0039710000 0.9092510000 -0.6879970000
C -2.0718670000 -0.1097690000 -0.4571700000
N -0.7333210000 0.1512720000 -0.4899630000
C -0.2665190000 1.4156910000 -0.5554370000
C -1.1587600000 2.4744930000 -0.7848620000
C -3.6584370000 -2.0139780000 0.1238860000
C -2.3723640000 -1.4804870000 -0.0373860000
C -3.8003300000 -3.3138200000 0.6189580000
C -2.6515240000 -4.0500360000 0.9409290000
C -1.3962380000 -3.4740540000 0.7363240000
N -1.2562270000 -2.2149530000 0.2680450000
C 1.2394990000 1.5994410000 -0.2695590000
C 1.6037230000 3.0939030000 -0.2573890000
C 2.0494850000 0.8433140000 -1.3363720000
C 1.5123480000 0.9502590000 1.1175290000
N 1.1881350000 -0.3587390000 1.2639410000
C 1.3453470000 -0.9618040000 2.4634110000
C 1.8624890000 -0.2961660000 3.5747430000
C 2.2320040000 1.0446380000 3.4295800000
C 2.0495860000 1.6744730000 2.1915850000
C 3.0277010000 1.4662760000 -2.1247150000
C 3.7179310000 0.7269110000 -3.0923860000

C 3.4108980000 -0.6271180000 -3.2640710000
C 2.4296000000 -1.1919190000 -2.4533460000
N 1.7765040000 -0.4757740000 -1.5033570000
H -3.2311100000 3.0246940000 -1.0906030000
H -4.7958700000 -3.7471030000 0.7503230000
H -2.7145140000 -5.0668010000 1.3368200000
H -0.4837390000 -4.0334540000 0.9515370000
H 1.0122850000 3.6289380000 0.5007270000
H 2.6696660000 3.2347140000 -0.0251810000
H 1.4022660000 3.5486780000 -1.2389940000
H 1.0380160000 -2.0093770000 2.5347030000
H 1.9701310000 -0.8268100000 4.5242270000
H 2.6532170000 1.6043640000 4.2700970000
H 2.3253450000 2.7227850000 2.0742110000
H 3.2530250000 2.5241520000 -1.9892090000
H 4.4822170000 1.2113710000 -3.7075220000
H 3.9134720000 -1.2440580000 -4.0132980000
H 2.1288530000 -2.2373710000 -2.5608740000
Fe 0.4315840000 -1.3871970000 -0.3567750000
H -0.7947830000 3.4988020000 -0.8693140000
N 1.6672700000 -2.9420320000 -0.0010600000
H 2.6526100000 -2.6754600000 -0.1326070000
N -0.0816540000 -2.2467590000 -1.8904340000
H -4.5350370000 -1.4151450000 -0.1335820000
H -4.0748990000 0.6945140000 -0.6842690000
H 1.6215250000 -3.3093650000 0.9600240000
H 1.4927740000 -3.7409330000 -0.6239530000

[(bpyPy$_2$Me)Fe(NH)(NH$_2$)]$^{2+}$, multiplicity = 4
C -2.5919440000 2.2288220000 -0.9356270000
C -3.0658410000 0.9388490000 -0.6692960000
C -2.1288180000 -0.0801260000 -0.4545380000
N -0.7988540000 0.1789750000 -0.5730700000
C -0.3267860000 1.4338590000 -0.6612220000
C -1.2163030000 2.4971760000 -0.8807080000
C -3.6835930000 -1.9462760000 0.3253920000
C -2.4082940000 -1.4334300000 0.0561700000
C -3.7979470000 -3.2144270000 0.9091490000
C -2.6361870000 -3.9356680000 1.2091110000
C -1.3911620000 -3.3771510000 0.8973350000
N -1.2843310000 -2.1568660000 0.3425300000
C 1.1774340000 1.5878710000 -0.3438020000
C 1.5527850000 3.0772850000 -0.2738750000
C 2.0310210000 0.8473640000 -1.3885720000
C 1.4147700000 0.8818080000 1.0238580000
N 1.1072010000 -0.4393370000 1.1216790000

C 1.2894940000 -1.0997890000 2.2869220000
C 1.7940290000 -0.4712080000 3.4248830000
C 2.1274950000 0.8839910000 3.3425720000
C 1.9363400000 1.5634320000 2.1326440000
C 2.9951060000 1.4964990000 -2.1771260000
C 3.7664650000 0.7580090000 -3.0796400000
C 3.5619890000 -0.6230780000 -3.1770320000
C 2.5850260000 -1.2102710000 -2.3771110000
N 1.8385460000 -0.4873290000 -1.5068030000
H -3.2977790000 3.0427220000 -1.1245440000
H -4.7856210000 -3.6313980000 1.1260610000
H -2.6797510000 -4.9261700000 1.6694380000
H -0.4522930000 -3.9110220000 1.0718170000
H 0.9486270000 3.5924770000 0.4880830000
H 2.6155580000 3.2029770000 -0.0191020000
H 1.3707880000 3.5641400000 -1.2438920000
H 1.0269970000 -2.1608460000 2.2871300000
H 1.9235160000 -1.0440670000 4.3466810000
H 2.5339140000 1.4154440000 4.2083040000
H 2.1939560000 2.6203730000 2.0606430000
H 3.1461790000 2.5724600000 -2.0870410000
H 4.5190160000 1.2595250000 -3.6955140000
H 4.1428650000 -1.2461560000 -3.8620690000
H 2.3750350000 -2.2813050000 -2.4155160000
Fe 0.3833060000 -1.4108340000 -0.4955710000
H -0.8544650000 3.5203240000 -0.9888360000
N 1.3725770000 -2.8022660000 -0.1754280000
H 2.3247480000 -3.0280780000 0.1555970000
N -0.2611060000 -2.0465650000 -2.0938740000
H -0.7331970000 -1.4660410000 -2.7971720000
H -0.1337480000 -3.0149300000 -2.4055100000
H -4.5736040000 -1.3603700000 0.0842130000
H -4.1373600000 0.7382910000 -0.5998530000

[(bpyPy$_2$Me)Fe(NH)(NH$_2$)]$^{2+}$, multiplicity = 2
C -2.5864650000 2.2049550000 -0.8193430000
C -3.0487510000 0.9137370000 -0.5403760000
C -2.1055790000 -0.1078840000 -0.3698480000
N -0.7823450000 0.1610990000 -0.5154340000
C -0.3110440000 1.4115800000 -0.6394430000
C -1.2101180000 2.4726480000 -0.8295050000
C -3.6371630000 -2.0044960000 0.3765200000
C -2.3706570000 -1.4859040000 0.0738270000
C -3.7359690000 -3.3078130000 0.8774300000
C -2.5682410000 -4.0595260000 1.0612890000
C -1.3345040000 -3.4926410000 0.7252490000

N -1.2401710000 -2.2354000000 0.2501820000
C 1.2026350000 1.5670820000 -0.3780410000
C 1.5840130000 3.0559470000 -0.3369200000
C 2.0387060000 0.8077940000 -1.4249050000
C 1.4352790000 0.8846820000 0.9992510000
N 1.0592150000 -0.4140240000 1.1292500000
C 1.1509730000 -1.0345370000 2.3274990000
C 1.6526020000 -0.3903220000 3.4582850000
C 2.0824340000 0.9342710000 3.3357010000
C 1.9671890000 1.5764290000 2.0967370000
C 3.0056400000 1.4388570000 -2.2227540000
C 3.7751220000 0.6827770000 -3.1136760000
C 3.5700610000 -0.6992540000 -3.1897470000
C 2.5902920000 -1.2716680000 -2.3819270000
N 1.8411360000 -0.5292960000 -1.5279690000
H -3.2998650000 3.0186340000 -0.9779510000
H -4.7153820000 -3.7291880000 1.1212340000
H -2.6007100000 -5.0795320000 1.4529470000
H -0.3920980000 -4.0400910000 0.8230850000
H 0.9963410000 3.5833300000 0.4294070000
H 2.6517600000 3.1812580000 -0.1037100000
H 1.3846710000 3.5289600000 -1.3103910000
H 0.8183180000 -2.0749040000 2.3655080000
H 1.7061450000 -0.9309360000 4.4067210000
H 2.4961180000 1.4724110000 4.1937510000
H 2.2844380000 2.6144010000 1.9923860000
H 3.1622370000 2.5151850000 -2.1491250000
H 4.5303680000 1.1728820000 -3.7353120000
H 4.1541540000 -1.3341420000 -3.8609070000
H 2.3769510000 -2.3436530000 -2.3977790000
Fe 0.4106810000 -1.4346240000 -0.5245350000
H -0.8505920000 3.4937860000 -0.9617860000
N 1.4607610000 -2.6924620000 -0.0243450000
H 2.3633930000 -2.5920210000 0.4773750000
N -0.2770660000 -1.9196490000 -2.1325450000
H 0.0166770000 -1.4383350000 -2.9907720000
H -1.2380130000 -2.2680340000 -2.2335960000
H -4.5307390000 -1.3939320000 0.2274540000
H -4.1170420000 0.7092350000 -0.4405700000

[(bpyPy$_2$Me)Fe(NH)(NH$_3$)]$^{3+}$, multiplicity = 2
C -2.5712280000 2.2178060000 -0.9244260000
C -3.0404620000 0.9284080000 -0.6477880000
C -2.1012650000 -0.0852620000 -0.4272160000
N -0.7705480000 0.1827520000 -0.5421920000
C -0.3008830000 1.4384110000 -0.6547530000

C -1.1957630000 2.4919110000 -0.8845300000
C -3.6404530000 -1.9649730000 0.3409270000
C -2.3720780000 -1.4467620000 0.0496240000
C -3.7418760000 -3.2539960000 0.8773340000
C -2.5754500000 -3.9942470000 1.1044650000
C -1.3371510000 -3.4344950000 0.7740110000
N -1.2433500000 -2.1872140000 0.2691490000
C 1.2024080000 1.6004320000 -0.3559550000
C 1.5760260000 3.0896330000 -0.2897540000
C 2.0512150000 0.8559290000 -1.3993340000
C 1.4395390000 0.8939320000 1.0069640000
N 1.0901310000 -0.4136590000 1.1217190000
C 1.2095750000 -1.0691570000 2.3009040000
C 1.7191110000 -0.4396080000 3.4351800000
C 2.1123280000 0.8976740000 3.3382280000
C 1.9656540000 1.5675760000 2.1175620000
C 3.0240870000 1.4969890000 -2.1807580000
C 3.8024400000 0.7539990000 -3.0734640000
C 3.6037640000 -0.6283190000 -3.1627700000
C 2.6207620000 -1.2121900000 -2.3696260000
N 1.8564830000 -0.4799050000 -1.5176300000
H -3.2806960000 3.0277400000 -1.1153540000
H -4.7232360000 -3.6725840000 1.1163780000
H -2.6075080000 -5.0004060000 1.5289180000
H -0.4009170000 -3.9833090000 0.9076010000
H 0.9733160000 3.6033420000 0.4735390000
H 2.6392690000 3.2151110000 -0.0383990000
H 1.3896230000 3.5731950000 -1.2604150000
H 0.8875760000 -2.1126150000 2.3252160000
H 1.8076020000 -1.0057220000 4.3658790000
H 2.5260010000 1.4244310000 4.2029140000
H 2.2539230000 2.6156760000 2.0349680000
H 3.1764320000 2.5726760000 -2.0894920000
H 4.5621340000 1.2526650000 -3.6823840000
H 4.1991890000 -1.2590480000 -3.8278560000
H 2.4350880000 -2.2893450000 -2.4051090000
Fe 0.4349780000 -1.3973700000 -0.4846550000
H -0.8364190000 3.5133510000 -1.0118580000
N 1.3753370000 -2.6806310000 -0.1166570000
H 2.3493850000 -2.9071240000 0.1738350000
N -0.3375670000 -2.0178310000 -2.2341420000
H -1.1797250000 -1.4962890000 -2.5132370000
H -0.5971940000 -3.0119080000 -2.1834890000
H 0.3275570000 -1.9216700000 -3.0134780000
H -4.5331570000 -1.3640010000 0.1543140000
H -4.1105950000 0.7214480000 -0.5781100000

[(bpyPy$_2$Me)Fe(NH)(NH$_3$)]$^{3+}$, multiplicity = 4
C -2.5929170000 2.2451530000 -0.9354480000
C -3.0619770000 0.9526910000 -0.6685440000
C -2.1216000000 -0.0597400000 -0.4482420000
N -0.7909410000 0.2088430000 -0.5506700000
C -0.3246110000 1.4637540000 -0.6516240000
C -1.2192660000 2.5195620000 -0.8832730000
C -3.6569570000 -1.9546550000 0.2937580000
C -2.3913700000 -1.4214080000 0.0300680000
C -3.7530760000 -3.2405040000 0.8417350000
C -2.5844050000 -3.9679150000 1.1084160000
C -1.3475000000 -3.3998640000 0.7997490000
N -1.2568460000 -2.1529450000 0.2846040000
C 1.1776710000 1.6209450000 -0.3439570000
C 1.5588170000 3.1081840000 -0.2807380000
C 2.0178410000 0.8714620000 -1.3917500000
C 1.4219550000 0.9150030000 1.0197140000
N 1.1329430000 -0.4127540000 1.1191730000
C 1.3300890000 -1.0917900000 2.2744410000
C 1.8233840000 -0.4598770000 3.4137300000
C 2.1362410000 0.9002770000 3.3377550000
C 1.9365270000 1.5886710000 2.1325170000
C 2.9806480000 1.5058550000 -2.1875150000
C 3.7704900000 0.7514620000 -3.0626920000
C 3.5981800000 -0.6362750000 -3.1137910000
C 2.6249020000 -1.2155790000 -2.3054620000
N 1.8404470000 -0.4716530000 -1.4831720000
H -3.3021360000 3.0546940000 -1.1286400000
H -4.7353850000 -3.6704470000 1.0559960000
H -2.6191290000 -4.9715600000 1.5379250000
H -0.4075030000 -3.9368060000 0.9530270000
H 0.9590770000 3.6265990000 0.4817570000
H 2.6231380000 3.2284530000 -0.0306300000
H 1.3730010000 3.5914460000 -1.2516490000
H 1.0844140000 -2.1566360000 2.2711110000
H 1.9653830000 -1.0387490000 4.3295860000
H 2.5394880000 1.4300240000 4.2056640000
H 2.1840920000 2.6483950000 2.0668480000
H 3.1219680000 2.5848480000 -2.1187050000
H 4.5219160000 1.2469320000 -3.6845250000
H 4.2041720000 -1.2734630000 -3.7628900000
H 2.4554850000 -2.2958290000 -2.3050280000
Fe 0.3914290000 -1.3530260000 -0.4459780000
H -0.8588970000 3.5417510000 -1.0019950000
N 1.3922250000 -2.7875190000 -0.2000910000

H 2.2779590000 -3.2133830000 0.1190460000
N -0.3095100000 -2.0449910000 -2.2145710000
H -1.1055230000 -1.4989100000 -2.5725060000
H -0.6114260000 -3.0248680000 -2.1358590000
H 0.4065770000 -2.0218470000 -2.9528260000
H -4.5538340000 -1.3702650000 0.0774810000
H -4.1322390000 0.7437010000 -0.6065320000

[(bpyPy$_2$Me)Fe(NH$_2$)(NH$_2$)]$^{3+}$, multiplicity = 4
C -2.5651280000 2.2335530000 -0.9511030000
C -3.0440630000 0.9440540000 -0.6874630000
C -2.1113290000 -0.0741810000 -0.4618350000
N -0.7804160000 0.1908020000 -0.5525520000
C -0.3010000000 1.4399560000 -0.6519850000
C -1.1905060000 2.5000320000 -0.8903980000
C -3.6554290000 -1.9619730000 0.2697230000
C -2.3865350000 -1.4313330000 0.0180820000
C -3.7605480000 -3.2408710000 0.8308580000
C -2.5955510000 -3.9620640000 1.1307550000
C -1.3535530000 -3.3976450000 0.8371850000
N -1.2531910000 -2.1609080000 0.2996840000
C 1.2025800000 1.5933220000 -0.3439920000
C 1.5865670000 3.0798940000 -0.2822090000
C 2.0382410000 0.8414180000 -1.3931760000
C 1.4436360000 0.8885710000 1.0202410000
N 1.1268210000 -0.4317570000 1.1216650000
C 1.2863510000 -1.0995050000 2.2890570000
C 1.7909480000 -0.4726970000 3.4266850000
C 2.1455050000 0.8762430000 3.3410280000
C 1.9681890000 1.5597700000 2.1299170000
C 3.0127720000 1.4706160000 -2.1794110000
C 3.7817690000 0.7167560000 -3.0731660000
C 3.5715370000 -0.6638470000 -3.1578000000
C 2.5898900000 -1.2392580000 -2.3564510000
N 1.8375450000 -0.4960070000 -1.5044210000
H -3.2679050000 3.0473560000 -1.1496520000
H -4.7459320000 -3.6699800000 1.0321160000
H -2.6364690000 -4.9589610000 1.5751030000
H -0.4195220000 -3.9334020000 1.0243470000
H 0.9875300000 3.5999950000 0.4797040000
H 2.6507070000 3.1979240000 -0.0306700000
H 1.4037340000 3.5628740000 -1.2538200000
H 0.9971760000 -2.1535600000 2.3060800000
H 1.9030830000 -1.0461720000 4.3500590000
H 2.5568570000 1.4021390000 4.2074120000
H 2.2388580000 2.6133520000 2.0583950000

H 3.1762580000 2.5449760000 -2.0912400000
H 4.5417600000 1.2077690000 -3.6880300000
H 4.1534400000 -1.2995430000 -3.8300360000
H 2.3824020000 -2.3104430000 -2.3913560000
Fe 0.3818730000 -1.3811050000 -0.4630510000
H -0.8235760000 3.5199950000 -1.0077450000
N 1.4570180000 -2.8580050000 -0.1571200000
H 1.4052930000 -3.7313660000 -0.6980010000
H 2.2612890000 -2.8647490000 0.4867180000
N -0.2172930000 -2.0416540000 -2.0852080000
H -0.8674670000 -2.8338130000 -2.1770260000
H -0.0062370000 -1.6103970000 -2.9948830000
H -4.5483600000 -1.3793740000 0.0333010000
H -4.1159860000 0.7415120000 -0.6321940000

[(bpyPy$_2$Me)Fe(NH$_2$)(NH$_2$)]$^{3+}$, multiplicity = 2
C -2.5498790000 2.2118680000 -0.9257390000
C -3.0282910000 0.9227650000 -0.6644420000
C -2.0970270000 -0.0967110000 -0.4410090000
N -0.7655800000 0.1700770000 -0.5331790000
C -0.2818320000 1.4215370000 -0.6414390000
C -1.1737080000 2.4777090000 -0.8744040000
C -3.6473360000 -1.9713940000 0.2981680000
C -2.3736380000 -1.4600170000 0.0195170000
C -3.7616890000 -3.2548950000 0.8440660000
C -2.5994180000 -3.9899250000 1.1043380000
C -1.3552510000 -3.4364340000 0.7835410000
N -1.2444730000 -2.2006980000 0.2549240000
C 1.2237940000 1.5864970000 -0.3558940000
C 1.5944500000 3.0762760000 -0.2859440000
C 2.0582660000 0.8514200000 -1.4173910000
C 1.4718580000 0.8736280000 1.0005930000
N 1.1062650000 -0.4312280000 1.1016670000
C 1.2026420000 -1.0812350000 2.2853740000
C 1.7202920000 -0.4653810000 3.4238600000
C 2.1436370000 0.8631010000 3.3291350000
C 2.0101240000 1.5385520000 2.1092250000
C 3.0446740000 1.4874480000 -2.1847670000
C 3.8059330000 0.7438670000 -3.0926030000
C 3.5749890000 -0.6313340000 -3.2117480000
C 2.5793940000 -1.2098370000 -2.4297120000
N 1.8352230000 -0.4767490000 -1.5612820000
H -3.2530200000 3.0269680000 -1.1180800000
H -4.7475300000 -3.6697780000 1.0706220000
H -2.6374150000 -4.9872390000 1.5484680000
H -0.4325250000 -3.9939700000 0.9616140000

H 0.9972450000 3.5854250000 0.4847500000
H 2.6591950000 3.2006850000 -0.0403470000
H 1.4033870000 3.5646720000 -1.2532850000
H 0.8538720000 -2.1167070000 2.3147900000
H 1.7850480000 -1.0300940000 4.3572890000
H 2.5647130000 1.3803670000 4.1960530000
H 2.3187580000 2.5810220000 2.0295650000
H 3.2211970000 2.5571960000 -2.0717200000
H 4.5765020000 1.2372930000 -3.6920880000
H 4.1543240000 -1.2598460000 -3.8929580000
H 2.3650960000 -2.2807400000 -2.4816360000
Fe 0.4097390000 -1.3899000000 -0.5387250000
H -0.8066660000 3.4969620000 -0.9966260000
N 1.4669290000 -2.7673260000 -0.0743320000
H 1.2832920000 -3.7510900000 -0.3225120000
H 2.3103580000 -2.6752740000 0.5113220000
N -0.2198610000 -2.0496860000 -2.0866110000
H -0.9533000000 -2.7698030000 -2.1769200000
H 0.0554430000 -1.6903170000 -3.0142380000
H -4.5346560000 -1.3674900000 0.0959480000
H -4.0999140000 0.7180730000 -0.6130730000

MeCN, multiplicity = 1
C -7.9305190000 -10.7267220000 1.0655210000
C -6.4737070000 -10.6286630000 1.1098320000
H -8.2821500000 -11.4458010000 1.8240930000
H -8.2537290000 -11.0687220000 0.0681850000
H -8.3795340000 -9.7405370000 1.2700280000
N -5.3082150000 -10.5499520000 1.1453180000

NH_3, multiplicity = 1
N -3.4062600000 2.0314360000 -0.0471600000
H -2.3807850000 1.9549480000 0.0223060000
H -3.6991510000 2.1535560000 0.9330710000
H -3.6990690000 1.0670120000 -0.2609860000

N_2H_4, multiplicity = 1
N -5.65593157558449 -0.68732489801612 0.06171968010262
N -5.58810331553809 0.79856577094464 -0.06171888099823
H -5.08293721478638 1.08382092202259 0.79073703827746
H -6.54838235021633 1.09907279415619 0.16372799703163
H -4.69565325326846 -0.98783209975199 -0.16372998040384
H -6.16110020380625 -0.97258000455531 -0.79073473880964

Ferrocene, multiplicity = 1
C 1.1627240000 0.3769360000 -1.6333370000

C 0.7167690000 -0.9903940000 -1.6334520000
C -0.7212130000 -0.9887400000 -1.6324780000
C -1.1639780000 0.3796340000 -1.6318610000
C 0.0003550000 1.2231080000 -1.6325230000
H 2.2018030000 0.7129070000 -1.6174890000
H 1.3578040000 -1.8747880000 -1.6190580000
H -1.3642490000 -1.8716700000 -1.6173630000
H -2.2022550000 0.7180140000 -1.6147190000
H 0.0016210000 2.3155870000 -1.6151990000
Fe 0.0000100000 -0.0004580000 0.0003460000
C -0.7168910000 -0.9906570000 1.6335370000
C -1.1627810000 0.3767810000 1.6335310000
C -0.0002810000 1.2228930000 1.6328970000
C 1.1640490000 0.3792990000 1.6321590000
C 0.7211570000 -0.9890990000 1.6326470000
H -1.3580070000 -1.8749910000 1.6189140000
H -2.2018330000 0.7128450000 1.6177600000
H -0.0014710000 2.3153770000 1.6157350000
H 2.2023510000 0.7176150000 1.6152970000
H 1.3641030000 -1.8720960000 1.6174310000

Ferrocenium, multiplicity = 2
C 1.0034420000 0.7144730000 -1.7331470000
C 1.0035960000 -0.7133810000 -1.7318490000
C -0.3564340000 -1.1611110000 -1.6909750000
C -1.2040500000 0.0005970000 -1.6691700000
C -0.3563670000 1.1620220000 -1.6928500000
H 1.8888220000 1.3527350000 -1.7038460000
H 1.8891410000 -1.3513810000 -1.7022350000
H -0.6866650000 -2.2006720000 -1.6539200000
H -2.2949760000 0.0008010000 -1.6290140000
H -0.6864970000 2.2016360000 -1.6560550000
Fe -0.0000040000 -0.0000010000 -0.0000120000
C -1.0034430000 -0.7144700000 1.7331380000
C -1.0035920000 0.7133860000 1.7318380000
C 0.3564410000 1.1611120000 1.6909570000
C 1.2040500000 -0.0006030000 1.6691450000
C 0.3563630000 -1.1620260000 1.6928340000
H -1.8888300000 -1.3527250000 1.7039000000
H -1.8891400000 1.3513880000 1.7022790000
H 0.6866770000 2.2006740000 1.6539250000
H 2.2949790000 -0.0008130000 1.6289990000
H 0.6864890000 -2.2016420000 1.6560600000

TEMPO, multiplicity = 2
O -1.2492590000 -0.2906870000 0.4243790000

N -2.4129740000 -0.5340430000 -0.0687860000
C -3.4514420000 0.5490390000 0.1228870000
C -4.6960800000 0.2509660000 -0.7421770000
H -5.5014500000 0.9355480000 -0.4207760000
H -4.4638250000 0.5014720000 -1.7949570000
C -5.1476780000 -1.2107660000 -0.6758460000
H -5.4361800000 -1.4866460000 0.3554200000
H -6.0455870000 -1.3534200000 -1.3025480000
C -4.0144930000 -2.1081980000 -1.1806130000
H -3.7869970000 -1.8351070000 -2.2285590000
H -4.3164130000 -3.1712540000 -1.1859230000
C -2.7198870000 -1.9890100000 -0.3460300000
C -3.8038920000 0.6307340000 1.6263430000
H -2.8760220000 0.7150000000 2.2158510000
H -4.3596980000 -0.2576200000 1.9695330000
H -4.4287020000 1.5213850000 1.8144360000
C -2.8078220000 1.8741840000 -0.3275270000
H -2.5005240000 1.8157310000 -1.3861620000
H -1.9229070000 2.1052830000 0.2851840000
H -3.5423850000 2.6909560000 -0.2199830000
C -2.8390140000 -2.7330520000 1.0051460000
H -1.9496110000 -2.5175820000 1.6208750000
H -2.8942580000 -3.8211660000 0.8270550000
H -3.7387810000 -2.4294760000 1.5664850000
C -1.5302660000 -2.5558200000 -1.1433170000
H -0.6015970000 -2.4934790000 -0.5549750000
H -1.3917840000 -1.9954650000 -2.0842510000
H -1.7274370000 -3.6127590000 -1.3915770000

TEMPOH, multiplicity = 1

O 1.7239200000 0.5195110000 0.6071560000
N 0.5534440000 0.3613860000 -0.2439160000
C -0.4595910000 1.3790490000 0.1817410000
C -1.7239750000 1.1449220000 -0.6810960000
H -2.5119790000 1.8386490000 -0.3351500000
H -1.4870780000 1.4192890000 -1.7271180000
C -2.2101380000 -0.3080670000 -0.6503750000
H -2.5384080000 -0.5847590000 0.3688100000
H -3.0925410000 -0.4249890000 -1.3052220000
C -1.0831280000 -1.2344750000 -1.1182140000
H -0.8361020000 -0.9931040000 -2.1697860000
H -1.3998570000 -2.2935460000 -1.0955690000
C 0.2054860000 -1.0948060000 -0.2712530000
C -0.7963730000 1.3664520000 1.6928030000
H 0.1334780000 1.3495940000 2.2837190000

H -1.4123610000 0.5014020000 1.9846770000
H -1.3576380000 2.2812190000 1.9552670000
C 0.1382480000 2.7576460000 -0.1734590000
H 0.4358270000 2.7807910000 -1.2365620000
H 1.0277660000 2.9682800000 0.4435080000
H -0.6054260000 3.5545730000 0.0045100000
C 0.0393240000 -1.7467730000 1.1238350000
H 0.8885640000 -1.4675830000 1.7693970000
H 0.0283560000 -2.8466450000 1.0207360000
H -0.8953500000 -1.4484380000 1.6253240000
C 1.3640760000 -1.8028180000 -1.0063710000
H 2.2919150000 -1.7559690000 -0.4116310000
H 1.5480220000 -1.3194310000 -1.9820880000
H 1.1147770000 -2.8646390000 -1.1788790000
H 2.4087420000 0.8122760000 -0.0237950000

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