Activation of Ammonia and Hydrazine by Electron Rich Fe(II) Complexes Supported by a Dianionic Pentadentate Ligand Platform Through a Common Terminal Fe(III) Amido Intermediate

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General

Unless mentioned otherwise, manipulation and storage of all oxygen and moisture sensitive materials were performed under an argon atmosphere in an M-Braun glovebox. Air and moisture sensitive reactions were performed using a double manifold high vacuum line using standard Schlenk techniques. Passage of argon through an OxisorBW scrubber (Matheson Gas Products) removed any residual oxygen and moisture. Before use, all glassware was stored in a 135 °C oven for a minimum of one hour, and then subjected to dynamic vacuum for at least 20 min after transfer to the glovebox anti-chamber or the vacuum line. All anhydrous solvents were prepared by passing through an M-Braun SP-800 solvent purification system and were stored in 500 mL thick-walled vessels over sodium/benzophenone ketal or CaH₂. All dried solvents were degassed, and vacuum distilled prior to use. ¹⁵NH₃ (98% purity) was purchased from Millipore Sigma and used as received using a corrosive gas regulator for lecture bottles. ¹⁴NH₃ anhydrous was purchased from Praxair and passed through two columns of KOH pallets prior to use. Chemicals were obtained from common vendors and used as received unless mentioned otherwise. The syntheses of the dianionic pentadentate [²⁴Β₂Pz₂Py]H₂Li ligands,¹ ²¹Ph-THF¹ and ¹¹Ph¹ have previously been reported. 2,4,6-tri-tert-butyl phenoxy radical was synthesized according to a literature procedure.³

Physical Methods

¹H, ¹³C{¹H} chemical shifts are referenced to the residual solvent signals of C₆D₆ (¹H, 7.16 ppm; ¹³C{¹H}, 128.06 ppm), THF-d₈ (¹H, 3.58, 1.72 ppm; ¹³C{¹H}, 67.21, 25.31 ppm) and toluene-d₈ (¹H, 7.09, 7.01, 6.97, 2.08 ppm; ¹³C{¹H}, 137.48, 128.87, 127.96, 125.13, 20.43 ppm). ¹H, ¹¹B, ¹³C{¹H}, ¹⁵N, ¹⁵N{¹H}, ¹H-¹H-COSY, ¹H-¹³C-HSQC, ¹H-¹³C-HMBC and ¹H-¹⁵N-HMBC NMR experiments were performed at room temperature on Bruker RDQ-400, or Ascend-500 or Avance-600 MHz spectrometers and analyzed with MestReNova software (v8.1, Mestrelab Research S.L.). All ¹¹B chemical shifts are relative to BF₃-OEt₂. All ¹⁵N NMR spectra are externally referenced to 60% CH₃¹⁵NO₂ (δCH₃¹⁵NO₂ = δ₁⁵NH₃ - 380) in CDCl₃. Solution magnetic moments were measured using Evans method.⁴

Elemental analysis was performed on site by Johnson Li using a Perkin Elmer Model 2400 series II analyzer.

Solution high resolution-mass spectrometry experiments were performed on a Kratos MS-80 spectrometer by Wade White (direct ESI-MS or APCI-MS) on samples prepared in the glovebox in a gas tight syringe.
Resonance Raman spectra were recorded at room temperature on a ND:YAG source with a Bruker RAM II FT-Raman instrument with an excitation wavelength of 1064 nm.

Infrared spectra were collected on a Nicolet Avatar FT-IR spectrometer, and samples were prepared as a KBr pellet.

Absorption spectrum was measured using a Varian Cary-50 single-beam spectrophotometer. The solution was placed in a co-joint UV-vis cuvette of 2 mm path length.

Low temperature $^{57}$Fe Mössbauer measurements were performed using a See Co. MS4 Mössbauer spectrometer integrated with a Janis SVT-400T He/N2 cryostat for measurements at 80 K. All samples were prepared in an inert atmosphere glovebox equipped with a liquid nitrogen fill port to enable sample freezing to 77 K within the glovebox. Each sample was loaded into a Delrin Mössbauer sample cup for measurements and loaded under liquid nitrogen. Isomer shifts were determined relative to α-Fe at 298 K. All Mössbauer spectra were fit using the program WMoss (See Co). Errors of the fit analyses were the following: δ ± 0.02 mm/s and ΔE_Q ± 3%. For multi-component fits the quantitation errors were ± 3% (e.g. 70 ± 3%).

Electrochemical measurements were carried out in a glovebox under an argon atmosphere with a CH instrument potentiostat and C-3 cell stand. A glassy carbon working electrode, a platinum counter electrode and a silver wire pseudo reference electrode were used for cyclic voltammetry in THF with 0.1 M [Bu$_4$N][PF$_6$] electrolyte. Ferrocene (E$_{Fc+/0}$ = 0.64 V vs SHE) was added during each experiment as an internal reference.

X-ray crystallography was carried out on either a Nonius Kappa CCD diffractometer using graphite-monochromated Mo Kα radiation or a Bruker Smart APEX II three-circle diffractometer using Cu Kα radiation. Crystals suitable for X-ray diffraction were coated in Paratone 8277 oil (Exxon) and mounted on a glass fiber before data collection. The crystals were kept at 173 K during data collection. Diffractions spots were integrated and scaled with SAINT$^5$ and the space group was determined with XPREP.$^6$ Using Olex2,$^7$ the structures were solved with the ShelXT$^8$ structure solution program using Intrinsic Phasing and refined with the ShelXL$^9$ refinement package using Least Squares minimization. Full crystallography details can be found in independently uploaded .cif files.

**Computational Details**

All calculations were carried out with the Gaussian09 program$^{10}$ at the DFT level using the hybrid functional B3PW91.$^{11,12}$ For Fe, the relativistic energy-consistent pseudopotential of the Stuttgart-Köln ECP library was used in combination with its adapted segmented basis.$^{13}$ For all other atoms, a standard 6-31G** basis set was used.$^{14,15}$ Electronic energies and enthalpies
were computed at $T = 298$ K in the gas phase. All stationary points have been identified as minima (number of imaginary frequencies $N_{\text{imag}} = 0$) or transition states ($N_{\text{imag}} = 1$) and IRC calculations were carried out from all transition states.
Syntheses.

Synthesis of $^{57}\text{FeBr}_2$. $^{57}\text{Fe}$ metal (100 mg, 1.76 mmol) and a small stirrer bar were transferred to a 25 mL Schlenk flask equipped with a 14/20 septa under an argon atmosphere. Under a flow of Ar, a needle was added to the septa and fresh concentrated hydrobromic acid (48%, 500 μL) was added dropwise using a 3 mL syringe resulting in hydrogen evolution. Once hydrogen evolution had slowed, the septa was replaced with a glass stopper and the flask was heated to 80 °C with stirring for 2 hours under a light dynamic flow of Ar. The solution was then allowed to cool to room temperature and the glass stopper was replaced with a 14/20 septa. Degassed methanol (1 mL) was added via syringe all at once. The resulting mixture was stirred for 30 min at room temperature until it went colorless (see picture below). The solvents were then removed under vacuum. The remaining white/yellow solid was heated at 100 °C under a vacuum of 30 mtorr for 4 hours. The flask was allowed to cool to room temperature under vacuum and then moved to the glovebox where the pale-yellow solid was collected to yield $^{57}\text{FeBr}_2$ (360 mg, 93%). The same procedure was used to make $^{56}\text{FeBr}_2$ (1.8 g, 92%) using 0.50 g of $^{56}\text{Fe}$ metal.

Schlenk flask used for the reaction (mixture after 30 mins of stirring with MeOH):
Synthesis of $^{57}\text{Fe(HMDS)}_2$. $^{57}\text{Fe(HMDS)}_2$ was synthesized by modification of a literature procedure.\textsuperscript{16} LiHMDS was sublimed at 80 °C. 350 mg of freshly synthesized $^{57}\text{FeBr}_2$ (1 eq) was added to a 50 mL Schlenk flask equipped with a Teflon cap. 10 mL of Et\textsubscript{2}O was transferred. The solution was cooled to 0 °C and freshly sublimed LiHMDS (2 eq) dissolved in 15 mL of Et\textsubscript{2}O was added dropwise via canula. The suspension was allowed to stir at 0 °C for 30 min and slowly turned grey. The resulting mixture was stirred at room temperature for 20 h. All volatiles were removed \textit{in vacuo} and the resulting green residue was extracted with pentane (3 x 5 mL). The pentane extractions were combined, passed through a Celite plug and concentrated under vacuum to give a dark green oil. The oil was distilled under vacuum (30 mtorr) to afford a green fraction at 110 °C (oil bath temperature). The product was brought to a glovebox and stored at -40 °C. It solidified as a green solid (350 mg, 60%). $^1$H NMR (500 MHz, C\textsubscript{6}D\textsubscript{6}): δ 64.9 (36 H, broad singlet). The same procedure was used to make $^{56}\text{Fe(HMDS)}_2$ using $^{56}\text{FeBr}_2$.

Notes: $\text{Fe(HMDS)}_2$ is a highly reactive compound that reacts vigorously with water and oxygen. Handle with care in an inert atmosphere.

Extraction of $^{15}\text{N}_2\text{H}_4$.

Notes: We recommend doing this procedure first without the hydrazine sulfate to get a feel for the extraction process using liquid NH\textsubscript{3}. \textit{Hydrazine is highly toxic and explosive.} We do not recommend doing this procedure on a bigger scale than reported below. If you choose to do so, adjust the size of the apparatus. The frit is a medium porous frit.

Extraction. $^{15}\text{N}_2\text{H}_4$ was prepared according to a modified procedure.\textsuperscript{17} In an Ar glovebox, 95 % $^{15}$N-labeled hydrazine sulfate (0.500 g), purchased from Millipore-Sigma, was placed on the designed extraction apparatus (see picture below) equipped with a cold finger. The cold finger is roughly 2 cm above the frit. A 25 mL round bottom flask (RBF) was put on the other side of the extraction apparatus. The assembled apparatus was taken out of the glovebox and placed under vacuum on a Schlenk line, and then back filled with argon three times. The cold finger is equipped with a pressure-release Kontes cap and linked to a series of two empty bubblers and a third bubbler filled with 2 M HCl to quench NH\textsubscript{3}. An ice bath was put under the HCl bubbler during the NH\textsubscript{3} quench. After 30 mins under vacuum, 10 mL of liquid $^{14}$NH\textsubscript{3}, passed through two columns of KOH pallets, was condensed into the RBF by cooling the RBF with a liquid N\textsubscript{2} bath. The liquid N\textsubscript{2} bath was discarded and replaced with an acetone/dry ice bath to allow NH\textsubscript{3} to melt. In the meantime, the cold finger was charged with crushed dry ice and acetone and kept at -78 °C for the entire extraction procedure. The apparatus was then
filled with Ar and kept under static Ar. The acetone/dry ice bath was warmed to -15 to -5 °C to allow NH₃ to reflux gently. NH₃ (g) passed through the side arm (open through a Kontes cap), condensed on the cold finger (kept at -78 °C), and dipped onto the hydrazine sulfate. The white crystalline powder slowly “swells” upon NH₃ absorption. Once the solid was covered with a 5 mm layer of liquid NH₃, the liquid containing the ¹⁵N₂H₄/NH₃ mixture was pulled through the frit by cooling the RBF with a liquid N₂ bath and closing the side-arm Kontes cap. This represents the first extraction. The extraction procedure was repeated three times. The frit was kept cold by swabbing the exterior as needed with a dry ice/acetone mixture. After the fourth extraction (4 h) only ammonium sulfate was left on the frit (presumably). The apparatus was put under a gentle flow of Ar, the cold finger was emptied by pipetting the dry ice/acetone mixture out, and the ¹⁵N₂H₄/NH₃ solution mixture was allowed to warm up slowly to -10 °C. The pressure-release Kontes valve linked to the HCl bubbler was opened and the leftover ammonia was quenched slowly (30 mins) at -10 °C. The flask containing the hydrazine residue was quickly transferred onto the Schlenk line using a Y-Joint. Three freeze-pump-thaw cycles were performed to remove any trace amount of NH₃. The flask containing clean ¹⁵N₂H₄ was brought to the Ar glovebox and kept in the freezer at -40 °C (107 mg, 84%). ¹H NMR (500 MHz, C₆D₆) δ 2.28 (d, J₁₅N-₁H = 63.9 Hz, 4H). ¹⁵N NMR (51 MHz, C₆D₆) δ -331.0 (t, J₁₅N-₁H = 61.0 Hz, 2N). ¹⁵N{¹H} NMR (51 MHz, C₆D₆) δ -331.0 (s, 2N).

**Special apparatus designed for ¹⁵N₂H₄ extraction:**
Synthesis of $1_{\text{Tol}}$.

In a 100 mL round bottom flask equipped with a Y-joint and a Teflon cap, the lithium salt of the ligand $[\text{Tol}B_2\text{Pz}_3\text{Py}]\text{HLi}$ (0.40 g, 0.72 mmol) was dissolved in 10 mL of THF. Fe(HMDS)$_2$ (0.30 g, 0.79 mmol) dissolved in 5 mL of THF was added dropwise to the ligand solution. The resulting yellow solution was stirred at room temperature for 4 h and all volatiles were removed \textit{in vacuo}. The residual yellow/green solid was washed with 20 mL of pentane and dissolved in 40 mL of toluene. The green solution was left in the freezer (-40 °C) overnight. The solution was then passed through a short plug of Celite and the solvent was removed \textit{in vacuo}. The solid sample was transferred to a 100 mL thick-walled glass vessel equipped with a Kontes Teflon cap and placed in an oil bath at 25 °C. The vessel was evacuated under full dynamic
vacuum and the temperature in the oil bath was gradually increased to 150 °C and kept at this temperature for 4 h. During this time the yellow solid slowly turned green. After this time, the glass vessel was sealed, cooled down, and immediately brought to the glovebox. 0.34 g (70%) of 1Tol was collected and stored at -40 °C in the freezer. The product is paramagnetic and highly air and moisture sensitive. 1H NMR (500 MHz, C6D6) δ 74.4, 45.1, 19.8, 13.9, 9.8, 7.5, 7.0, 2.1. 11B NMR (161 MHz, C6D6) δ +38.4 (s). **Elemental Analysis** for C31H29B2N9Fe: C, 61.53; H, 4.83; N, 20.83. Found (%): C, 60.93; H, 5.02; N, 20.71. HRMS (APCI) m/z calcd for C31H29B2N9Fe: 605.2076 (M+) m/z found: 605.2093 (M+). **Evans Method**: Sample mass, 5.0 mg; Solvent, C6D6; Standard, Si2OMes (6%); μeff = 4.99; s = 2, n = 4. The same procedure was used to make 57Fe(HMDS)2 and 1ph using [^7B2Pz4Py]HLi.

**Synthesis of 1tol-15NH3.**

A 100 mL round bottom flask equipped with a Y-joint and a Teflon cap was charged with 1Tol (0.10 g, 0.17 mmol) dissolved in 20 mL of toluene. The solution was degassed and cooled to -78 °C. 15NH3 (3 eq.) was added and condensed using a liquid N2 bath. The frozen solution with frozen 15NH3 was allowed to melt using an isopropanol bath and was stirred at room temperature for 2 h. The solvent and excess 15NH3 were removed in vacuo. The brown solid was washed with 5 mL of pentane and dried to afford 99 mg (96%) of 1Tol-15NH3 as a brown solid. Crystals suitable for X-ray diffraction were grown by slow diffusion of pentane into a saturated solution of 1tol-15NH3 in benzene. 1H NMR (500 MHz, C6D6) δ 9.00 (4H, s), 8.33 (2H, d, JHH = 7.5 Hz), 8.23 (4H, d, JHH = 7.5 Hz), 7.35 (8H, m), 7.25 (4H, m), 6.60 (1H, s), 2.73 (3H, d, 1J15N-1H = 62.4 Hz, 15NH3), 2.40 (6H, s, -CH3). 11B NMR (161 MHz, C6D6) δ -1.6 (s). 15N signal was not observed. **Elemental Analysis** for C31H29B215NFen3C6H6: C, 63.46; H, 5.57; N, 20.00. Found (%): C, 63.75; H, 5.68; N, 19.46. IR (KBr) (cm⁻¹) for 1tol-15NH3: 3642; 3566. The same procedure was used to make 1tol-14NH3 using 14NH3; 571tol-15NH3 using 571tol and 1ph-15NH3 using 1ph.

**Synthesis of 2ph-15N.**

A two neck 100 mL round bottom flask equipped with a Y-joint and a Teflon cap, and a 14/20 septum was charged with 1ph-15NH3 (0.10 g, 1 eq, 0.17 mmol) dissolved in 20 mL of toluene. A solution of ArO- (0.22 g, 5 eq, 0.84 mmol) in 10 mL of toluene was added to the RBF through
the 14/20 septum under static Ar. The resulting dark green solution was stirred for 16 h at room temperature in the dark. All volatiles were removed in vacuo. The solid mixture was washed with 2x15 mL of pentane and dried under vacuum to afford 0.10 g (78%) of \( \text{2}_{\text{Ph}}^{-15}\text{N} \) as a green solid. \(^1\text{H} \text{NMR} \) (500 MHz, \( \text{C}_6\text{D}_6 \)) \( \delta \) 17.82 (1H, d, \(^1\text{J}_{\text{H}-1\text{H}} = 66.6 \text{ Hz, } 15\text{NH} \), 8.19 (2H, s), 8.00 (2H, s), 7.85 (2H, s), 7.77 (2H, s), 7.67 (2H, s), 7.53 (3H, s), 7.44 (4H, s), 6.93 (2H, s), 6.50 (2H, s), 5.76 (2H, s), 5.62 (2H, s), 4.60 (2H, s), 1.64 (9H, s, \( \text{O}^2\text{B}\text{u} \)), 0.83 (9H, \( \text{p}^2\text{B}\text{u} \)). \(^{11}\text{B} \text{NMR} \) (161 MHz, \( \text{C}_6\text{D}_6 \)) no signal. \(^{15}\text{N}^{(1)}\text{H} \text{NMR} \) (61 MHz, \( \text{C}_6\text{D}_6 \)) \( \delta \) +351.59.

**Elemental Analysis** for \( \text{C}_{43}\text{H}_{46}\text{B}_2\text{ON}_{10}\text{Fe} \): C, 64.85; H, 5.82; N, 17.59. Found (%): C, 64.94; H, 6.16; N, 17.01. HRMS (APCI) m/z calcd for \( \text{C}_{43}\text{H}_{46}\text{B}_2\text{ON}_{10}\text{Fe} \): 797.3345 (M\(^+\)) m/z found: 797.3356 (M\(^+\)). The same protocol was repeated with \( \text{1}_{\text{Ph}}^{-14}\text{NH}_3 \). The same protocol was repeated with \( \text{1}_{\text{Tol}}^{-15}\text{NH}_3 \) and the solid mixture was dissolved in 15 mL of pentane and put in the freezer (-40 °C). X-ray quality crystals of \( \text{2}_{\text{Tol}} \) were obtained after three weeks left in the freezer in the dark.

**Synthesis of \( \text{3}_{\text{Tol}}^{-\text{NH}_3} \).**

A 100 mL round bottom flask equipped with a Y-joint and a Teflon cap was charged with \( \text{1}_{\text{Tol}}^{-\text{NH}_3} \) (0.10 g, 0.16 mmol) dissolved in 20 mL of toluene. AgSbF\(_6\) (66 mg, 0.19 mmol) was added as a solid all at once. The resulting bright red solution was stirred for 1 h at room temperature. The solution was filtered through a syringe filter to remove Ag(0) and the solvent was removed in vacuo. The red solid was washed with 10 mL of pentane and dried in vacuo to afford 0.13 g (93%) of \( \text{3}_{\text{Tol}}^{-\text{NH}_3} \). Crystals suitable for X-ray diffraction were grown by slow diffusion of pentane into a saturated solution of \( \text{3}_{\text{Tol}}^{-\text{NH}_3} \) in benzene. \(^1\text{H} \text{NMR} \) (500 MHz, \( \text{C}_6\text{D}_6 \)) \( \delta \) 76.9, 12.1, 9.14, 7.4, 4.8, 3.6, 1.4, 0.5, -3.4, -18.8, -34.0. \(^{11}\text{B} \text{NMR} \) (161 MHz, \( \text{C}_6\text{D}_6 \)) +7.0 (s).

**Elemental Analysis** for \( \text{C}_{31}\text{H}_{35}\text{B}_2\text{Ni}_{10}\text{SbF}_6\text{Fe} \): C, 43.40; H, 3.76; N, 16.33. Found (%): C, 43.52; H, 3.99; N, 16.10. **Evans Method**: Sample mass, 4.6 mg; Solvent, \( \text{C}_6\text{D}_6 \); Standard, \( \text{Si}_2\text{OMe}_6 \) (6%); \( \mu_{\text{eff}} \) = 1.80; \( s = 1/2 \), \( n = 1 \). The same protocol was used to make \( \text{3}_{\text{Tol}}^{-15}\text{NH}_3 \) using \( \text{1}_{\text{Tol}}^{-15}\text{NH}_3 \).

**Synthesis of \( \text{3}_{\text{Tol}}^{-\text{Br}} \).**

A 100 mL round bottom flask equipped with a Y-joint and a Teflon cap was charged with \( \text{1}_{\text{Tol}} \) (0.10 g, 0.17 mmol) dissolved in 20 mL of toluene. Trityl bromide (59 mg, 0.18 mmol) dissolved in 5 mL of toluene was added dropwise. The resulting bright orange solution was stirred for 1 h at room temperature. The solvent was removed in vacuo. The orange solid was washed with
15 mL of hexanes and dried in vacuo to afford 0.11 g (95%) of 3_Tol-Br. Crystals suitable for X-ray diffraction were grown by slow diffusion of pentane into a saturated solution of 3_Tol-Br in benzene. \(^1\)H NMR (500 MHz, C\(_6\)D\(_6\)) \(\delta\) 107.7, 86.3, 55.8, 30.3, 2.6. \(^{11}\)B NMR (161 MHz, C\(_6\)D\(_6\)) no signal. **Elemental Analysis** for C\(_{31}\)H\(_{29}\)B\(_2\)FeN\(_9\)Br, C\(_6\)H\(_6\): C, 59.89; H, 4.78; N, 15.72. Found (%): C, 59.85; H, 4.50; N, 15.59. **HRMS (APCI)** m/z calcd for C\(_{31}\)H\(_{29}\)B\(_2\)FeN\(_9\)Br: 685.1338 (M+H)\(^+\) m/z found: 685.1338 (M+H)\(^+\). **Evans Method**: Sample mass, 5.0 mg; Solvent, C\(_6\)D\(_6\); Standard, Si\(_2\)OMe\(_6\) (6%); \(\mu_{\text{eff}}\) = 5.73; s = 5/2, n = 5.

**Synthesis of 3_Tol-Br.**

A 100 mL round bottom flask equipped with a Y-joint and a Teflon cap was charged with 1_Tol (0.10 g, 0.17 mmol) dissolved in 20 mL of toluene. XeF\(_2\) (14 mg, 0.083 mmol) dissolved in 5 mL of toluene was added dropwise. The resulting bright orange solution was stirred for 1 h at room temperature. All volatiles were removed in vacuo. The orange solid was washed with 10 mL of pentane and dried in vacuo to afford 92 mg (89%) of 3_Tol-Br. Crystals suitable for X-ray diffraction were grown by slow diffusion of pentane into a saturated solution of 3_Tol-Br in benzene. \(^1\)H NMR (500 MHz, C\(_6\)D\(_6\)) \(\delta\) 106.8, 85.8, 59.6, 55.8, 29.8, 20.4, 2.6. \(^{11}\)B NMR (161 MHz, C\(_6\)D\(_6\)) no signal. \(^{19}\)F\(^{\{1\}H}\) NMR (471 MHz, C\(_6\)D\(_6\)) no signal. **Elemental Analysis** for C\(_{31}\)H\(_{29}\)B\(_2\)FeN\(_9\)BrF: C, 59.66; H, 4.68; N, 20.20. Found (%): C, 59.52; H, 4.92; N, 19.79. **HRMS (APCI)** m/z calcd for C\(_{31}\)H\(_{29}\)B\(_2\)FeN\(_9\)BrF: 625.2070 (M+H)\(^+\) m/z found: 625.2097 (M+H)\(^+\). **Evans Method**: Sample mass, 5.0 mg; Solvent, C\(_6\)D\(_6\); Standard, Si\(_2\)OMe\(_6\) (6%); \(\mu_{\text{eff}}\) = 5.99; s = 5/2, n = 5.

**Synthesis of 4_Tol.**
A 100 mL round bottom flask equipped with a Y-joint and a Teflon cap was charged with 1_{Tol} (0.15 g, 0.25 mmol) dissolved in 25 mL of toluene. Neat anhydrous hydrazine (3.9 μL, 0.12 mmol) was added. The resulting dark forest green solution was stirred for 2 h at room temperature. The solvent was removed in vacuo. The solid mixture was washed with 5 mL of cold Et₂O and 4_{Tol} was isolated as a deep blue solid (52%). Crystals suitable for X-ray diffraction were grown by slow diffusion of pentane into a saturated solution of 4_{Tol} in benzene. ¹H NMR (500 MHz, C₆D₆) δ 18.66 (2H, s, H12), 7.97 (8H, d, ³J_HH = 7.6 Hz, H5), 7.88 (8H, d, ³J_HH = 2.5 Hz, H9), 7.84 (8H, d, ³J_HH = 2.5 Hz, H11), 7.47 (4H, d, ³J_HH = 7.6 Hz, H2), 7.28 (8H, d, ³J_HH = 7.6 Hz, H6), 6.88 (2H, t, ³J_HH = 7.6 Hz, H3), 5.95 (8H, t, ³J_HH = 2.5 Hz, H10), 2.36 (12H, s, H8). ¹³C{¹H} NMR (151 MHz, C₆D₆) δ 144.5 (s, C9), 138.1 (s, C11), 136.5 (s, C7), 135.8 (s, C5), 133.3 (s, C3), 129.1 (s, C6), 127.0 (s, C2), 106.4 (s, C10), 21.4 (s, C8). C1 and C4 not seen. ¹¹B NMR (161 MHz, C₆D₆) no signal. **Elemental Analysis** for C₆₂H₆₀B₄N₂₀Fe,C₆H₆: C, 61.95; H, 5.05; N, 21.25. Found (%): C, 61.61; H, 4.86; N, 20.72. **UV-vis** (C₆H₆) [λ_max]: 723, 388 nm. **rRaman** (1064 nm, cm⁻¹): 1321; 1248. 4_{Tol}⁻¹⁵N₂ was made via the same protocol using ¹⁵N₂H₄. ¹⁵N{¹H} NMR (61 MHz, C₆D₆) δ +476.44. **rRaman** (1064 nm, cm⁻¹): 1279; 1206.
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Figures S1-S32:

Figure S1. $^1$H NMR spectrum of 1$_{Ph}$-THF in C$_6$D$_6$.

Figure S2. $^1$H NMR spectrum of 1$_{Ph}$-MeCN in CD$_3$CN.
Figure S3. Mössbauer spectrum of a solid sample of $1_{\text{Tol}}$ collected at 80 K. The species in green corresponds to leftover $1_{\text{Tol}}$-THF as the parameters match the ones already reported for $1_{\text{Ph}}$-THF.\textsuperscript{1}

| $\delta$ (mm/s) | 1.04 | 1.13 | -0.03 |
|-----------------|------|------|-------|
| $\Delta E_0$ (mm/s) | 0.93 | 2.40 | 0.64 |
| % | 84 | 12 | 6 |

Figure S4. Mössbauer spectrum of a benzene solution of $1_{\text{Tol}}$ collected at 80 K under a dinitrogen atmosphere. The major species (orange) corresponds to a dinitrogen adduct and the parameters are indicative of a low spin Fe(II) complex. These parameters are also similar to the ones obtained for the diazone adduct, complex $4_{\text{Tol}}$ (Figure S29). The species in green corresponds to leftover $1_{\text{Tol}}$-THF as the parameters match the ones already reported for $1_{\text{Ph}}$-THF.\textsuperscript{1}

| $\delta$ (mm/s) | 0.44 | 1.13 |
|-----------------|------|------|
| $\Delta E_0$ (mm/s) | 0.43 | 2.40 |
| % | 90 | 10 |
Figure S5. Cyclic voltammograms of 1_{Tol} in THF at different scan rates (0.02 to 0.5 V/s) under argon. Reversible Fe(II)/Fe(III) redox couple at -0.44 V vs Fc/Fc⁺. Concentration of 1_{Tol}: 0.1 mM.

Figure S6. Stack ^1H NMR spectra of 1_{Tol}^{14}NH₃ (spectrum 1) and 1_{Tol}^{15}NH₃ (spectrum 2) in C₆D₆ with the proton assignments of the NH₃ ligand.
Figure S7. Mössbauer spectrum of a benzene solution of $^{1}$Tol-$^{15}$NH$_3$ collected at 80 K under a dinitrogen atmosphere. The major species (red) corresponds to $^{1}$Tol-$^{15}$NH$_3$ (LS) and the parameters for the species in orange match the dinitrogen adduct reported in Figure S4. The species in blue corresponds to leftover $^{1}$Tol-THF as the parameters match the ones already reported for $^{1}$Ph-THF.¹
Procedure for the reactivity of \( \text{Ph-nNH}_3 \) with ArO· to isolate \( \text{2Ph-nN} \)

A 25 mL two neck round bottom flask equipped with a Y-Joint with a Teflon cap and a 14/20 septum was charged with 20 mg of \( \text{1Ph-nNH}_3 \) (1 eq, 0.034 mmol) in 5 mL of toluene. A solution of ArO· (44 mg, 5 eq, 0.17 mmol) in 2 mL of toluene was added to the RBF through the 14/20 septum under static Ar. The resulting dark green solution was stirred for 16 h at room temperature in the dark. The solvent was removed in vacuo. The solid mixture was washed with 10 mL of pentane and dried under vacuum.

**Figure S8.** \(^1\text{H} \) NMR spectrum of \( \text{2Ph-}^{15}\text{N} \) in \( \text{C}_6\text{D}_6 \).
**Figure S9.** Zoomed $^1$H NMR stack spectra of $2_{\text{Ph}^{\text{15}} \text{N}}$ (spectrum 1) and $2_{\text{Ph}^{\text{14}} \text{N}}$ (spectrum 2) in C$_6$D$_6$.

| δ (mm/s) | 0.29 | 0.69 |
| ΔE$_0$ (mm/s) | 0.97 | 1.09 |
| % | 83 | 17 |

**Figure S10.** Mössbauer spectrum of a solid sample of $2_{\text{Ph}^{\text{15}} \text{N}}$ collected at 80 K under a dinitrogen atmosphere. The parameters are consistent with a low spin Fe(II) species.

**Figure S11.** $^1$H NMR spectrum of the reaction between $1_{\text{Tol}^{\text{15}} \text{NH}_3}$ and ArO· after 16 h at room temperature in C$_6$D$_6$. $2_{\text{Tol}^{\text{15}} \text{N}}$ is present, as well as ArOH.
**Procedure for the reactivity of $2_{Ph}^{15}N$ with ArO· and $^{15}NH_3$**

A J-Young tube equipped with a Teflon cap was charged with 5 mg of $2_{Ph}^{15}N$ (1 eq, 0.006 mmol) in ~0.5 mL of C$_6$D$_6$. ArO· (8 mg, 5 eq, 0.03 mmol) was added as a solid. The J-Young tube was degassed via three freeze-pump-thaw cycles and $^{15}NH_3$ (~ 5 eq) was added to the J-Young tube. The J-Young tube was covered with aluminum foil and stirred at room temperature for 16 h.

![Figure S12. $^1$H NMR spectrum of $2_{Ph}^{15}N$ + ArO· and $^{15}NH_3$ in C$_6$D$_6$.](image)
Procedure for the reactivity of $1_{\text{Ph}}$-$\text{NH}_3$ with ArO·

A J-Young tube equipped with a Teflon cap was charged with 20 mg of $1_{\text{Ph}}$-$\text{NH}_3$ (1 eq, 0.034 mmol) in ~0.5 mL of C$_6$D$_6$. ArO· (44 mg, 5 eq, 0.17 mmol) was added as a solid and the J-Young was stirred for 16 h at room temperature, covered with aluminum foil.

![Figure S13. Stack $^1$H NMR spectra of $1_{\text{Ph}}$-$\text{NH}_3$ + ArO· (spectrum 1) and ArOH (spectrum 2) in C$_6$D$_6$.](image-url)
Procedure for the analysis of the headspace of the reaction between \( \text{Ph}^-\text{NH}_3 \) and \( \text{ArO}^- \)

A 25 mL two neck round bottom flask (RBF) equipped with a Y-Joint with a Teflon cap and a 14/20 septum was charged with 20 mg of \( \text{Ph}^-\text{NH}_3 \) (1 eq, 0.034 mmol) in 5 mL of toluene. A solution of \( \text{ArO}^- \) (44 mg, 5 eq, 0.17 mmol) in 2 mL of toluene was added to the RBF through the 14/20 septum under static Ar. The resulting dark green solution was stirred for 16 h at room temperature in the dark. The headspace of the reaction was taken through the 14/20 septum using a 500 μL syringe. The headspace sample was analyzed by GC-MS.

**Figure S14.** GC-MS analysis of the headspace of the reaction between \( \text{Ph}^-\text{NH}_3 \) and \( \text{ArO}^- \) in toluene. The peak at m/z 56.1 corresponds to the formation of isobutene. Notably, no isobutane is observed at m/z 58.
**Procedure for the reaction between $3_{\text{Tol}}\text{-NH}_3^+$ and DBU**

A J-Young tube equipped with a septum screw cap was charged with 10 mg of $3_{\text{Tol}}\text{-NH}_3^+$ (1 eq, 0.012 mmol) in ~0.5 mL of $\text{C}_6\text{D}_6$. A $^1\text{H}$ NMR spectrum was recorded. DBU (stock solution, 1 eq) was added through the septum screw cap. Another $^1\text{H}$ NMR spectrum was recorded.

![Stack $^1\text{H}$ NMR spectra of $3_{\text{Tol}}\text{-NH}_3^+$ (spectrum 1) and $3_{\text{Tol}}\text{-NH}_3^+$ + DBU (spectrum 2) in $\text{C}_6\text{D}_6$. Large window.](image)

**Figure S15.** Stack $^1\text{H}$ NMR spectra of $3_{\text{Tol}}\text{-NH}_3^+$ (spectrum 1) and $3_{\text{Tol}}\text{-NH}_3^+$ + DBU (spectrum 2) in $\text{C}_6\text{D}_6$. Large window.
Figure S16. Stack $^1$H NMR spectra of $^1$Tol-NH$_3$ (spectrum 1) and $3_{^1}$Tol-NH$_3^+$ + DBU (spectrum 2) in C$_6$D$_6$.

Procedure for the reaction between $3_{^1}$Tol-$^{15}$NH$_3^+$, ArO· and DBU

A J-Young tube equipped with a septum screw cap was charged with 10 mg of $3_{^1}$Tol-$^{15}$NH$_3^+$ (1 eq, 0.012 mmol) and ArO· (15 mg, 5 eq, 0.058 mmol) in ~0.5 mL of C$_6$D$_6$. DBU (stock solution, 1 eq) was added through the septum screw cap. The reaction was stirred in the dark for 16 h at room temperature.

Figure S17. Stack $^1$H NMR spectra of $3_{^1}$Tol-$^{15}$NH$_3^+$ + ArO· + DBU (spectrum 1), $^1$Tol-$^{15}$NH$_3$ + ArO· (spectrum 2) and ArOH (spectrum 3) in C$_6$D$_6$. 
Figure S18. ORTEP diagrams for $3_{\text{Tor}}$-Br. Hydrogen, boron, carbon, nitrogen, bromine and iron atoms are white, pink, grey, light blue, gold and orange respectively. Thermal ellipsoids are shown at the 50% probability level. Calculated hydrogen atoms and the molecule of solvent are omitted for clarity. Selected bond distances (Å): Fe-Br, 2.455(1); Fe-N1, 2.214(3); Fe-N2, 2.067(3); Fe-N4, 2.110(4); Fe-N6, 2.075(4); Fe-N8, 2.094(3). Selected bond angles (°): N1-Fe-N2, 85.9(1); N2-Fe-N4, 91.9(1); N1-Fe-N10, 176.3(9). Selected metrical data are given in Table S2.

Figure S19. ORTEP diagrams for $3_{\text{Tor}}$-F. Hydrogen, boron, carbon, nitrogen, fluorine and iron atoms are white, pink, grey, light blue, bright yellow and orange respectively. Thermal ellipsoids are shown at the 50% probability level. Calculated hydrogen atoms and the molecule of solvent are omitted for clarity. Selected bond distances (Å): Fe-F, 1.8349(16); Fe-N1, 2.193(2); Fe-N2, 2.0737(18); Fe-N4, 2.1086(17). Selected bond angles (°): N1-Fe-N2, 85.69(6); N2-Fe-N4, 92.36(10); N1-Fe-F, 179.54(8). Selected metrical data are given in Table S2.
Procedure for the reaction between 3_{Tol}-Br and LiNH₂

A J-Young tube equipped with a Teflon cap was charged with 10 mg of 3_{Tol}-Br (1 eq, 0.015 mmol) in ~0.5 mL of THF-d₈. A ¹H NMR spectrum was recorded. LiNH₂ (1.2 eq, 0.018 mmol) was added as a solid. Another ¹H NMR spectrum was recorded.

Figure S20. ¹H NMR spectrum of 3_{Tol}-Br in THF-d₈.
Figure S21. Stack $^1$H NMR spectra of $3_{\text{Tol}}$-Br + LiNH$_2$ (spectrum 1) and $1_{\text{Tol}}$-$^{15}$NH$_3$ (spectrum 2) in THF-$d_8$. 
Procedure for the reaction between $3_{\text{Tol}}$-Br, ArO· and LiNH₂

A J-Young tube equipped with a Teflon cap was charged with 10 mg of $3_{\text{Tol}}$-Br (1 eq, 0.015 mmol) and ArO· (5 eq, 19 mg, 0.073 mmol) in ~0.5 mL of THF-$d_8$. LiNH₂ (1.2 eq, 0.018 mmol) was added as a solid. The reaction mixture was stirred for 2 days at room temperature in the dark.

![Figure S22. Stack $^1$H NMR spectra of $3_{\text{Tol}}$-Br + ArO· + LiNH₂ (spectrum 1), $2_{\text{Ph}}$-$^{15}$N (spectrum 2) and $1_{\text{Tol}}$-$^{15}$NH₃ (spectrum 3) in THF-$d_8$. Based on the $^1$H integration in spectrum 1 between the peaks corresponding to $2_{\text{Tol}}$ and the peaks corresponding to $1_{\text{Tol}}$-$^{15}$NH₃, a 30% NMR yield is found for the formation of $2_{\text{Tol}}$.](image-url)
Procedure for the reaction between $3_{\text{Tol}}$-F, ArO· and LiNH$_2$

A J-Young tube equipped with a Teflon cap was charged with 10 mg of $3_{\text{Tol}}$-F (1 eq, 0.016 mmol) and ArO· (5 eq, 21 mg, 0.080 mmol) in ~0.5 mL of THF-$d_8$. LiNH$_2$ (1.2 eq, 0.5 mg, 0.019 mmol) was added as a solid. The reaction mixture was stirred overnight at room temperature in the dark.

Figure S23. Stack $^1$H NMR spectra of $3_{\text{Tol}}$-F + ArO· + LiNH$_2$ (spectrum 1), $2_{\text{Ph}}$-$^{15}$N (spectrum 2) and $1_{\text{Tol}}$-$^{15}$NH$_3$ (spectrum 3) in THF-$d_8$. Based on the $^1$H integration in spectrum 1 between the peaks corresponding to $2_{\text{Tol}}$ and the peaks corresponding to $1_{\text{Tol}}$-$^{15}$NH$_3$, a 40% NMR yield is found for the formation of $2_{\text{Tol}}$. 
Procedure for the reaction between 1_{Tol} and ^{14}N_2H_4

A J-Young tube equipped with a Teflon cap was charged with 10 mg of 1_{Tol} (1 eq, 0.017 mmol) in ~0.5 mL of C_6D_6. Neat anhydrous ^{14}H_2H_4 (0.5 eq) was added and the J-Young was stirred for 2 h at room temperature.

Figure S24. Stack ^1H NMR spectra of 1_{Tol} + ^{14}N_2H_4 (spectrum 1), 1_{Tol}^{14}NH_3 (spectrum 2) and 4_{Tol} (spectrum 3) in C_6D_6.
Procedure for the reaction between $1_{\text{Tol}}$ and $^{14}\text{N}_2\text{H}_4$ at low temperature

A J-Young tube equipped with a Teflon cap was charged with 10 mg of $1_{\text{Tol}}$ (1 eq, 0.017 mmol) in ~0.5 mL of tol-$d_8$. Neat anhydrous $^{1}\text{H}_2\text{H}_4$ (0.5 eq) was added as a drop at the top of the J-Young tube and closed with a Teflon cap. The J-Young was cooled to -78 ºC using an acetone/dry ice bath. The solution was mixed just before inserting the J-Young tube into the NMR instrument for recording.

![Figure S25. $^1$H NMR spectrum of $1_{\text{Tol}} + ^{14}\text{N}_2\text{H}_4$ at 210 K in Tol-$d_8$.](image)
**Figure S26.** Stack $^1$H NMR spectra of $1_{\text{Tol}} + ^{14}$N$_2$H$_4$ (spectrum 1) and of $1_{\text{Tol}} + ^{15}$N$_2$H$_4$ (spectrum 2) at 210 K in Tol-$d_8$.

**Figure S27.** Stack $^1$H NMR spectra of $1_{\text{Tol}} + ^{14}$N$_2$H$_4$ at different temperatures (starting at 210 K) in Tol-$d_8$. 
Figure S28. UV-vis spectrum of $4_{\text{Tol}}$ in C$_6$H$_6$.

![UV-vis spectrum](image)

**Figure S29.** Mössbauer spectrum of a solid sample of $4_{\text{Tol}}$ collected at 80 K under a dinitrogen atmosphere. The parameters are consistent with a low spin Fe(II) species.

$\delta$ (mm/s) 0.41

$\Delta E_0$ (mm/s) 0.49
Figure S30. IR (KBr pallet) spectrum of $1_{10}$-^{15}NH$_3$. 
**Figure S31.** IR (KBr pallet) spectrum of $1_{\text{Tol}}^{14}\text{NH}_3$.

**Figure S32.** IR (KBr pallet) spectrum of $2_{\text{Ph}}^{15}\text{N}$.
NMR spectra of characterized compounds

Figure S33. $^1$H NMR spectrum of $^{15}$N$_2$H$_4$ in C$_6$D$_6$.

Figure S34. $^{15}$N($^1$H) NMR spectrum of $^{15}$N$_2$H$_4$ in C$_6$D$_6$. 
Figure S35. $^{15}\text{N}$ NMR spectrum of $^{15}\text{N}_2\text{H}_4$ in $\text{C}_6\text{D}_6$. 
Figure S36. $^1$H NMR spectrum of 1_Tol in C$_6$D$_6$.

Figure S37. $^{11}$B NMR spectrum of 1_Tol in C$_6$D$_6$. 
Figure S38. $^1$H NMR spectrum of $\text{1}_{\text{Tol}}{^{15}\text{NH}_3}$ in $\text{C}_6\text{D}_6$.

Figure S39. $^{11}$B NMR spectrum of $\text{1}_{\text{Tol}}{^{15}\text{NH}_3}$ in $\text{C}_6\text{D}_6$. 
Figure S40. $^1$H NMR spectrum of $1_{\text{ph}}^{15}\text{NH}_3$ in $\text{C}_6\text{D}_6$.

Figure S41. $^1$H NMR spectrum of $2_{\text{ph}}^{15}\text{N}$ in $\text{C}_6\text{D}_6$. 
**Figure S42.** $^{15}$N($^1$H) NMR spectrum of $2_{\text{Ph}-15\text{N}}$ in $\text{C}_6\text{D}_6$.

**Figure S43.** $^{15}$N-$^1$H HMBC of $2_{\text{Ph}-15\text{N}}$ in $\text{C}_6\text{D}_6$. 
Figure S44. $^1$H NMR spectrum of $\text{Tol-NH}_3^+$ in $\text{C}_6\text{D}_6$.

Figure S45. $^{11}$B NMR spectrum of $\text{Tol-NH}_3^+$ in $\text{C}_6\text{D}_6$. 
Figure S46. $^1$H NMR spectrum of $3_{\text{Tol-Br}}$ in C$_6$D$_6$.

Figure S47. $^1$H NMR spectrum of $3_{\text{Tol-F}}$ in C$_6$D$_6$. 
Figure S48. $^1$H NMR spectrum of 4$_{\text{Tol}}$ in C$_6$D$_6$.

Figure S49. $^{13}$C($^1$H) NMR spectrum of 4$_{\text{Tol}}$ in C$_6$D$_6$. 
Figure S50. $^1$H NMR spectrum of $4_{\text{Tol}}$($^{15}\text{N}$)$_2$ in C$_6$D$_6$.

Figure S51. $^{15}\text{N}(^1\text{H})$ NMR spectrum of $4_{\text{Tol}}$($^{15}\text{N}$)$_2$ in C$_6$D$_6$. 
Figure S52. $^{15}$N-1H HMBC of 4$_{\text{Tol}}$-$^{15}$N$_2$ in C$_6$D$_8$. 
Table S1

|                      | 1_{Tol}-NH₃ | 2_{Tol} | 3_{Tol}-NH₃⁺ |
|----------------------|-------------|---------|--------------|
| chemical formula     | C₃₇H₃₈B₂N₁₀Fe | C₄₅H₆₅B₂N₁₀OFe | C₃₇H₃₈B₂FeN₁₀SbFe |
| crystal colour       | Red         | blue    | Red          |
| Fw; F(000)           | 700.24; 2928.0 | 824.42; 3472.0 | 935.99; 1884.0 |
| T (K)                | 173         | 173     | 173          |
| wavelength (Å)       | 1.54178     | 1.54178 | 1.54178      |
| space group          | C2/c        | P2/c    | P2₁/n        |
| a (Å)                | 16.6461(14) | 18.7182(7) | 11.9800(2)  |
| b (Å)                | 17.2299(16) | 24.1607(11) | 25.1657(5)  |
| c (Å)                | 24.132(2)   | 23.6620(9) | 14.4893(3)  |
| α (deg)              | 90          | 90      | 90           |
| β (deg)              | 102.636(4)  | 98.957(3) | 114.2040(10) |
| γ (deg)              | 90          | 90      | 90           |
| Z                    | 8           | 8       | 4            |
| V (Å³)               | 6753.7(10)  | 10570.5(7) | 3984.29(14) |
| ρ_{calc} (g·cm⁻³)    | 1.377       | 1.036   | 1.560        |
| μ (mm⁻¹)             | 3.928       | 2.588   | 8.900        |
| θ range (deg);      | 7.48 to 136.582; 98.9% | 3.656 to 136.696; 98.4% | 7.024 to 140.13; 99.8% |
| completeness         |             |         |              |
| collected reflections; |           |         |              |
| R_o                  | 18406; 0.0778 | 19096; 0.0660 | 28060; 0.0373 |
| unique reflections;  |             |         |              |
| R_{int}              | 6138; 0.0545 | 19096; 0.0704 | 7559; 0.0422 |
| R₁; wR₂ [I > 2σ(I)] | 0.0441; 0.1222 | 0.0677; 0.1758 | 0.0447; 0.1117 |
| R₁; wR₂ [all data]  | 0.0937; 0.1395 | 0.0915; 0.1953 | 0.0593; 0.1195 |
| GOF                  | 1.057       | 1.029   | 1.040        |
| largest diff peak and hole | 0.59 and -0.48 | 1.15 and -0.57 | 1.42 and -0.97 |

^a R₁=Σ||F_o|-|F_c||/ΣF_o|

^b wR₂=Σ[w(F_o²-F_c²)^2]/Σ[w(F_o²)]^{1/2}
Table S2

|                  | $3_{\text{Tol}}$-Br       | $3_{\text{Tol}}$-F       | $4_{\text{Tol}}$         |
|------------------|---------------------------|--------------------------|--------------------------|
| chemical formula | C$_{43}$H$_{41}$B$_2$BrN$_9$Fe | C$_{31}$H$_{29}$B$_2$FeN$_9$ | C$_{65}$H$_{63}$B$_4$Fe$_2$N$_{20}$ |
| crystal colour   | Red                       | yellow                   | blue                     |
| $F_{w}$; $F(000)$| 841.23; 866.0              | 624.10; 1292.0            | 1279.29; 1330.0           |
| $T$ (K)          | 173                       | 173                      | 173                      |
| wavelength (Å)   | 0.71073                   | 0.71073                  | 1.54178                  |
| space group      | P-1                       | Pnma                     | P-1                      |
| $a$ (Å)          | 10.252(5)                 | 8.2450(4)                | 12.5636(9)               |
| $b$ (Å)          | 12.025(5)                 | 19.3287(10)              | 13.6840(10)              |
| $c$ (Å)          | 18.400(8)                 | 18.0484(9)               | 20.5835(17)              |
| $\alpha$ (deg)  | 104.192(5)                | 90                       | 98.128(5)                |
| $\beta$ (deg)   | 92.618(5)                 | 90                       | 100.359(5)               |
| $\gamma$ (deg)  | 112.901(5)                | 90                       | 115.218(5)               |
| $Z$              | 2                         | 4                        | 2                        |
| $V$ (Å$^3$)      | 2000.3(15)                | 2876.3(2)                | 3053.3(4)                |
| $\rho_{\text{calc}}$ (g·cm$^{-3}$) | 1.397                    | 1.441                    | 1.391                    |
| $\mu$ (mm$^{-1}$) | 1.420                    | 0.571                    | 4.291                    |
| $\theta$ range (deg); completeness | 3.836 to 51.996; 99.7% | 6.878 to 56.59; 99.7% | 4.502 to 136.71; 97.3% |
| collected reflections; $R_{\sigma}$ | 26732; 0.1247 | 19799; 0.0347 | 10913; 0.0660 |
| unique reflections; $R_{\text{int}}$ | 7875; 0.1088 | 3656; 0.0420 | 10913; 0.0678 |
| $R_1^a$; $wR_2^b$ [$I > 2\sigma(I)$] | 0.0521; 0.0779 | 0.0432; 0.1125 | 0.0546; 0.1325 |
| $R_1$; $wR_2$ [all data] | 0.1238; 0.0964 | 0.0657; 0.1285 | 0.0888; 0.1502 |
| GOF              | 0.997                     | 1.073                    | 1.036                    |
| largest diff peak and hole | 0.43 and -0.40 | 0.43 and -0.58 | 0.57 and -0.48 |

$^a$ $R_1 = \Sigma ||I_F - |F_c||| / \Sigma I_F$

$^b$ $wR_2 = (\Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2])^{1/2}$
## Cartesian Coordinates for calculated structures

### $1_{\text{Tol}}$ (HS)

| Atom | $x$          | $y$          | $z$          |
|------|--------------|--------------|--------------|
| Fe   | 5.80866300   | 11.15160000  | 18.06350400  |
| N    | 4.46838600   | 12.56937600  | 17.68814100  |
| N    | 3.26567600   | 12.52820600  | 18.31051300  |
| N    | 4.26962100   | 9.86949300   | 17.73424900  |
| N    | 3.11619500   | 10.09750300  | 18.40966000  |
| N    | 5.46621400   | 11.17912200  | 20.11993600  |
| N    | 7.12111800   | 9.71253000   | 18.27839500  |
| N    | 7.98043100   | 9.78550500   | 19.31660700  |
| N    | 7.35315700   | 12.45211900  | 18.26849300  |
| N    | 8.15496600   | 12.29194900  | 19.35224400  |
| C    | 4.35842200   | 13.43089200  | 16.67036400  |
| H    | 5.19673600   | 13.61180900  | 16.01245500  |
| C    | 3.06714700   | 13.96028500  | 16.61662700  |
| H    | 2.67084300   | 14.68190200  | 15.91735400  |
| C    | 2.40577600   | 13.34624600  | 17.66735600  |
| H    | 1.37847200   | 13.42736900  | 17.98603200  |
| C    | 4.02586400   | 8.90138900   | 16.84530900  |
| H    | 4.80539700   | 8.55759100   | 16.18116500  |
| C    | 2.69358800   | 8.49062700   | 16.92574800  |
| H    | 2.19411100   | 7.73032600   | 16.34338200  |
| C    | 2.15419100   | 9.28473800   | 17.92404500  |
| H    | 1.14793100   | 9.33249100   | 18.30980500  |
| C    | 1.56125700   | 11.46995000  | 20.08386400  |
| C    | 0.93319600   | 10.33272600  | 20.62504200  |
| H    | 1.38952800   | 9.35378300   | 20.49525500  |
| C    | -0.24391900  | 10.40991300  | 21.36716700  |
| H    | -0.68830300  | 9.49683000   | 21.76051200  |
| C    | -0.85522200  | 11.63984600  | 21.62978400  |
| C    | -0.21587000  | 12.78604500  | 21.14965700  |
| H    | -0.63790500  | 13.76564700  | 21.36928200  |
| C    | 0.96124500   | 12.70013500  | 20.40682100  |
| H    | 1.43952500   | 13.62958800  | 20.10746600  |
| C    | -2.14766400  | 11.72542400  | 22.39822700  |
| H    | -2.23630300  | 10.91276400  | 23.12763300  |
| H    | -2.23237200  | 12.67513800  | 22.93769000  |
| H    | -3.01452000  | 11.65488800  | 21.72724600  |
| C    | 4.18546300   | 11.38063500  | 20.49941500  |
| C    | 3.92141000   | 11.64147400  | 21.84983300  |
| H    | 2.89971200   | 11.79097000  | 22.17922200  |
| C    | 4.97390000   | 11.74292900  | 22.75303500  |
| H    | 4.77827400   | 11.98490500  | 23.79590400  |
| C    | 6.27792400   | 11.54124300  | 22.31321800  |
| H    | 7.11057200   | 11.64364500  | 23.00102200  |
| C    | 6.51530400   | 11.21981900  | 20.97287000  |
| C    | 7.40555900   | 8.59354100   | 17.60435200  |
| H    | 6.85077500   | 8.33149500   | 16.71572500  |
| C    | 8.46158600   | 7.91446100   | 18.21725800  |
| H    | 8.91762200   | 6.98294700   | 17.91554100  |
| C    | 8.79628100   | 8.70971600   | 19.30033000  |
| Atom | X             | Y             | Z             |
|------|---------------|---------------|---------------|
| H    | 9.55763600    | 8.58790700    | 20.05501500   |
| C    | 7.61149000    | 13.66822600   | 17.76836800   |
| H    | 7.09596600    | 14.01763700   | 16.88686200   |
| C    | 8.57254900    | 13.42091800   | 18.53779200   |
| H    | 8.98913000    | 15.30645500   | 18.38978900   |
| C    | 8.73334000    | 13.41356200   | 19.54374700   |
| H    | 9.54128000    | 13.49749200   | 20.38527600   |
| C    | 9.24797400    | 10.81070300   | 21.28727200   |
| H    | 10.56512000   | 11.60022000   | 20.93853300   |
| C    | 10.75851400   | 11.65267000   | 19.98828000   |
| H    | 11.65709400   | 10.86345200   | 21.75314400   |
| C    | 12.65660000   | 11.15838000   | 21.43683800   |
| H    | 11.49359700   | 10.17907200   | 22.96154300   |
| C    | 10.19767100   | 9.78024400    | 23.30227100   |
| H    | 10.03558100   | 9.21436100    | 24.21845700   |
| C    | 9.11059100    | 10.85533000   | 22.48441600   |
| H    | 8.13012600    | 9.71956000    | 22.77894900   |
| C    | 12.66562000   | 9.88727200    | 23.86135200   |
| H    | 12.82887300   | 10.70358100   | 24.57798800   |
| H    | 12.50761900   | 8.97260400    | 24.44319400   |
| B    | 3.00276200    | 11.36765400   | 19.35785700   |
| B    | 7.99001200    | 11.02250200   | 20.28952700   |

$1_{\text{Tol-NH}_3}(LS)$

| Atom | X             | Y             | Z             |
|------|---------------|---------------|---------------|
| Fe   | 5.81693400    | 11.12955200   | 18.04236600   |
| N    | 4.43585200    | 12.58083500   | 17.67886800   |
| N    | 3.22723800    | 12.51880300   | 18.28208200   |
| N    | 4.27603800    | 9.86396900    | 17.77605300   |
| N    | 3.10669000    | 10.08572200   | 18.41683900   |
| N    | 5.48501300    | 11.22082700   | 19.99168500   |
| N    | 7.10870700    | 9.65753800    | 18.32743500   |
| N    | 8.03539000    | 9.78650000    | 19.29743500   |
| N    | 7.31837700    | 12.45927200   | 18.30156500   |
| N    | 8.20055100    | 12.30066900   | 19.31345800   |
| N    | 6.23969400    | 11.07411800   | 16.03427800   |
| C    | 4.31989300    | 13.47173000   | 16.68551000   |
| H    | 5.15976900    | 13.70609000   | 16.04486600   |
| C    | 3.02329900    | 13.99022100   | 16.62877600   |
| H    | 2.62818300    | 14.72877000   | 15.94636900   |
| C    | 2.35956500    | 13.34185800   | 17.65618400   |
| H    | 1.32904700    | 13.40003700   | 17.96999900   |
| C    | 4.04601900    | 8.89649300    | 16.88030800   |
| H    | 4.83683000    | 8.53971300    | 16.23618200   |
| C    | 2.71072200    | 8.48469400    | 16.92606000   |
| H    | 2.22702300    | 7.72063200    | 16.33921000   |
| C    | 2.14865700    | 9.28014500    | 17.90271100   |
| H    | 1.13302000    | 9.33714200    | 18.26892700   |
| C    | 1.56073900    | 11.45973900   | 20.08220700   |
| C    | 0.94156500    | 10.31752400   | 20.62242600   |
| H    | 1.39921300    | 9.34104300    | 20.47965200   |
| C    | -0.22852600   | 10.38656400   | 21.37673300   |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | -0.66603400 | 9.46985700 | 21.76961100 |
| C    | -0.84190200 | 11.61275500 | 21.65092900 |
| C    | -0.21281500 | 12.76393200 | 21.16854200 |
| H    | 0.63792000  | 13.74062600 | 21.39550300 |
| C    | 0.95737500  | 12.68605200 | 20.41420100 |
| H    | 1.42791100  | 13.61817700 | 20.11056100 |
| C    | -2.12709400 | 11.68980300 | 22.43258700 |
| H    | -2.20827200 | 10.86963400 | 23.15446300 |
| H    | -2.20690100 | 12.63382500 | 22.98282300 |
| H    | -3.00068500 | 11.62590800 | 21.76963600 |
| C    | 4.20871100  | 11.39744200 | 20.41472800 |
| C    | 3.95920600  | 11.64769800 | 21.76883200 |
| H    | 2.93697100  | 11.78258800 | 22.10189700 |
| C    | 5.01134800  | 11.75463400 | 22.66670000 |
| H    | 4.82691600  | 11.99246100 | 23.71234100 |
| C    | 6.30402000  | 11.55075000 | 22.20340200 |
| H    | 7.14820100  | 11.64261200 | 22.87558000 |
| C    | 6.53591100  | 11.24502000 | 20.85997600 |
| C    | 7.34427800  | 8.48774700  | 17.72011300 |
| H    | 6.70847600  | 8.14021900  | 16.91930100 |
| C    | 8.43986200  | 7.84358800  | 18.30352600 |
| H    | 8.86535800  | 6.88550800  | 18.04251300 |
| C    | 8.84581800  | 8.70688200  | 19.30572100 |
| H    | 9.64780000  | 8.62813400  | 20.02300100 |
| C    | 7.55954800  | 13.66397600 | 17.76837800 |
| H    | 6.96406200  | 14.03450900 | 16.94780900 |
| C    | 8.59133600  | 14.31115000 | 18.45301800 |
| H    | 9.00250400  | 15.29264700 | 18.26687400 |
| C    | 8.95687400  | 13.41060600 | 19.43945200 |
| H    | 9.68988100  | 13.49327500 | 20.22685000 |
| C    | 9.25936000  | 10.82384100 | 21.27696400 |
| C    | 10.58634400 | 11.16959200 | 20.96242800 |
| H    | 10.80579500 | 11.66231700 | 20.01830700 |
| C    | 11.65869500 | 10.86431200 | 21.80001000 |
| H    | 12.66596900 | 11.15840900 | 21.50828600 |
| C    | 11.46581000 | 10.17266900 | 22.99935300 |
| C    | 10.16123800 | 9.77297200  | 23.30479700 |
| H    | 9.97627300  | 9.19668300  | 24.21145100 |
| C    | 9.09477100  | 10.08588700 | 22.46360800 |
| H    | 8.10822300  | 9.71568200  | 22.73120000 |
| C    | 12.61485800 | 9.87294000  | 23.92574000 |
| H    | 12.74688500 | 10.67293500 | 24.66682100 |
| H    | 12.45164300 | 8.94232600  | 24.48045500 |
| H    | 13.55924900 | 9.77997500  | 23.37817000 |
| B    | 2.98989000  | 11.36511500 | 19.32920100 |
| B    | 8.03049700  | 11.04026500 | 20.24132200 |
| H    | 5.40495800  | 11.09497100 | 15.45016300 |
| H    | 6.83100500  | 11.86087000 | 15.76997600 |
| H    | 6.77059300  | 10.23517400 | 15.80277600 |

$1_{\text{tol}}{\text{NH}}_3 (\text{HS})$

Fe  
5.80658200  10.98431900  17.96800300
| Element | X Component | Y Component | Z Component |
|---------|-------------|-------------|-------------|
| N       | 4.44568400  | 12.41768400 | 17.64145900 |
| N       | 3.23279100  | 12.35474300 | 18.37088800 |
| N       | 0.65187800  | 9.90880100  | 17.83366200 |
| N       | 5.50053100  | 11.09712700 | 19.92094600 |
| N       | 7.19498800  | 9.61301300  | 18.27897700 |
| N       | 8.16592800  | 9.85786600  | 19.17909000 |
| N       | 8.16592800  | 9.85786600  | 19.17909000 |
| N       | 7.68903600  | 12.49712500 | 18.08683200 |
| N       | 8.24281100  | 12.39931600 | 19.31671900 |
| C       | 4.39054500  | 13.39787800 | 16.73020900 |
| H       | 5.27005800  | 13.66095300 | 16.15911500 |
| C       | 3.11609600  | 13.96849500 | 16.70416300 |
| H       | 2.76057800  | 14.78152400 | 16.08793700 |
| C       | 2.41102500  | 13.26365900 | 17.66779600 |
| H       | 1.82461100  | 9.25259200  | 17.82716000 |
| C       | 0.84923900  | 9.49630700  | 18.10877300 |
| C       | 1.55734100  | 11.42828900 | 20.06523900 |
| H       | 0.78938900  | 10.35585000 | 20.55320700 |
| H       | -0.34663100 | 10.54716900 | 21.33912800 |
| C       | -0.90530900 | 9.68079100  | 21.69036300 |
| C       | -0.27755800 | 13.91963600 | 21.54555000 |
| C       | 1.13751600  | 12.70759000 | 20.47425500 |
| C       | 1.72903900  | 13.57920500 | 20.20281200 |
| C       | -2.02243000 | 12.04279200 | 22.51023400 |
| H       | -2.22482700 | 11.88902000 | 23.16006000 |
| H       | -1.94588700 | 12.93916800 | 23.13564600 |
| H       | -2.90213000 | 12.17219200 | 21.86513200 |
| C       | 4.20752900  | 11.15985200 | 20.34037200 |
| C       | 3.95620300  | 11.26018600 | 21.71371100 |
| C       | 2.93179300  | 11.28891900 | 22.06422600 |
| C       | 5.00574100  | 11.36501700 | 22.61662100 |
| C       | 4.80737200  | 11.48578500 | 23.67973700 |
| C       | 6.30897700  | 11.32243200 | 22.14215300 |
| C       | 7.14663200  | 11.42362700 | 22.82333500 |
| C       | 6.55565100  | 11.14393600 | 20.77772000 |
| C       | 7.50575800  | 8.47028600  | 17.65758800 |
| C       | 6.84529000  | 8.05611400  | 16.90749500 |
| C       | 8.70743800  | 7.95907000  | 18.15687500 |
| C       | 9.21578100  | 7.05012800  | 17.86979600 |
| C       | 9.90990800  | 8.87511900  | 19.12254700 |
| H       | 9.94782600  | 8.89107100  | 19.77762300 |
| C       | 7.83666200  | 13.77430600 | 17.71286900 |
| C       | 7.48859400  | 14.10043200 | 16.74059400 |
| C       | 8.46776300  | 14.52540200 | 18.70954800 |
3\textbf{Tol-NH}_2 (LS)

|  |  |  |  |  |
|---|---|---|---|---|
| Fe | 5.81865100 | 11.14268500 | 17.97319400 |
| N  | 4.41736300 | 12.57204700 | 17.68129500 |
| N  | 3.21654000 | 12.53940700 | 18.30269400 |
| N  | 4.26918200 | 9.88986300 | 17.77821800 |
| N  | 3.10390800 | 10.10430900 | 18.48277700 |
| N  | 5.47127800 | 11.22455300 | 19.99947500 |
| N  | 7.13086400 | 9.70711200 | 18.27754700 |
| N  | 8.00054000 | 9.79239500 | 19.30217500 |
| N  | 7.34073400 | 12.41402700 | 18.26827200 |
| N  | 8.18408900 | 12.29126400 | 19.31591600 |
| N  | 6.15070300 | 11.14319100 | 16.18393700 |
| C  | 4.32451400 | 13.45691100 | 16.68405300 |
| H  | 5.16083700 | 13.60305700 | 16.01872800 |
| C  | 3.04528200 | 14.01640200 | 16.64989600 |
| H  | 2.66272300 | 14.76146500 | 15.96753600 |
| C  | 2.37034000 | 13.38996000 | 17.68503100 |
| H  | 1.34447000 | 13.47818400 | 18.00547100 |
| C  | 4.06000700 | 8.89668600 | 16.90783100 |
| H  | 4.85376200 | 8.56674000 | 16.25644300 |
| C  | 2.73807700 | 8.45451000 | 16.98304800 |
| H  | 2.26610200 | 7.66739500 | 16.41334500 |
| C  | 2.16479000 | 9.26159600 | 17.95184900 |
| H  | 1.15126500 | 9.30308600 | 18.31934900 |
| C  | 1.54709200 | 11.46341500 | 20.09774300 |
| C  | 0.95040900 | 10.31499600 | 20.65073800 |
| H  | 1.42410500 | 9.34523800 | 20.5152500 |
| C  | -0.21690700 | 10.36982500 | 21.41007400 |
| H  | -0.63649700 | 9.44888600 | 21.81225400 |
| Atoms | X     | Y     | Z     |
|-------|-------|-------|-------|
| C     | -0.84998300 | 11.58750100 | 21.67774500 |
| C     | -0.24239100 | 12.74529500 | 21.18416700 |
| H     | -0.68232400 | 13.71645100 | 21.40607100 |
| C     | 0.92531600  | 12.68172700 | 20.42440000 |
| H     | 1.37902900  | 13.61989600 | 20.11486900 |
| C     | -2.13258700 | 11.64823400 | 22.46479300 |
| H     | -2.19620000 | 10.83228400 | 23.19310400 |
| H     | -2.22664300 | 12.59499100 | 23.00787700 |
| C     | -3.00741400 | 11.56382700 | 21.80588900 |
| C     | 4.19622300  | 11.41672700 | 20.41735900 |
| C     | 3.94800600  | 11.68648600 | 21.76788400 |
| H     | 2.92649600  | 11.83245200 | 22.09778300 |
| C     | 5.00048200  | 11.79847800 | 22.66401600 |
| H     | 4.81650000  | 12.05094100 | 23.70628400 |
| C     | 6.29231300  | 11.58081000 | 22.20563700 |
| H     | 7.13780200  | 11.67405400 | 22.87762600 |
| C     | 6.51833600  | 11.25485400 | 20.86649900 |
| C     | 7.39991600  | 8.57536100  | 17.61833200 |
| H     | 6.83859800  | 8.30627600  | 16.73775500 |
| C     | 8.45642300  | 7.90033100  | 18.23280200 |
| C     | 8.90140600  | 6.95974400  | 17.94282500 |
| C     | 8.80857100  | 8.71213800  | 19.29847800 |
| H     | 9.57650000  | 8.60070500  | 20.04813000 |
| C     | 7.62759500  | 13.56746300 | 17.65818000 |
| H     | 7.09286200  | 13.85405400 | 16.76743100 |
| C     | 8.65165100  | 14.23033900 | 18.33801500 |
| H     | 9.10007400  | 15.18357400 | 18.09890000 |
| C     | 8.96567500  | 13.38682700 | 19.39247600 |
| H     | 9.68369300  | 13.49750000 | 20.19038900 |
| C     | 9.23309600  | 10.81578100 | 21.29019700 |
| C     | 10.56267100 | 11.15600900 | 20.98106200 |
| H     | 10.78843100 | 11.64820200 | 20.03840200 |
| C     | 11.62928100 | 10.84480700 | 21.82328000 |
| H     | 12.63909500 | 11.13436900 | 21.53629900 |
| C     | 11.42777400 | 10.15274600 | 23.02105900 |
| C     | 10.12012700 | 9.75898200  | 23.32098800 |
| H     | 9.92859100  | 9.18499700  | 24.22636400 |
| C     | 9.05872100  | 10.07837500 | 22.47571200 |
| H     | 8.06886500  | 9.71417600  | 22.74014400 |
| C     | 12.57174800 | 9.84624100  | 23.95137600 |
| H     | 12.71314700 | 10.65151200 | 24.68491100 |
| H     | 12.3951200  | 8.92300900  | 24.51430900 |
| H     | 13.51534800 | 9.73633000  | 23.40570800 |
| B     | 2.97238000  | 11.38374700 | 19.33798900 |
| B     | 8.01065300  | 11.04146600 | 20.25259000 |
| H     | 5.40699100  | 10.92392400 | 15.52710100 |
| H     | 7.04994400  | 10.80978800 | 15.84873900 |

**C-N_{para}**

| Atoms | X     | Y     | Z     |
|-------|-------|-------|-------|
| Fe    | 6.68269800 | 11.19368800 | 18.74487200 |
| N     | 5.56386100 | 12.75091900 | 18.14250400 |
| N     | 4.26325300 | 12.82249500 | 18.50898100 |
|  |  |  |  |
|---|---|---|---|
| N  | 5.13551900 | 10.08164400 | 18.13316600 |
| N  | 3.88617600 | 10.41716800 | 18.53380700 |
| N  | 5.90017600 | 12.32882900 | 19.37557900 |
| N  | 7.85073500 | 12.03648000 | 20.57174800 |
| N  | 5.52069400 | 11.31838500 | 14.44235100 |
| C  | 5.75576000 | 13.65235000 | 17.17284800 |
| H  | 6.72605100 | 13.75763200 | 16.70824500 |
| C  | 4.39263300 | 15.10890300 | 16.16893200 |
| H  | 4.56111000 | 14.31899600 | 16.88648000 |
| N  | 8.78012300 | 13.74845500 | 17.75153100 |
| C  | 5.01387300 | 9.09334400 | 17.23937700 |
| C  | 3.66623600 | 8.78922900 | 17.03073000 |
| H  | 3.02243300 | 11.60292800 | 17.93149100 |
| H  | 4.60674400 | 11.57005000 | 17.02324000 |
| C  | 4.10655800 | 11.86565600 | 17.09003300 |
| H  | 3.06855700 | 12.15501300 | 17.20905600 |
| C  | 4.95317600 | 11.81096600 | 18.19181100 |
| H  | 4.58041800 | 12.06933300 | 18.48111200 |
| C  | 6.28064700 | 11.43076800 | 19.02151100 |
| H  | 6.95713700 | 11.40926400 | 19.86923800 |
| C  | 6.74746700 | 11.09831100 | 20.74550100 |
| H  | 8.21812200 | 8.55218800 | 18.42969900 |
| H  | 7.91035800 | 8.41206200 | 17.40393300 |
| C  | 9.02108300 | 7.73668400 | 19.23009400 |
| H  | 9.47225900 | 6.78959200 | 18.97303600 |
| C  | 9.11468900 | 8.42171900 | 20.43018200 |
| H  | 9.63944600 | 8.17694600 | 21.34036400 |
| C  | 8.68927000 | 13.52195400 | 18.99734100 |
| H  | 8.38304600 | 13.96277700 | 18.06092800 |
| C  | 9.55997800 | 14.02915200 | 19.96218200 |
| H  | 10.09940800 | 14.96480300 | 19.94660400 |
| C  | 9.57306300 | 13.05777100 | 20.95121900 |
|   |         |         |         |         |
|---|---------|---------|---------|---------|
| H | 11.08383200 | 13.03185500 | 21.90158900 |
| C | 9.28606600  | 10.37018100 | 22.60070000 |
| C | 8.81539800  | 9.62825400  | 23.15490000 |
| C | 11.52615500 | 10.14056500 | 23.57644200 |
| H | 12.59383000 | 10.33247600 | 23.49951400 |
| C | 11.03183600 | 9.44177300  | 24.68239700 |
| C | 9.65924500  | 9.17834800  | 24.71340400 |
| H | 10.12336800 | 11.07661000 | 21.70400600 |
| C | 11.52615500 | 10.58080700 | 22.56285100 |
| H | 11.12336800 | 11.07661000 | 21.70400600 |
| C | 10.67670700 | 10.58080700 | 22.56285100 |
| H | 11.94065200 | 9.99520000  | 25.79727000 |
| H | 12.02605600 | 9.76817700  | 26.57297700 |
| H | 11.56419600 | 8.08869400  | 26.28364300 |
| H | 12.95313000 | 8.78917900  | 25.43021000 |
| B | 3.68742700  | 11.68810100 | 19.45969500 |
| B | 8.30508700  | 10.75488200 | 21.37135500 |
| H | 5.16317700  | 12.20971600 | 14.78289400 |
| H | 5.05277200  | 10.61057700 | 15.00754900 |
| C | 5.13468600  | 11.12765100 | 13.02437900 |
| C | 5.50983000  | 9.71762900  | 12.68086000 |
| C | 5.33117000  | 11.36398000 | 12.85457000 |
| C | 4.69048000  | 8.79014800  | 12.15339000 |
| H | 2.76710800  | 10.48521200 | 12.36465100 |
| H | 3.31835800  | 12.33574700 | 13.20069700 |
| C | 3.26281200  | 9.15815300  | 11.88924500 |
| C | 5.97300300  | 12.15084000 | 12.13351100 |
| C | 5.52232400  | 12.07320100 | 10.66908300 |
| H | 6.15962300  | 12.71527200 | 10.04909600 |
| H | 5.59766600  | 11.05182300 | 10.28022800 |
| H | 4.48647700  | 12.40574700 | 10.54144300 |
| C | 7.47316000  | 11.82770400 | 12.22083900 |
| H | 7.78556300  | 11.70489800 | 13.26284200 |
| H | 7.72844100  | 10.91641000 | 11.66897700 |
| H | 8.05477000  | 12.64634100 | 11.77982300 |
| C | 5.77207400  | 13.59041300 | 12.63771900 |
| H | 4.72049600  | 13.89849600 | 12.63612100 |
| H | 6.17702200  | 13.72913100 | 13.64629000 |
| H | 6.30919900  | 14.28220400 | 11.97800400 |
| C | 1.26649500  | 10.79290900 | 12.26753700 |
| C | 5.15970100  | 7.36662000  | 11.82214000 |
| C | 5.03393300  | 7.11270300  | 10.30499200 |
| H | 5.39071400  | 6.10242900  | 10.06778200 |
| H | 3.99819400  | 7.20302400  | 9.97392900  |
| H | 5.64686200  | 7.82531200  | 9.73931900  |
| C | 6.62847700  | 7.14922800  | 12.21285400 |
| H | 7.30502500  | 7.81898300  | 11.66847100 |
| H | 6.79446300  | 7.29040900  | 13.28792400 |
| H | 6.91828700  | 6.12104400  | 11.96789000 |
| C | 4.31296800  | 6.33437200  | 12.59499900 |
| H | 4.41265900  | 6.48135000  | 13.67792500 |
| H | 3.25709200  | 6.40437300  | 12.32784600 |
| H | 4.66180400  | 5.32031000  | 12.36329300 |
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | 0.92995700 | 12.16580300| 12.86772500|
| H    | 1.20210700 | 12.23036500| 13.92847900|
| C    | 1.42552800 | 12.98484900| 12.33199900|
| C    | -0.15021800| 12.33624700| 12.79426200|
| C    | 0.99863400 | 10.80414400| 10.78921600|
| H    | 1.20210700 | 12.23036500| 13.92847900|
| H    | 1.42552800 | 12.98484900| 12.33199900|
| H    | -0.15021800| 12.33624700| 12.79426200|
| C    | 0.82530800 | 10.80414400| 10.78921600|
| C    | 0.82530800 | 10.80414400| 10.78921600|
| H    | 0.99863400 | 10.80414400| 10.78921600|
| H    | 0.99863400 | 10.80414400| 10.78921600|
| O    | 2.50757800 | 8.37075200 | 11.31936300|

C-N<sub>ortho</sub>

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| Fe   | 5.63623600 | 11.04954700| 18.15073600|
| N    | 4.11441800 | 12.60829400| 17.87255800|
| N    | 2.95914400 | 12.50367200| 18.56875100|
| N    | 3.92046100 | 9.65061600 | 18.29257900|
| N    | 2.82114400 | 10.06678100| 18.96215100|
| N    | 5.40896700 | 11.22975600| 20.24858000|
| N    | 7.09162400 | 9.52379000 | 18.37009700|
| N    | 7.95153200 | 9.69860400 | 19.40169000|
| N    | 7.30938300 | 12.44194400| 18.28799700|
| N    | 8.15718700 | 12.25384000| 19.32956800|
| N    | 5.43950000 | 10.40244700| 15.65996100|
| C    | 3.89204100 | 13.46917500| 16.87548200|
| H    | 4.68977200 | 13.71666600| 16.18821500|
| C    | 2.56946900 | 13.92384000| 16.89991700|
| H    | 2.09044200 | 14.63149300| 16.23864600|
| C    | 2.01048500 | 13.26716200| 17.98496200|
| H    | 1.00306700 | 13.28910800| 18.37053200|
| C    | 3.58839400 | 8.51666500 | 17.66246800|
| H    | 4.32356700 | 7.97987400 | 17.07765600|
| C    | 2.24816200 | 8.19876600 | 17.89637400|
| H    | 1.68823800 | 7.34993400 | 17.53127100|
| C    | 1.79900400 | 9.21977800 | 18.71932900|
| H    | 0.82219300 | 9.39762300 | 19.14206000|
| C    | 1.51271300 | 11.64747200| 20.64099000|
| C    | 0.96883000 | 10.58308700| 21.38444300|
| H    | 1.40796500 | 9.59141000 | 21.30171400|
| C    | -0.09806500| 10.75166000| 22.26503900|
| H    | -0.47947300| 9.89115200 | 22.81285500|
| C    | -0.67664600| 12.00797200| 22.47005800|
| C    | -0.11602800| 13.08806100| 21.78304000|
| H    | -0.51153600| 14.08958100| 21.94650600|
| C    | 0.95093200 | 12.91030000| 20.90245500|
| H    | 1.37529000 | 13.79662600| 20.43720700|
| C    | -1.85351500| 12.18931500| 23.39237600|
| H    | -1.84738900| 11.45072400| 24.20152400|
| X       | Y       | Z       |
|---------|---------|---------|
| -1.85945700 | 13.18708900 | 23.84490400 |
| -2.80359600 | 12.07209100 | 22.85350500 |
| 4.17500700  | 11.54447900 | 20.71623000 |
| 4.05235600  | 11.98127400 | 22.04155500 |
| 3.07480100  | 12.22981300 | 22.43693000 |
| 5.18259400  | 12.12145200 | 22.83714200 |
| 5.09351600  | 12.49157000 | 23.85564000 |
| 6.42581500  | 11.78283200 | 22.31932500 |
| 7.32044300  | 11.90435600 | 22.92007700 |
| 6.53017100  | 11.30147200 | 21.00937400 |
| 7.34749900  | 8.31862900  | 17.84642000 |
| 6.79807200  | 7.95771900  | 16.98620300 |
| 8.38167400  | 7.69086900  | 18.54169400 |
| 8.81468200  | 6.71793800  | 18.36026200 |
| 8.73502100  | 8.60500600  | 19.52071000 |
| 9.49141000  | 8.54841200  | 20.28734300 |
| 7.50486600  | 13.69117300 | 17.84969400 |
| 6.93373600  | 14.06945300 | 17.01399300 |
| 8.47752100  | 14.33781100 | 18.61361400 |
| 8.85485400  | 15.34408000 | 18.50511000 |
| 8.85063800  | 13.38891000 | 19.55319900 |
| 9.55317800  | 13.45288800 | 20.37027100 |
| 9.24636000  | 10.82358700 | 21.28905100 |
| 10.56223600 | 11.13091000 | 20.89804600 |
| 10.74274600 | 11.57174500 | 19.92009000 |
| 11.66489000 | 10.85768000 | 21.70626100 |
| 12.66286100 | 11.11794600 | 21.35628400 |
| 11.51390900 | 10.23976300 | 22.95140800 |
| 10.21790600 | 9.88476900  | 23.33834900 |
| 10.06423300 | 9.37208300  | 24.28634300 |
| 9.12019700  | 10.16708600 | 22.52657200 |
| 8.13815800  | 9.84005500  | 22.86029900 |
| 12.69824200 | 9.97224100  | 23.84279600 |
| 13.61591700 | 9.83259100  | 23.26085400 |
| 12.87486000 | 10.80971000 | 24.53136500 |
| 12.54596300 | 9.07677300  | 24.45555500 |
| 2.84731500  | 11.44506400 | 19.73959100 |
| 7.97823900  | 11.00420700 | 20.29042800 |
| 4.44877700  | 10.25330300 | 15.85541000 |
| 5.89623100  | 9.52788600  | 15.92347200 |
| 5.58819100  | 10.45809200 | 14.18323800 |
| 5.48157200  | 9.00903400  | 13.64823800 |
| 4.52670100  | 11.35972500 | 13.63001600 |
| 4.77416400  | 8.75199200  | 12.37790700 |
| 3.77397700  | 11.04772300 | 12.55839100 |
| 4.39369400  | 12.29886200 | 14.15599400 |
| 3.97363000  | 9.74777000  | 11.91734600 |
| 3.39273600  | 9.56112800  | 11.01949400 |
| 7.04061400  | 11.02904300 | 13.81485300 |
| 7.32741700  | 10.87079700 | 12.31507600 |
| 8.25763400  | 11.39586400 | 12.06722400 |
| 7.45927700  | 9.82188100  | 12.02924500 |
| 6.52833200  | 11.29816300 | 11.69963600 |
| Atoms | X-Coordinate | Y-Coordinate | Z-Coordinate |
|-------|--------------|--------------|--------------|
| C     | 8.12568800   | 10.29474800  | 14.61494600  |
| H     | 8.03034600   | 10.48030700  | 15.68911900  |
| H     | 8.11015200   | 9.21427800   | 14.44565000  |
| C     | 9.10849900   | 10.66828200  | 14.30211400  |
| H     | 8.03034600   | 10.48030700  | 15.68911900  |
| H     | 8.11015200   | 9.21427800   | 14.44565000  |
| C     | 7.10556300   | 12.51933400  | 14.74554000  |
| H     | 6.48278500   | 13.13248500  | 13.51375600  |
| H     | 6.79424700   | 12.67807700  | 15.21038100  |
| H     | 8.13894000   | 12.87253300  | 14.07936900  |
| C     | 2.69690800   | 11.96760100  | 11.97659300  |
| H     | 6.48278500   | 13.13248500  | 13.51375600  |
| H     | 6.79424700   | 12.67808700  | 15.21038100  |
| H     | 8.13894000   | 12.87253300  | 14.07936900  |
| C     | 4.86074300   | 7.37144400   | 10.79656300  |
| H     | 4.14245200   | 7.34704300   | 10.36125400  |
| H     | 4.27435700   | 6.36148600   | 9.90061200   |
| H     | 3.06320400   | 7.51517200   | 10.46006600  |
| C     | 4.58315000   | 8.09376300   | 9.66772000   |
| H     | 6.33494900   | 6.98787200   | 11.48099900  |
| H     | 6.82024900   | 7.69425800   | 10.79656300  |
| H     | 6.89643500   | 6.96371500   | 12.41765600  |
| H     | 6.38958000   | 5.99201400   | 11.02457400  |
| C     | 4.19522000   | 6.31602600   | 12.62790800  |
| H     | 4.70852100   | 6.24227000   | 13.58851200  |
| H     | 3.14344500   | 6.56681600   | 12.81137200  |
| H     | 4.22739000   | 5.33387300   | 12.13976500  |
| C     | 2.57589400   | 13.27890500  | 12.76218600  |
| H     | 2.30854000   | 13.10221400  | 13.81007600  |
| H     | 3.50862200   | 13.85453000  | 12.73645300  |
| H     | 1.79139900   | 13.90270100  | 12.31868600  |
| C     | 3.04634000   | 12.31126400  | 10.51452900  |
| H     | 3.11864600   | 11.42047200  | 9.88059600   |
| H     | 2.27115500   | 12.95671500  | 10.08404800  |
| H     | 4.00239700   | 12.84419200  | 10.45474000  |
| C     | 1.33270500   | 11.24981700  | 12.02469200  |
| H     | 1.33198300   | 10.31721100  | 11.44939300  |
| H     | 1.05455800   | 11.00773800  | 13.05673500  |
| H     | 0.55197400   | 11.89521100  | 11.60430600  |
| O     | 5.98134200   | 8.10677000   | 14.32016900  |

(1Tol)2-NH2NH2 (LS)

| Fe    | 6.38575300   | 3.72948300   | 11.95054600  |
| Fe    | 2.67915000   | 5.76218600   | 14.71528200  |
| N     | 1.17930600   | 4.45259100   | 14.31795900  |
| N     | 7.27460700   | 4.68521800   | 9.38735100   |
| N     | 2.93185700   | 4.69149500   | 16.42276800  |
| N     | 7.68919600   | 2.35236700   | 11.21737600  |
| N     | 2.37380500   | 6.77386700   | 12.99803100  |
| N     | 0.29352200   | 4.14740000   | 15.29459500  |
| N     | 4.04453500   | 4.50971200   | 13.73717400  |
| N     | 4.91521800   | 2.44440500   | 11.58274200  |
| N     | 4.09129000   | 8.33394900   | 14.86483100  |
| N     | 7.90678000   | 5.07678000   | 12.19203900  |
| N     | 4.17595200   | 7.02556400   | 15.18750400  |
| N     | 5.05030000   | 5.05154900   | 12.82419200  |
| N     | 6.69537700   | 2.87187900   | 13.77869400  |
N          1.43774200  6.98301300  15.59944700
N          5.04856900  1.16086600  11.96974000
N          1.84614300  4.36826300  17.16311000
N          6.17974100  4.58316800  10.16951600
     8.87829100  5.14750100  11.25178900
N          6.60988400  1.16086600  11.96974000
N          2.54703900  8.11225500  12.96179000
C          1.54135300  8.31408000  15.34758800
C          7.64460600  1.08139200  11.70598000
C          -0.75537100  4.51223800  17.71976400
C          8.73249000  2.77190700  10.45744700
C          0.49542100  6.48231500  16.43359000
C          3.95228100  3.97349200  16.91185200
H          4.94553800  4.04081300  16.49145500
C          2.21351900  6.37279400  11.72920000
H          2.00075300  5.33793600  11.50736400
C          5.17135500  5.15018600  9.49743500
H          4.18735700  5.23428500  9.93423600
C          9.84349200  1.94003000  10.27961400
H          10.69945500  2.31259500  9.72795900
C          7.06806400  1.17079500  15.14407800
H          7.11946500  0.13119000  15.42849600
C          6.15245200  0.91168400  12.96684100
C          8.74384300  0.23538600  11.53290000
H          8.72754700  0.27505000  11.98075600
C          0.64783400  9.19674800  15.96138200
H          0.72990800  10.25819400  15.75914100
C          5.60456300  5.60939600  8.25062500
H          5.02477700  6.10075500  7.48299400
C          7.18269200  3.35049300  14.93323500
H          7.37309800  4.40472000  15.05114900
C          -0.40499600  7.35962200  17.05543300
H          -1.15847800  6.94896800  17.72077000
C          10.07775400  3.76748800  7.74508900
H          9.68547000  2.75501300  7.80226000
C          9.74863800  4.69525500  8.75021000
C          3.74656900  2.53059800  10.93112100
H          3.43571300  3.46079200  10.48236500
C          0.97423000  3.57041400  13.33106200
H          1.56496000  3.58996300  12.42738400
C          5.41298100  6.82585500  15.66278400
H          5.70154200  5.85709700  16.04029600
C          2.17949900  3.43869900  18.08320200
C          1.43386900  3.02527600  18.74421300
C          3.53043300  3.16375800  17.96905600
H          4.12156300  2.47932200  18.55965900
C          -0.43369300  3.06983500  14.93269800
H          -1.16733000  2.64976100  15.60278000
C          8.26806100  5.91554000  13.17202700
H          7.62371000  6.09326000  14.02075400
C          9.86158300  5.96960600  11.66890100
H          10.74793400  6.11672200  11.07184700
C          6.95042500  5.29301300  8.22471000
|   |    |     |    |    |    |    |    |    |    |    |    |    |
|---|----|-----|----|----|----|----|----|----|----|----|----|----|
| H | 6.94540100 | -1.65172000 | 11.09839400 |
| C | 3.09375800 | 12.70609300 | 15.13476700 |
| H | 3.59271700 | 13.30947200 | 15.89171700 |
| C | 2.16285200 | 14.83142600 | 14.11803500 |
| H | 2.21102400 | 15.27522300 | 15.11867700 |
| H | 2.96955000 | 15.28282000 | 13.52469300 |
| H | 1.21495500 | 15.13291100 | 13.65922500 |
| C | -4.04291500 | 3.90571300 | 20.54966100 |
| H | -4.12238200 | 2.84169800 | 20.81090800 |
| H | -3.89096600 | 4.45720400 | 21.48415700 |
| H | -5.00844700 | 4.20941600 | 20.13057500 |
| B | 8.70268300 | 4.30677600 | 9.92878000 |
| C | 6.16786500 | -3.26200200 | 12.26258600 |
| H | 6.43628200 | -4.00254300 | 11.51060900 |
| B | 6.37332800 | 0.65907600 | 12.63770400 |
| B | 2.70632100 | 8.86253700 | 14.33547100 |
| C | 5.22768200 | -5.12751000 | 13.69426700 |
| H | 4.34694200 | -5.25209600 | 14.33363600 |
| H | 5.05151300 | -5.67785700 | 12.76348100 |
| H | 6.07055200 | -5.61384800 | 14.20367800 |
| B | 0.43442400 | 4.87292300 | 16.68327600 |
| C | 12.26908900 | 5.74858100 | 5.32673500 |
| H | 12.05420700 | 5.12846600 | 4.44955400 |
| H | 12.15323200 | 6.79858700 | 5.03618500 |
| H | 13.32720000 | 5.59715300 | 5.57980500 |
| H | 4.51681400 | 5.59099800 | 12.13777900 |
| H | 4.58890200 | 3.95752000 | 14.40317000 |
| H | 3.57316200 | 3.78423800 | 13.19196000 |
| H | 5.52515500 | 5.77625800 | 13.36735700 |

\((1\text{ Tol})_2\text{NH}_2\text{NH}_2\text{ (HS)}\)
N  2.82402400  8.37531000  13.16730300
C  1.56474000  8.40862500  15.51059600
C  7.93847700  5.93853800  11.97369000
C  2.57083500  6.88866800  11.62086300
C  7.93847700  5.93853800  11.97369000
C  2.57083500  6.88866800  11.62086300
C  7.93847700  5.93853800  11.97369000
H  2.27004000  5.93853800  11.19736900
C  4.90520700  4.58314800  9.37853700
H  3.93913800  4.55254800  9.85958900
C  9.94585100  2.02104000  10.11854300
H  10.72488200  2.43524000  9.48820800
C  7.47960800  1.36761200  15.21916100
H  6.74959600  0.98129200  13.22858400
C  9.11528300  0.31773400  11.56632000
H  9.23219000  0.62460200  12.08961000
C  0.68350400  9.31795000  16.10772800
H  0.85107700  10.38305700  15.99893500
C  5.21012600  4.98416000  8.07520100
H  4.53143800  5.31986700  7.30476600
C  7.28080000  3.51999100  11.84956100
H  7.31371700  4.59611000  14.92044000
C  0.53288000  3.81295800  13.02294000
H  1.07210700  3.85120000  12.11660500
C  5.47639900  6.67352700  15.89761300
H  5.72353900  5.62162000  16.19376000
C  1.44311800  3.17946700  17.88016800
H  0.57577000  1.93651400  18.49088900
C  3.30082700  0.74398700  11.36200800
H  4.45198300  3.58381300  16.70500100
C  3.40794500  3.57838800  16.99353400
C  8.75946100  2.74022000  10.29790000
C  3.07734100  6.58423200  13.60216000
C  5.47253200  1.93651400  18.49088900
C  2.75749500  2.74073100  17.90275800
C  3.17533200  1.93651400  18.49088900
C  6.58421700  4.84766700  7.99527000
H  7.26513600  5.04709500  7.18296200
C  3.68697100  4.55116000  17.68019000
H  -4.67368400  4.55299100  17.21962000
C  6.17215000  1.40134100  14.44115600
C  5.78360400  -0.66187000  15.13803200
C  3.30082700  0.74398700  11.36200800
S63
| Atom | x    | y    | z    |
|------|------|------|------|
| H    | 2.33263900 | 0.37394200 | 11.05836600 |
| C    | 2.92947400 | 10.55397400 | 14.69186300 |
| C    | -2.55530200 | 4.66392000 | 16.87410800 |
| H    | -2.70490800 | 4.78671000 | 15.80394400 |
| C    | 2.26479800 | 11.35919500 | 13.74984600 |
| H    | 1.74492500 | 10.89541800 | 12.91499800 |
| C    | -0.40277100 | 8.85231400 | 16.83889700 |
| H    | -1.08948200 | 9.55546500 | 17.30642600 |
| C    | 10.14059200 | 0.81314100 | 10.77230300 |
| H    | 11.07469000 | 0.26576900 | 10.66420000 |
| C    | 3.19404100 | 8.95560800 | 12.00533200 |
| H    | 3.54430600 | 9.97621600 | 11.98326000 |
| C    | 4.32355700 | 0.04208800 | 11.97414800 |
| H    | 4.38638000 | -0.99127600 | 12.27692200 |
| C    | 9.75524400 | 5.95023900 | 8.04588800 |
| H    | 9.40671300 | 6.76006000 | 8.68209600 |
| C    | 6.25821700 | 7.83236100 | 15.95127700 |
| H    | 7.28066600 | 7.93875800 | 16.28464300 |
| C    | 2.20490700 | 12.74814200 | 13.86132900 |
| H    | 1.67778800 | 13.32209300 | 13.10063400 |
| C    | 5.40621000 | 8.83157500 | 15.50269300 |
| H    | 5.58065600 | 9.88712700 | 15.36232600 |
| C    | -3.57868800 | 4.45074100 | 19.07070200 |
| C    | -1.16645300 | 4.61859700 | 18.80288500 |
| H    | -0.19602300 | 4.70365700 | 19.28673000 |
| C    | -0.54443400 | 2.97097300 | 13.30703300 |
| H    | -0.99987600 | 2.22450500 | 12.67251800 |
| C    | 6.45165900 | -3.75656500 | 13.90476700 |
| C    | 2.79580100 | 13.41538900 | 14.93767500 |
| C    | 9.27678900 | 6.69603300 | 12.40635100 |
| H    | 9.78897100 | 7.49430500 | 12.92322800 |
| C    | 7.67528900 | 2.59887200 | 15.82392100 |
| H    | 8.06433100 | 2.79790000 | 16.81130700 |
| C    | 10.53458200 | 3.98461500 | 6.27204600 |
| H    | 10.81079900 | 3.19701000 | 5.57257600 |
| C    | 3.03531800 | 8.03960500 | 10.97608800 |
| H    | 3.22102500 | 8.19040400 | 9.92260800 |
| C    | -2.29262700 | 4.50545300 | 19.61671900 |
| H    | -2.16863000 | 4.47092900 | 20.69817700 |
| C    | 3.46988500 | 11.24155000 | 15.79530700 |
| H    | 3.92025600 | 10.68001100 | 16.61072000 |
| C    | 10.44516900 | 6.29030400 | 6.88310400 |
| H    | 10.64897000 | 7.33861300 | 6.66952300 |
| C    | 6.03416600 | -2.74720900 | 14.77745000 |
| H    | 5.58163900 | -3.01728700 | 15.73043800 |
| C    | 10.86445000 | 5.31061900 | 5.97780000 |
| C    | 7.12080900 | -2.01218400 | 12.34676500 |
| H    | 7.50753500 | -1.76160100 | 11.36193800 |
| C    | 3.41462800 | 12.62886000 | 15.91431300 |
| H    | 3.85038000 | 13.10758000 | 16.79010100 |
| C    | 2.76823500 | 14.91753300 | 15.04238300 |
| H    | 2.73800200 | 15.24713500 | 16.08685700 |
| H    | 3.66285000 | 15.36419600 | 14.58762000 |
IRCA (prior to TSA)

Fe  
5.79313000  11.85843600  17.58365800
N  
5.67160700  13.89499500  17.54533100
N  
4.89528700  14.52545800  18.45782400
N  
3.78439500  11.94392400  17.75668100
N  
3.23509600  12.75683300  18.68763000
N  
6.03483200  11.84491700  19.55647400
N  
5.78219300  9.87907800  17.62855800
N  
6.76934100  9.23436400  18.27981700
N  
7.81522000  11.89615200  17.45012400
N  
8.56275400  11.02996000  18.17264600
N  
5.67713600  11.78490200  15.52010700
C  
5.95353100  14.80027900  16.59787400
H  
6.55911900  14.54885900  15.73798300
C  
5.35029800  16.02722600  16.88419800
H  
5.39674700  16.94181600  16.31132400
C  
4.67468200  15.79914700  18.06986900
H  
4.03975800  16.45026200  18.65003000
C  
2.77994000  11.52387800  16.97655100
H  
2.95463800  10.86638000  16.13493900
C  
1.56378600  12.07104900  17.39356900
H  
0.58357300  11.91841300  16.96620100
C  
1.90536300  12.86041800  18.47651800
H  
1.29719100  13.49996000  19.09677700
C  
3.38470400  14.51913800  20.66689500
C  
2.30975000  13.96222700  21.38474600
H  
1.97032000  12.95589800  21.14879400
C  
1.67650000  14.63652100  22.42704300
| C      | 2.88875100 | 14.69749300 | 11.07632500 |
|--------|------------|-------------|-------------|
| H      | 3.30324500 | 15.04398300 | 12.02040300 |
| C      | 1.80218000 | 15.39296800 | 10.54720900 |
| H      | 1.42494600 | 15.39296800 | 10.54720900 |
| C      | 1.17766400 | 14.97082600 | 9.36979300  |
| C      | 1.66713700 | 13.80852200 | 8.76581400  |
| H      | 1.18264800 | 13.42813500 | 7.86779500  |
| C      | 2.75623100 | 13.51214700 | 9.29919700  |
| C      | 3.06834000 | 12.20193500 | 8.81074800  |
| C      | 0.02613900 | 15.73778800 | 8.77426000  |
| H      | -0.65530600| 15.07826400 | 8.22638300  |
| H      | -0.38033500| 9.13062000  | 10.83779700 |
| B      | 8.30033500 | 16.49914900 | 8.06701900  |
| B      | 4.59086600 | 12.66506900 | 11.14886900 |
| H      | 6.35305500 | 9.94429100  | 15.25195200 |
| H      | 7.49160800 | 11.05693800 | 15.22968000 |

**TSA**

| Fe     | 5.44756200 | 11.83967500 | 17.73680600 |
|--------|------------|-------------|-------------|
| N      | 3.87036800 | 12.92387300 | 17.80431000 |
| N      | 2.84564600 | 12.76915000 | 18.83803000 |
| N      | 4.27216400 | 10.30662500 | 18.27294000 |
| N      | 3.39234000 | 10.43352000 | 19.29377000 |
| N      | 5.80123700 | 12.32032700 | 19.65577000 |
| N      | 7.08114400 | 10.72614600 | 17.74300000 |
| N      | 8.21957200 | 11.24646300 | 18.27313700 |
| N      | 6.57356500 | 13.43422800 | 17.21293700 |
| N      | 7.75065000 | 13.68474400 | 17.82684100 |
| N      | 5.07379200 | 11.53391700 | 15.86014300 |
| C      | 3.03749000 | 13.58813400 | 16.85158800 |
| H      | 3.50598300 | 13.81776400 | 15.90626600 |
| C      | 1.72952700 | 13.86151600 | 17.25978900 |
| H      | 0.95684700 | 14.38622800 | 16.71642000 |
| C      | 1.64899300 | 13.30546000 | 18.52514000 |
| H      | 0.81814100 | 13.24215600 | 19.21032300 |
| C      | 3.98416200 | 9.15783500  | 17.65216300 |
| H      | 4.55068700 | 8.84937900  | 16.78672500 |
| C      | 2.90083600 | 8.52362400  | 18.26694200 |
| H      | 2.44175300 | 7.58160700  | 18.00397000 |
| C      | 2.55085000 | 9.37992600  | 19.29646600 |
| H      | 1.74980900 | 9.31809100  | 20.01745400 |
| C      | 2.24908000 | 11.79251800 | 21.25968700 |
| C      | 2.18650800 | 10.68322900 | 22.12377100 |
| H      | 2.80145200 | 9.80904000  | 21.92026200 |
| C      | 1.38984800 | 10.66329000 | 23.26687000 |
| H      | 1.37908000 | 9.78157700  | 23.89907000 |
| C      | 0.61543600 | 11.77638900 | 23.62431100 |
| C      | 0.70490100 | 12.90776200 | 22.80890900 |
| H      | 0.14851400 | 13.80503500 | 23.07615800 |
| C      | 1.50515000 | 12.91447300 | 21.66662000 |
| H      | 1.57537100 | 13.84174400 | 21.10325100 |
|   | X          | Y          | Z          |
|---|------------|------------|------------|
| C | 8.02188200 | 7.81638100 | 13.53116400|
| H | 8.21594500 | 8.34008000 | 14.45376600|
| C | 8.36424100 | 6.51396400 | 13.16456700|
| H | 8.92675200 | 5.78879500 | 13.73436600|
| C | 7.81258900 | 6.35790700 | 11.90330200|
| H | 7.79599300 | 6.50130500 | 11.24800700|
| C | 3.53650100 | 8.49549000 | 12.66360000|
| H | 3.18916200 | 9.04897800 | 13.52693600|
| C | 7.81258900 | 6.35790700 | 11.90330200|
| H | 7.81258900 | 6.35790700 | 11.90330200|
| Element | X (Å) | Y (Å) | Z (Å) |
|---------|-------|-------|-------|
| H       | 6.54310800 | 16.40403100 | 8.18517700 |
| C       | 6.79139100  | 14.80013000  | 9.59388800  |
| H       | 6.40097700  | 14.07305700  | 8.86043000  |
| C       | 7.40375500  | 18.56788700  | 9.62625200  |
| H       | 6.66980800  | 18.80638400  | 8.84750000  |
| H       | 6.40097700  | 14.07307500  | 8.88604300  |
| C       | 7.24828500  | 19.25797100  | 10.46275600 |
| H       | 8.39783500  | 18.78094500  | 9.21057100  |
| H       | 6.27448900  | 7.88276300   | 10.34127500 |
| B       | 6.79139100  | 14.80013000  | 9.59388800  |
| H       | 6.40097700  | 14.07307500  | 8.88604300  |
| C       | 7.40375500  | 18.56788700  | 9.62625200  |
| H       | 6.66980800  | 18.80638400  | 8.84750000  |
| H       | 6.40097700  | 14.07307500  | 8.88604300  |
| C       | 7.24828500  | 19.25797100  | 10.46275600 |
| H       | 8.39783500  | 18.78094500  | 9.21057100  |
| H       | 6.27448900  | 7.88276300   | 10.34127500 |
| B       | 6.79139100  | 14.80013000  | 9.59388800  |
| H       | 6.40097700  | 14.07307500  | 8.88604300  |
| C       | 7.40375500  | 18.56788700  | 9.62625200  |
| H       | 6.66980800  | 18.80638400  | 8.84750000  |
| H       | 6.40097700  | 14.07307500  | 8.88604300  |
| C       | 7.24828500  | 19.25797100  | 10.46275600 |
| H       | 8.39783500  | 18.78094500  | 9.21057100  |

IRCA’ (after TSA)

| Element | X (Å) | Y (Å) | Z (Å) |
|---------|-------|-------|-------|
| Fe      | 5.73673800  | 12.25601800  | 17.91394300 |
| N       | 4.33253700  | 13.73167300  | 18.01698100 |
| N       | 3.36942100  | 13.67254000  | 18.96487200 |
| N       | 4.17602500  | 11.01468900  | 18.15014800 |
| N       | 3.27385500  | 11.23750500  | 19.13248600 |
| N       | 6.03675700  | 12.35707400  | 19.87715200 |
| N       | 7.03810800  | 10.76398000  | 17.80418800 |
| N       | 8.22025700  | 10.89063000  | 18.43959000 |
| N       | 7.26857800  | 13.56117600  | 17.67665000 |
| N       | 8.41584600  | 13.40187800  | 18.37953000 |
| N       | 5.47029100  | 12.19533100  | 15.88360000 |
| C       | 3.93270600  | 14.64629200  | 17.12442000 |
| H       | 4.53684000  | 14.87410000  | 16.25811000 |
| C       | 2.69197600  | 15.18224800  | 17.48107500 |
| H       | 2.11873300  | 15.93985000  | 16.96651500 |
| C       | 2.36647300  | 14.52056000  | 18.65257700 |
| H       | 1.48552600  | 14.58609000  | 19.27157000 |
| C       | 3.66629400  | 10.05978100  | 17.36435100 |
| H       | 4.20172200  | 9.72855600   | 16.48681100 |
| C       | 2.41141000  | 9.65481500   | 17.83212600 |
| H       | 1.76562000  | 8.89996400   | 17.42046800 |
| C       | 2.19679900  | 10.44268000  | 18.94923500 |
| H       | 1.34780600  | 10.50189300  | 19.61253000 |
| C       | 2.34058500  | 12.61932700  | 21.19683400 |
| C       | 1.91059000  | 11.47943800  | 21.90095300 |
| H       | 2.29128200  | 10.50025800  | 21.62002800 |
| C       | 1.03395000  | 11.55357700  | 22.98220800 |
| H       | 0.73241500  | 10.63816600  | 23.48950700 |
| C       | 0.54684800  | 12.78275600  | 23.43630000 |
| C       | 1.00409000  | 13.93149400  | 22.78531500 |
| H       | 0.68026800  | 14.91038200  | 23.15665000 |
| C       | 1.88169800  | 13.84826200  | 21.70414500 |
| H       | 2.24266100  | 14.77809600  | 21.27112700 |
| C       | -0.43122000 | 12.86607000  | 24.57859000 |
| H       | -0.30356800 | 12.03634300  | 25.27912000 |
| H       | -0.31631900 | 13.80053200  | 25.13921500 |
| H       | -1.46873300 | 12.83008300  | 24.21854100 |
| C       | 4.95880000  | 12.54157900  | 20.67929100 |
| C       | 5.14767100  | 12.79819900  | 22.04238700 |
| Atm | X     | Y     | Z   |
|-----|-------|-------|-----|
| H   | 3.46041800 | 12.51608200 | 20.03201500 |
| H   | 8.52915200  | 12.90337000 | 22.56513200 |
| H   | 6.58164500  | 13.14657000 | 23.61467800 |
| C   | 7.50942500  | 12.68944000 | 21.72121700 |
| H   | 8.52305000  | 12.77530000 | 22.09632200 |
| C   | 7.30397200  | 12.37496000 | 20.37539100 |
| C   | 7.03804400  | 9.57475700  | 17.20417400 |
| H   | 6.18143200  | 9.24674500  | 16.63737800 |
| C   | 8.24296700  | 8.90390700  | 17.45030600 |
| H   | 8.53274200  | 7.91424200  | 17.12672700 |
| C   | 8.96462200  | 9.78031600  | 18.24940000 |
| H   | 9.94459800  | 9.68962400  | 18.68474300 |
| C   | 7.35078700  | 14.75221700 | 17.07185000 |
| H   | 6.54397800  | 15.11175900 | 16.45229100 |
| C   | 8.54901300  | 15.39317900 | 18.24144000 |
| H   | 8.89443200  | 16.36582200 | 17.07965700 |
| C   | 9.18767500  | 14.50098700 | 18.24404600 |
| H   | 10.12519100 | 14.58299900 | 18.77167100 |
| C   | 10.01882800 | 11.92372100 | 19.92356200 |
| C   | 11.18563500 | 12.25282700 | 19.21060600 |
| H   | 11.10532100 | 12.74044500 | 18.24214400 |
| C   | 12.46261900 | 11.94056000 | 19.67708700 |
| H   | 13.32643000 | 12.22374700 | 19.08617500 |
| C   | 12.64517600 | 11.25682000 | 20.88191600 |
| C   | 11.49585500 | 10.87110700 | 21.57949000 |
| H   | 11.59604100 | 10.30270300 | 22.50315400 |
| C   | 10.22490000 | 11.19216900 | 21.10831200 |
| H   | 9.36531100  | 10.83491900 | 21.67074900 |
| C   | 14.02164900 | 10.94912400 | 21.41050500 |
| H   | 14.76582900 | 10.93002300 | 20.60684300 |
| H   | 14.34648100 | 11.70592700 | 22.13734300 |
| H   | 14.04951600 | 9.97974300  | 21.92096900 |
| B   | 3.46041800  | 12.51608200 | 20.03201500 |
| B   | 8.52915200  | 12.15224200 | 19.32101200 |
| H   | 6.16523500  | 12.78322800 | 15.42374200 |
| H   | 4.55192100  | 12.54569100 | 15.61184300 |
| Fe  | 6.02242200  | 9.92085000  | 12.47558700 |
| N   | 7.54857600  | 8.60873400  | 12.47014900 |
| N   | 7.72701200  | 7.72074900  | 11.46587600 |
| N   | 4.91939000  | 8.40039800  | 11.80118100 |
| N   | 5.37338600  | 7.55267400  | 10.85268700 |
| N   | 6.42362600  | 10.37001700 | 10.45291400 |
| N   | 4.52998300  | 11.20843200 | 12.43839400 |
| N   | 4.63946800  | 12.37447900 | 11.77670100 |
| N   | 7.18937400  | 11.49140000 | 12.89974300 |
| N   | 7.08808400  | 12.65555200 | 12.21779700 |
| N   | 5.64967600  | 9.57030100  | 14.08017400 |
| C   | 8.31381800  | 8.20695700  | 13.49520200 |
| H   | 8.31692300  | 8.74726200  | 14.43125200 |
| C   | 9.00045600  | 7.04086600  | 13.15802600 |
| H   | 9.69537100  | 6.47994300  | 13.76552200 |
| C   | 8.58359100  | 6.76059600  | 11.86678500 |
| H   | 8.82579700  | 5.93342700  | 11.21850600 |
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | 3.793981   | 7.875608   | 12.302043  |
| H       | 3.255391   | 8.381665   | 13.087698  |
| C       | 3.508733   | 6.662213   | 11.677133  |
| H       | 2.673274   | 6.001998   | 11.857803  |
| C       | 4.546749   | 6.491080   | 10.775148  |
| H       | 4.757524   | 5.679923   | 10.096054  |
| C       | 7.146549   | 6.780420   | 9.027013   |
| C       | 6.173383   | 6.366286   | 8.098198   |
| H       | 5.145195   | 6.703150   | 8.208433   |
| C       | 6.479784   | 5.566641   | 6.998944   |
| H       | 5.685600   | 5.274068   | 6.313871   |
| C       | 7.790459   | 5.147376   | 6.750864   |
| C       | 8.809660   | 5.597467   | 7.267894   |
| H       | 9.820125   | 5.329002   | 7.444400   |
| C       | 8.465092   | 6.396816   | 8.726466   |
| H       | 9.288280   | 6.760526   | 9.337504   |
| C       | 8.119726   | 4.250436   | 5.586966   |
| H       | 9.149348   | 4.398597   | 5.243908   |
| H       | 8.017547   | 3.191803   | 5.861233   |
| C       | 7.450429   | 4.430536   | 4.738535   |
| C       | 6.833429   | 9.354097   | 6.955895   |
| C       | 7.320669   | 9.635231   | 8.374607   |
| H       | 7.643359   | 8.818753   | 7.739782   |
| C       | 7.415803   | 10.947798  | 7.935572   |
| H       | 7.829967   | 11.175436  | 6.955629   |
| C       | 6.972648   | 11.964108  | 8.770422   |
| H       | 7.046982   | 13.001272  | 8.464034   |
| C       | 6.443546   | 11.658741  | 10.026514  |
| C       | 3.335257   | 11.193328  | 13.037933  |
| H       | 3.051501   | 10.370564  | 13.674872  |
| C       | 2.637267   | 12.366214  | 12.740634  |
| H       | 1.647216   | 12.648952  | 13.067009  |
| C       | 3.506493   | 13.089740  | 11.940069  |
| H       | 3.403360   | 14.061952  | 11.483851  |
| C       | 8.243269   | 11.597003  | 13.718564  |
| H       | 8.495471   | 10.802640  | 14.402543  |
| C       | 8.863622   | 12.834586  | 13.546366  |
| H       | 9.729577   | 13.218527  | 14.064656  |
| C       | 8.104097   | 13.466204  | 12.573029  |
| H       | 8.225438   | 14.431156  | 12.106019  |
| C       | 5.779219   | 14.303581  | 10.552419  |
| C       | 5.945408   | 15.440083  | 11.364871  |
| H       | 6.292538   | 15.326480  | 12.389020  |
| C       | 5.642038   | 16.726564  | 10.922464  |
| H       | 5.793681   | 17.571833  | 11.591996  |
| C       | 5.131974   | 16.949161  | 9.639603   |
| C       | 4.909134   | 15.827467  | 8.835591   |
| H       | 4.477996   | 15.957321  | 7.844235   |
| C       | 5.219957   | 14.544630  | 9.284158   |
| H       | 4.991681   | 13.706266  | 8.630361   |
| C       | 4.838306   | 18.340538  | 9.144337   |
| H       | 4.054401   | 18.337577  | 8.379368   |
| H       | 4.515146   | 18.998012  | 9.958942   |
|    | 5.73036200 | 18.79675300 | 8.69446500 |
|----|------------|-------------|-------------|
| B  | 6.78509900 | 7.82115300  | 10.20976200 |
| B  | 5.98775700 | 12.79279500 | 11.09468200 |
| H  | 5.83274000 | 8.55980300  | 14.23052000 |
| H  | 5.56033800 | 11.27661200 | 15.43206300 |

**Fe(IV)=NH (LS)**

|    | 5.81771100 | 11.17683200 | 17.95903600 |
|----|------------|-------------|-------------|
| N  | 4.40817600 | 12.59057200 | 17.66545000 |
| N  | 3.20872600 | 12.56367000 | 18.28761700 |
| N  | 4.31209000 | 9.85849100  | 17.86901700 |
| N  | 3.11952300 | 10.12562000 | 18.44745100 |
| N  | 5.45561400 | 11.22071200 | 20.01216200 |
| N  | 7.17886700 | 9.78227700  | 18.18906800 |
| N  | 8.00207900 | 9.81060300  | 19.25389900 |
| N  | 7.28321500 | 12.48684300 | 18.32842000 |
| N  | 8.14527600 | 12.31062000 | 19.35441100 |
| N  | 6.07516800 | 11.16665400 | 16.21154600 |
| C  | 4.30889100 | 13.44769200 | 16.64394300 |
| H  | 5.14185500 | 13.58011700 | 15.97022300 |
| C  | 3.02633300 | 13.99745100 | 16.59763800 |
| H  | 2.63784100 | 14.72156400 | 15.89647500 |
| C  | 2.35638100 | 13.39172800 | 17.64775500 |
| H  | 1.32933700 | 13.48016900 | 17.96522800 |
| C  | 4.15700200 | 8.75191500  | 17.13228600 |
| H  | 4.98821900 | 8.33291200  | 16.58747600 |
| C  | 2.84136600 | 8.29733100  | 17.21188000 |
| H  | 2.40620400 | 7.43333300  | 16.73152100 |
| C  | 2.21682700 | 9.20608000  | 18.04898800 |
| H  | 1.19155400 | 9.26840800  | 18.37908300 |
| C  | 1.53842400 | 11.50952600 | 20.08763700 |
| C  | 0.93733700 | 10.37432000 | 20.66286500 |
| H  | 1.40892300 | 9.40066200  | 20.55136500 |
| C  | -0.23148200| 10.44729200 | 21.41826500 |
| H  | -0.65426600| 9.53541400  | 21.83730800 |
| C  | -0.86163600| 11.67154600 | 21.66128900 |
| C  | -0.24809300| 12.81775300 | 21.14865000 |
| H  | -0.68412700| 13.79459300 | 21.35236700 |
| C  | 0.92065300 | 12.73585600 | 20.39239700 |
| H  | 1.37860100 | 13.66683300 | 20.06803700 |
| C  | -2.14632000| 11.75101700 | 22.44305500 |
| H  | -2.21570700| 10.94800700 | 23.18508100 |
| H  | -2.23827600| 12.70738600 | 22.96936800 |
| H  | -3.01921900| 11.65875900 | 21.78269700 |
| C  | 4.18460500 | 11.44504700 | 20.42310800 |
| C  | 3.93671900 | 11.71315700 | 21.77369000 |
| H  | 2.91854800 | 11.88898100 | 22.09975000 |
| C  | 4.98794600 | 11.77939900 | 22.67681300 |
| H  | 4.80559800 | 12.02362800 | 23.72131500 |
| C  | 6.27584900 | 11.52935400 | 22.22363800 |
| H  | 7.11906200 | 11.58975500 | 22.90231400 |
| C  | 6.50013000 | 11.21921600 | 20.87967400 |
|  | X   | Y   | Z   |
|---|-----|-----|-----|
| C | 7.54770900 | 8.75185200 | 17.42290000 |
| H | 7.06131300 | 8.07222200 | 18.01338600 |
| C | 8.61524200 | 8.78402200 | 19.17214200 |
| H | 9.13049200 | 7.19725700 | 17.64524300 |
| C | 8.87517200 | 8.75185200 | 17.42290000 |
| H | 9.62312500 | 8.64016000 | 19.93621000 |
| C | 8.87517200 | 7.06131300 | 16.47688000 |
| H | 9.13049200 | 7.19725700 | 17.64524300 |
| C | 7.53490500 | 13.68322000 | 17.79086800 |
| H | 6.97878900 | 14.02047500 | 16.93132500 |
| C | 8.61524200 | 14.31968300 | 18.49572300 |
| H | 9.13049200 | 15.29459500 | 18.31147200 |
| C | 7.53490500 | 14.31968300 | 18.49572300 |
| H | 8.61524200 | 15.29459500 | 18.31147200 |
| C | 11.05060000 | 10.82270200 | 21.82644000 |
| H | 12.61258000 | 11.13320900 | 21.55630200 |
| C | 11.40590900 | 10.91339000 | 23.00345100 |
| H | 10.10187900 | 9.67244800 | 23.28432900 |
| C | 9.91313400 | 9.06859500 | 24.17064400 |
| H | 9.04074800 | 10.05130000 | 22.44379900 |
| C | 8.05348500 | 9.62244800 | 22.69161900 |
| H | 12.54892100 | 9.77025000 | 23.92997500 |
| C | 12.67619600 | 10.55389400 | 24.68908200 |
| H | 12.38201600 | 8.82770500 | 24.46281600 |
| H | 13.49663000 | 9.68936600 | 23.38605000 |
| B | 2.96710600 | 11.42153000 | 19.33429000 |
| B | 7.98840800 | 11.02207400 | 20.25268000 |
| H | 5.60063500 | 10.45162800 | 15.64525100 |

\[4_{\text{Tot}} \text{ (LS)}\]

|  | X   | Y   | Z   |
|---|-----|-----|-----|
| Fe | 6.21009400 | 3.52411400 | 12.15761000 |
| Fe | 2.81725200 | 5.91211200 | 14.55051900 |
| N  | 1.24194600 | 5.06656200 | 13.59359000 |
| N  | 6.43786400 | 4.13784900 | 9.34426800 |
| N  | 2.57533400 | 4.50422500 | 15.98198500 |
| N  | 7.00361700 | 2.27433700 | 11.33732200 |
| N  | 3.08546000 | 7.28244900 | 13.09037200 |
| N  | 1.73539000 | 4.63750300 | 14.30592400 |
| N  | 4.01828100 | 4.67178700 | 13.71265600 |
| N  | 4.94987400 | 2.00710200 | 12.39903000 |
| N  | 4.41012400 | 8.17683400 | 15.54586100 |
| N  | 7.34569920 | 5.11055900 | 11.88280200 |
| N  | 4.31696700 | 8.27779100 | 15.53901400 |
| N  | 5.00244100 | 4.78420700 | 12.92727400 |
| N  | 7.00361700 | 3.01897800 | 13.96471000 |
| N  | 1.55050600 | 7.10258100 | 15.47342900 |
| N  | 5.43048000 | 0.80842300 | 12.78490600 |
| N  | 1.33848000 | 4.16424400 | 16.40623500 |
| N  | 5.54359200 | 3.89453100 | 10.32295000 |
| N  | 8.20523400 | 5.21476700 | 10.78256400 |
| N  | 7.23215200 | 1.72030800 | 14.27534000 |
H     2.25158000  0.12028500  12.46121700
C     3.33553000  10.59488800  15.14346100
C    -2.51909800  4.75698000  15.87730500
H    -2.53363300  4.75698000  15.87730500
C     2.72521700 11.50575900  14.26047600
H     2.21469800 11.13642800  13.37427500
C    -0.21421200  8.76679400  16.79806500
H    -0.90830300  9.42146100  17.32095100
C      9.98784900  0.96143400  10.74284800
H     10.94227200  0.47660700  10.54824700
C     3.70509100  9.25701100  12.31490000
H     3.95914900 10.30351900  12.37790100
C     4.42492800 -2.08952600  12.85040300
H     4.61914700 -1.10913800  13.14518900
C     8.80811000  8.48789000  17.76242400
C     8.45402200  6.66762200  16.38414100
C     6.30135500  7.40683000  16.42337500
H     7.27646400  7.35325000  16.88543200
C     9.98784900  12.87917000  14.49586100
H     9.61914700  13.53676900  13.77649000
C     5.60356400  8.54761300  16.05050000
H     5.88247200  9.58835500  16.10066200
C    -3.81111900  4.16399800  17.85129700
C    -1.38036000  4.26291300  17.90459500
H     8.31759200  7.76202100  12.48232000
H    -0.49988800  3.39693000  11.35673200
C     7.12019300 -3.63020600  14.57350300
C     3.28422300  13.42586900  15.64510600
C     8.82291700  6.88736400  12.08614900
H     9.31759200  7.76202100  12.48232000
C     8.13657700  2.92414400  15.90831400
H     8.65273800  3.21742400  16.81088000
C     9.58339700  8.83674600  6.03968000
H     9.85991500  3.02789600  5.36497700
C     3.73691700  8.38762300  11.23824400
H     4.00853400  8.60483300  10.21572000
C    -2.60185600  4.04732600  18.54251300
H    -2.61334800  3.79497800  19.60181600
C     3.85825600 11.16002200  16.32061200
H     4.25712500 10.51462200  17.09915900
C     9.31581900  6.16328300  6.50268700
H     9.37847800  7.20654600  6.19659200
C     6.76917600 -2.59768500  15.44882200
H     6.49618900 -2.83645100  16.47570100
C     9.73052600  5.16206900  5.61948500
C     7.39746200 -1.97151600  12.83908200
H     7.60535600 -1.73362200  11.79332600
C     3.84408600  12.53330100  16.56305400
H     4.26627400  12.91534900  17.49129300
C     3.30172800  14.91291200  15.88262900
H     3.35742200  15.14889300  16.95084600
H     4.16991800  15.38200900  15.40016300
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | 3.15679800| 7.33488900| 11.86518400|
| H    | 3.07751900| 6.38983200| 11.35089600|
| C    | 4.40299000| 0.03972400| 9.49256300  |
| H    | 3.48825000| 3.96246700| 10.06423800|
| C    | 9.74798700| 2.07633200| 10.05582400|
| H    | 10.43038800| 2.49909800| 9.32630900  |
| C    | 8.11880800| 1.54801100| 15.39721000|
| H    | 8.47314900| 0.57964900| 15.71932000|
| C    | 7.17798000| -0.90994200| 13.69415200|
| H    | 9.22651200| 0.44828700| 11.73069900|
| C    | 0.78161600| 9.34082300| 16.37189600|
| H    | 4.57669200| 4.17009100| 8.11217600  |
| C    | 7.65334200| 3.66715100| 15.06979400|
| H    | 7.56955000| 4.74433300| 15.09590000|
| C    | -0.62903200| 7.45715100| 16.77584900|
| H    | -1.52599500| 7.01530500| 17.19352300|
| C    | 9.23909200| 3.34019700| 7.22586700  |
| H    | 9.11031000| 2.30419500| 7.52998800  |
| C    | 8.84076200| 4.37153100| 8.09480300  |
| C    | 3.62013500| 1.71795100| 12.19834000|
| H    | 2.96408200| 2.52250300| 11.89486800|
| C    | 1.00147800| 4.67781700| 12.40894800|
| H    | 1.74420000| 4.90273300| 11.65932000|
| C    | 5.34415300| 6.46658400| 16.05006000|
| H    | 5.51792200| 5.40458500| 16.11783300|
| C    | 1.29294900| 3.09090200| 17.13662200|
| H    | 0.40278500| 2.62185900| 17.52744000|
| C    | 2.61855700| 2.69674500| 17.20155700|
| H    | 3.02873300| 1.82748500| 17.69411100|
| C    | -0.72760100| 3.96113900| 13.55236100|
| H    | -1.62021600| 3.49437100| 13.93848800|
| C    | 8.15244400| 6.19874300| 12.48643900|
| H    | 7.70795200| 6.43334400| 13.44510300|
| C    | 9.36258900| 6.09300600| 10.65907000|
| H    | 10.08340800| 6.18748200| 9.86110700  |
| C    | 5.95161400| 4.20308700| 7.94786800  |
| H    | 6.54742100| 4.29936700| 7.05389900  |
| C    | -3.87266500| 4.55364700| 16.52343800|
| H    | -4.79287100| 4.69294900| 15.95794100|
| C    | 6.82608700| -1.29624000| 15.00052500|
| H    | 6.48816700| -0.54327700| 15.70960300|
| C    | 3.32278600| 0.36905900| 12.39582600|
| H    | 2.37077600| -0.12849100| 12.28289900|
| C    | 3.15789000| 10.70247700| 15.29936100|
| C    | -2.64729000| 4.79326200| 15.90403000|
| H    | -2.65990100| 5.15227300| 14.87762300|
| C    | 2.53259100| 11.62986100| 14.44477600|
| H    | 2.01230100| 11.27819200| 13.55703700|
| C    | -0.37669000| 8.81342100| 16.92388200|
| H    | -1.07483900| 9.45140800| 17.46193200|
| Atoms | X    | Y    | Z    |
|-------|------|------|------|
| B     | 7.00683000 | 0.61667500 | 13.17157800 |
| B     | 3.05182900 | 9.10940200 | 15.04193800 |
| C     | 7.30522300 | -5.08307700 | 15.00543100 |
| H     | 6.58077900 | -5.28812700 | 15.80131200 |
| H     | 7.11028800 | -5.77896700 | 14.18212300 |
| H     | 8.30065600 | -5.32226100 | 15.40352100 |
| H     | -0.01416100 | 5.04713900 | 15.88609700 |
| C     | 10.54230400 | 5.17649800 | 4.14282900 |
| H     | 10.33700000 | 4.36760600 | 3.43300800 |
| H     | 10.16204300 | 6.10956700 | 3.71267700 |
| H     | 11.63395100 | 5.27419800 | 4.21606200 |
| H     | 5.05914000 | 6.01910800 | 12.89632400 |
| H     | 3.68924000 | 3.85437700 | 13.87578800 |

**TSB**

| Atoms | X    | Y    | Z    |
|-------|------|------|------|
| Fe    | -2.92297700 | -0.00300500 | -0.00331700 |
| Fe    | 2.83584400 | 0.18481200 | -0.28775300 |
| N     | 3.35549300 | -0.67732800 | -2.25433700 |
| N     | -3.80083200 | -1.92077800 | -1.97795000 |
| N     | 3.48766200 | 2.11783500 | -1.11566000 |
| N     | -5.01626300 | 0.03712500 | -0.06920700 |
| N     | 2.45151000 | -1.80423600 | 0.63174500 |
| N     | 4.42522000 | -0.17782400 | -2.90777100 |
| N     | 0.89063800 | 0.45809900 | -0.88367600 |
| N     | -2.89353400 | 1.77887600 | -0.83960200 |
| N     | 2.95027400 | 0.28208600 | 2.78622800 |
| N     | -3.06438900 | -1.84936900 | 0.82286400 |
| N     | 2.51454000 | 1.00415400 | 1.73119100 |
| N     | -1.10138900 | -0.08842200 | 0.19768800 |
| N     | -3.02961300 | 1.00013200 | 1.75876900 |
| N     | 4.82944000 | -0.10051200 | 0.24770400 |
| N     | -3.77401400 | 2.72266200 | -0.45468000 |
| N     | 4.51284200 | 2.11770400 | -1.99451200 |
| N     | -2.89297400 | -0.95886000 | -1.72151200 |
| N     | -3.95789700 | -2.75804500 | 0.36970900 |
| N     | -3.90897300 | 2.01186300 | 1.93880300 |
| N     | 2.89948700 | -2.02006800 | 1.88611200 |
| C     | 5.09833200 | -0.59489200 | 1.48221800 |
| C     | -5.66536500 | 1.13317600 | 0.40330500 |
| C     | 6.74933100 | 1.09834500 | -2.99563100 |
| C     | -5.68512800 | -1.11262400 | -0.34467800 |
| C     | 5.78719700 | 0.21319500 | -0.66156500 |
| C     | 2.84246800 | 3.27879300 | -1.26866000 |
| H     | 1.99297700 | 3.51610100 | -0.64133200 |
| C     | 1.53403000 | -2.74122900 | 0.37787500 |
| H     | 1.04789300 | -2.77732200 | -0.58849500 |
| C     | -2.09085300 | -0.87285100 | -2.78732600 |
| H     | -1.26817600 | -0.17782200 | -2.79692400 |
| C     | -7.04040900 | -1.21911100 | -0.01831600 |
| H     | -7.55062300 | -2.16121500 | -0.18400600 |
| C     | -3.91381700 | 2.38222500 | 3.23342700 |
| H     | -4.58448900 | 3.15223200 | 3.58221600 |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | -8.26893500 | -6.53095000 | -4.46399200 |
| H    | -7.06765800 | -7.68442000 | -3.85570300 |
| H    | -8.50352800 | -7.31341000 | -2.89785800 |
| H    | -0.66012000 | -1.00269500 | 0.24420000  |
| H    | 0.62894700  | 0.05646100 | -1.80503300 |
| H    | -0.66552700 | 0.51414300 | 0.88982500  |

[Fe(II)NH(·)-NH₂-Fe(II)] (LS)
H      -1.46040700  0.10777400  2.41695600

[Fe(II)NH(-)NH-Fe(II)] (HS)

|    |       |       |       |
|----|-------|-------|-------|
| Fe | -0.13745100 0.27255600 0.09442800 |
| Fe | 0.00897500 -0.20864900 5.05562500 |
| N  | 2.02815800 0.85052800 5.53226800 |
| N  | 0.79908300 -2.15516900 -1.13804400 |
| N  | 0.71740200 1.74657300 5.62433000 |
| N  | 0.12408800 0.68012900 -1.87908900 |
| N  | -0.74885300 -2.21466100 4.74028800 |
| N  | 2.69189700 -0.29022200 6.56852500 |
| N  | 0.25030700 0.16537400 3.16589000 |
| N  | 1.48926200 1.36537900 0.48810700 |
| N  | -3.06496400 -0.41504400 5.48264400 |
| N  | -1.74493600 0.11927200 -0.39343000 |
| N  | -2.10257400 0.39772700 4.99658800 |
| N  | -0.58009800 -0.18383200 2.06056000 |
| N  | -1.25095900 1.97913300 0.24865000 |
| N  | -0.39864600 0.54002400 7.12678000 |
| N  | 1.61830900 2.56280700 -0.12135900 |
| N  | 1.56170700 1.89870000 6.66988800 |
| N  | 0.91962800 -1.38487500 -0.04032400 |
| N  | -1.65183300 -1.74661600 -1.45474700 |
| N  | -0.82688500 3.12420600 -0.33310500 |
| N  | -1.92907400 -2.59907800 5.27544100 |
| C  | -1.54029700 -1.18730700 7.47646700 |
| C  | 0.25820000 1.97573900 -2.27231600 |
| C  | 2.77876300 1.04330500 8.86764700 |
| C  | -0.10237900 -0.30549200 -2.78646400 |
| C  | 0.51564900 -0.11575600 8.03635000 |
| C  | 0.74211200 2.88671400 4.92164800 |
| H  | 0.14041400 2.98979900 4.02921300 |
| C  | -0.43989800 -3.09935100 3.78168800 |
| H  | 0.47485000 -2.99571500 3.21398400 |
| C  | 1.78572100 1.99683600 0.77405300 |
| H  | 2.01810500 -1.56453400 1.73578600 |
| C  | -0.33560600 0.02342700 -4.12625200 |
| H  | -0.57862900 -0.76521600 -4.82903000 |
| C  | -1.78951700 4.06531300 -0.25766000 |
| H  | -1.65020000 5.03503100 -0.70970000 |
| C  | 1.02973200 4.56295200 -1.59492300 |
| C  | 0.01957000 2.32290800 -3.60554600 |
| H  | 0.05529000 3.36735000 -3.89509100 |
| C  | -1.78643900 -1.43413600 8.83180600 |
| H  | -2.69060800 -1.95435000 9.12358400 |
| C  | 2.25504000 -3.17895700 0.19107100 |
| H  | 2.97102800 -3.88261500 0.59065900 |
| C  | -2.47642800 2.23165700 0.72706100 |
| H  | -3.03737500 1.47311900 1.24950700 |
| C  | 0.27079400 -0.34897600 9.39507800 |
| H  | 0.98918500 -0.01094600 10.13181800 |
| C  | 0.66975700 -2.94065100 -4.42195900 |
