# 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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*Supporting Information*
Table of Contents

**Experimental Details.**

**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 $CaH_2$. All dried solvents were degassed, and vacuum distilled prior to use. $^{15}NH_3$ (98% purity) was purchased from Millipore Sigma and used as received using a corrosive gas regulator for lecture bottles. $^{14}NH_3$ 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 **[$^{Ar}$B$_2$Pz$_4$Py]HLi** ligands,[1,2] **1$_{Ph}$-THF**[1] and **1$_{Ph}$**[1] have previously been reported. 2,4,6-tri-*tert*-butyl phenoxy radical was synthesized according to a literature procedure.[3]

**Physical Methods**

$^1$H, $^{13}$C{$^1$H} chemical shifts are referenced to the residual solvent signals of $C_6D_6$ ($^1$H, 7.16 ppm; $^{13}$C{$^1$H}, 128.06 ppm), THF-*d8* ($^1$H, 3.58, 1.72 ppm; $^{13}$C{$^1$H}, 67.21, 25.31 ppm) and toluene-d8 ($^1$H, 7.09, 7.01, 6.97, 2.08 ppm; $^{13}$C{$^1$H}, 137.48, 128.87, 127.96, 125.13, 20.43 ppm). $^1$H, $^{11}$B, $^{13}$C{$^1$H}, $^{15}$N, $^{15}$N{$^1$H}, $^1$H-$^1$H-COSY, $^1$H-$^{13}$C-HSQC, $^1$H-$^{13}$C-HMBC and $^1$H-$^{15}$N-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 $^{11}$B chemical shifts are relative to $BF_3{\cdot}OEt_2$. All $^{15}$N NMR spectra are externally referenced to 60% $CH_3{}^{15}NO_2$ ($\delta_{CH315NO2} = \delta_{15NH3} - 380$) in $CDCl_3$. 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: $\delta \pm 0.02$ mm/s and $\Delta E_Q \pm 3\%$. 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 $[Bu_4N][PF_6]$ 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**

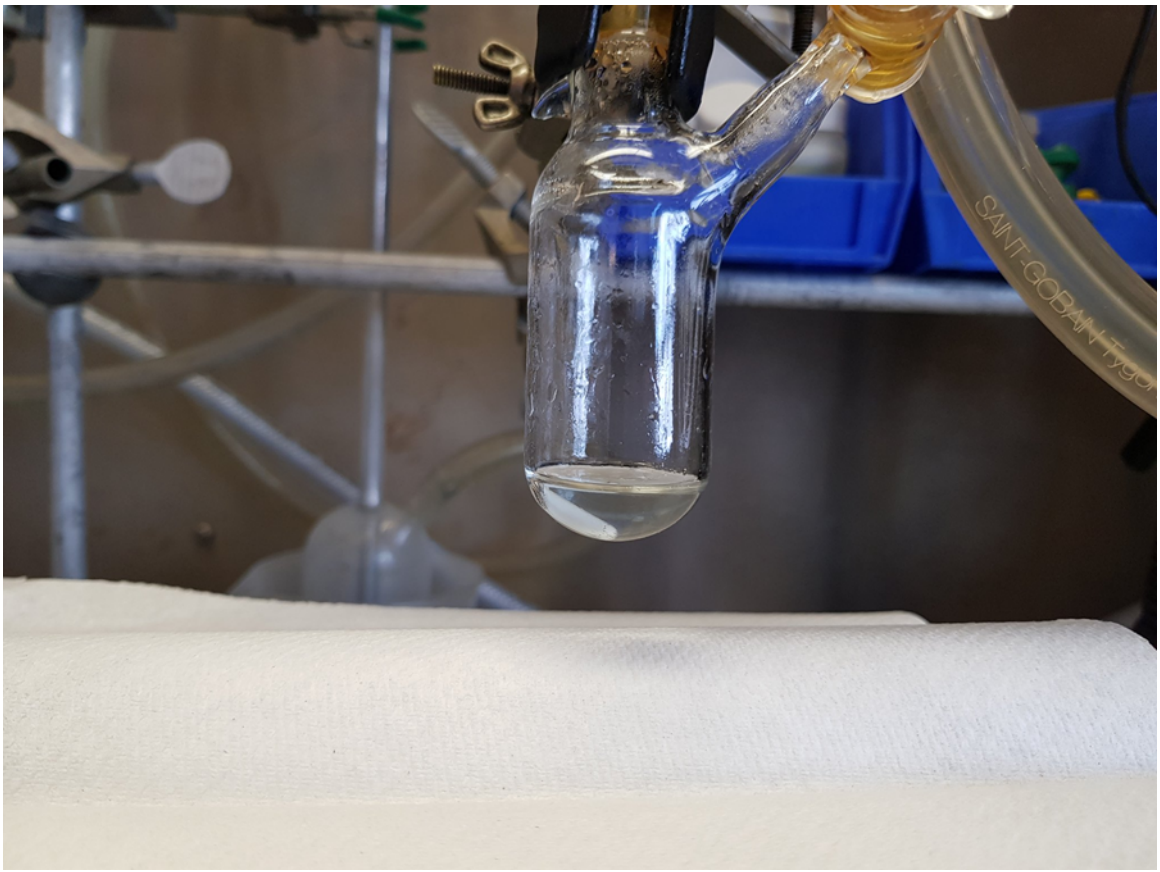
All calculations were carried out with the Gaussian09 program[10] at the DFT level using the hybrid functional B3PW91.[11,12] For Fe, the relativistic energy-consistent pseudopotential of the Stuttgart-Köln ECP library was used in combination with its adapted segmented basis.[13] For all other atoms, 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 Nimag = 0) or transition states (Nimag = 1) and IRC calculations were carried out from all transition states.

**Syntheses.**

**Synthesis of $^{n}FeBr_2$.** $^{57}Fe$ 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 $^{57}FeBr_2$ (360 mg, 93%). The same procedure was used to make $^{56}FeBr_2$ (1.8 g, 92%) using 0.50 g of $^{56}Fe$ metal.

**Schlenk flask used for the reaction (mixture after 30 mins of stirring with MeOH):**



**Synthesis of $^{n}$Fe(HMDS)$_2$.** $^{57}$Fe(HMDS)$_2$ was synthesized by modification of a literature procedure.[16] LiHMDS was sublimed at 80 ºC. 350 mg of freshly synthesized $^{57}$FeBr$_2$ (1 eq) was added to a 50 mL Schlenk flask equipped with a Teflon cap. 10 mL of $Et_2O$ was transferred. The solution was cooled to 0 ºC and freshly sublimed LiHMDS (2 eq) dissolved in 15 mL of $Et_2O$ was added dropwise via canula. The suspension was allowed to stir at 0 ºC for 30 min and slowly turned grey. The resulting mixture was stirred at room temperature for 20 h. All volatiles were removed *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 ºC (oil bath temperature). The product was brought to a glovebox and stored at -40 ºC. It solidified as a green solid (350 mg, 60%). $^1$H NMR (500 MHz, $C_6D_6$): δ 64.9 (36 H, broad singlet). The same procedure was used to make $^{56}$Fe(HMDS)$_2$ using $^{56}$FeBr$_2$.

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

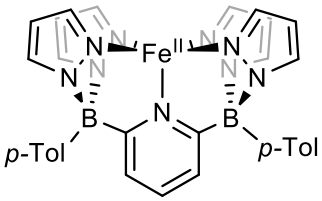
**Extraction of $^{15}N_2H_4$.**

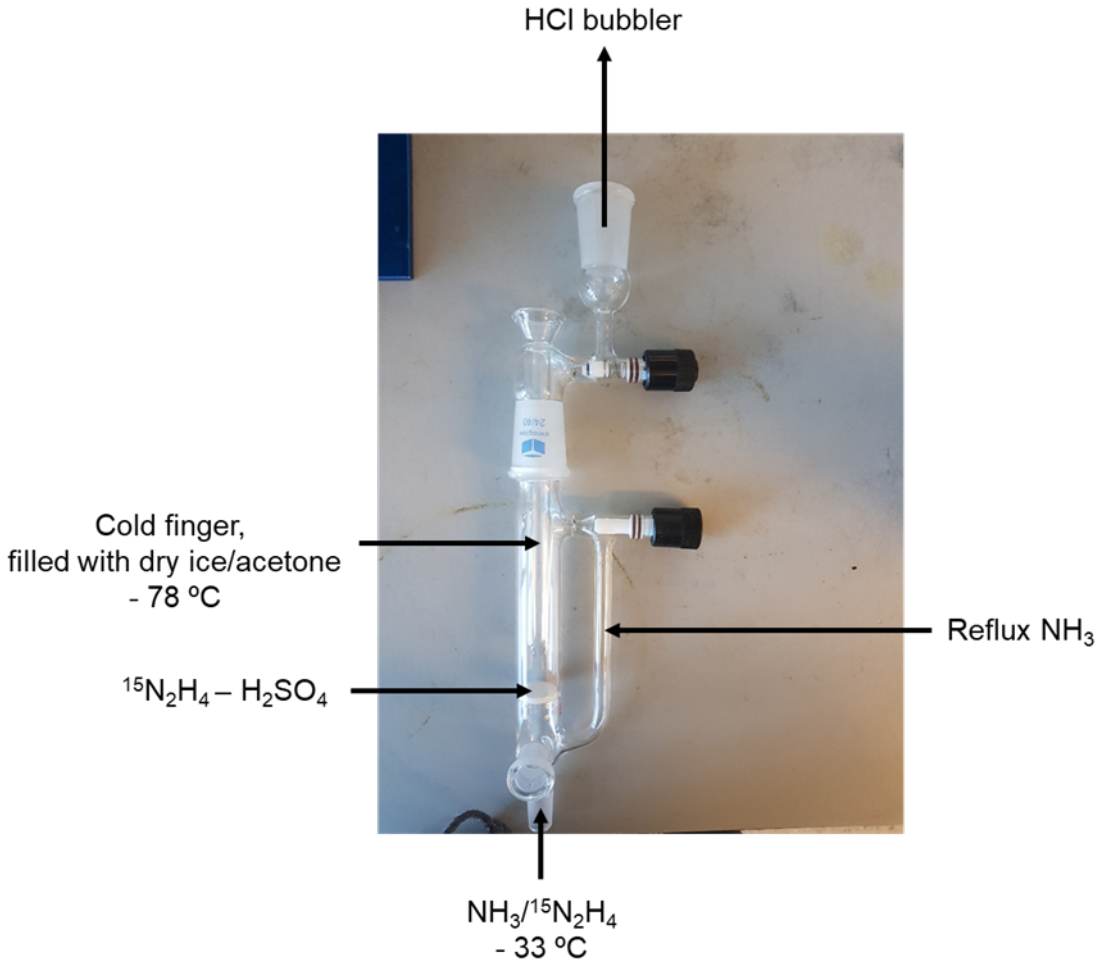
**Notes:** We recommend doing this procedure first without the hydrazine sulfate to get a feel for the extraction process using liquid $NH_3$. **Hydrazine is highly toxic and explosive.** We do not recommend doing this procedure on a bigger scale than reported below. If you choose to do so, adjust the size of the apparatus. The frit is a medium porous frit.

**Extraction.** $^{15}N_2H_4$ was prepared according to a modified procedure.[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 capand linked to a series of two empty bubblers and a third bubbler filled with 2 M HCl to quench $NH_3$. An ice bath was put under the HCl bubbler during the $NH_3$ quench. After 30 mins under vacuum, 10 mL of liquid $^{14}NH_3$, passed through two columns of KOH pallets, was condensed into the RBF by cooling the RBF with a liquid $N_2$ bath. The liquid $N_2$ bath was discarded and replaced with an acetone/dry ice bath to allow $NH_3$ to melt. In the meantime, the cold finger was charged with crushed dry ice and acetone and kept at -78 ºC **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 ºC to allow $NH_3$ to reflux gently. $NH_3$ (g) passed through the side arm (open through a Kontes cap), condensed on the cold finger (kept at -78 ºC), and dipped onto the hydrazine sulfate. The white crystalline powder slowly "swells" upon $NH_3$ absorption. Once the solid was covered with a 5 mm layer of liquid $NH_3$, the liquid containing the $^{15}N_2H_4/NH_3$ mixture was pulled through the frit by cooling the RBF with a liquid $N_2$ 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 $^{15}N_2H_4/NH_3$ solution mixture was allowed to warm up slowly to -10 ºC. The pressure-release Kontes valve linked to the HCl bubbler was opened and the leftover ammonia was quenched slowly (30 mins) at -10 ºC. 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 $NH_3$. The flask containing clean $^{15}N_2H_4$ was brought to the Ar glovebox and kept in the freezer at -40 ºC (107 mg, 84%). $^1$H NMR (500 MHz, $C_6D_6$) δ 2.28 (d, $^1J_{15N\text{-}1H}$ = 63.9 Hz, 4H). $^{15}$N NMR (51 MHz, $C_6D_6$) δ -331.0 (t, $^1J_{15N\text{-}1H}$ = 61.0 Hz, 2N). $^{15}N\{^1H\}$ NMR (51 MHz, $C_6D_6$) δ -331.0 (s, 2N).

**Special apparatus designed for $^{15}N_2H_4$ extraction:**

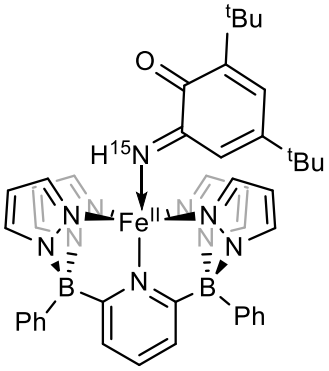



**Synthesis of $\mathbf{1_{Tol}}$.**

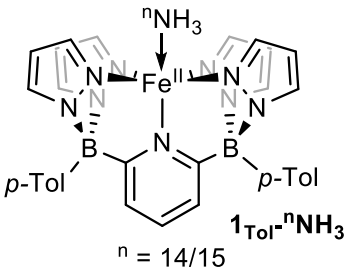
In a 100 mL round bottom flask equipped with a Y-joint and a Teflon cap, the lithium salt of the ligand **[$^{Tol}$B$_2$Pz$_4$Py]HLi** (0.40 g, 0.72 mmol) was dissolved in 10 mL of THF. Fe(HMDS)$_2$ (0.30 g, 0.79 mmol) dissolved in 5 mL of THF was added dropwise to the ligand solution. The resulting yellow solution was stirred at room temperature for 4 h and all volatiles were removed *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 *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 ºC 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 $\mathbf{1_{Tol}}$ was collected and stored at -40 °C in the freezer. The product is paramagnetic and highly air and moisture sensitive. **$^1$H NMR** (500 MHz, $C_6D_6$) δ 74.4, 45.1, 19.8, 13.9, 9.8, 7.5, 7.0, 2.1. **$^{11}$B NMR** (161 MHz, $C_6D_6$) δ +38.4 (s). **Elemental Analysis** for $C_{31}H_{29}B_2N_9Fe$: 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 $C_{31}H_{29}B_2N_9Fe$: 605.2076 ($M^{*+}$) m/z found: 605.2093 ($M^{*+}$). **Evans Method**: Sample mass, 5.0 mg; Solvent, $C_6D_6$; Standard, $Si_2OMe_6$ (6%); $\mu_{eff}$ = 4.99; s = 2, n = 4. The same procedure was used to make $^{57}\mathbf{1_{Ar}}$ using $^{57}Fe(HMDS)_2$ and $\mathbf{1_{Ph}}$ using **[$^{Ph}$B$_2$Pz$_4$Py]HLi**.




**Synthesis of $\mathbf{1_{Tol}}$-$^n$NH$_3$.**

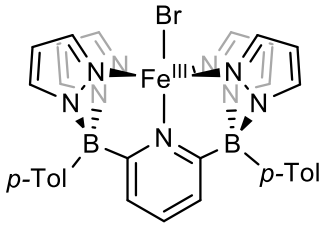
A 100 mL round bottom flask equipped with a Y-joint and a Teflon cap was charged with $\mathbf{1_{Tol}}$ (0.10 g, 0.17 mmol) dissolved in 20 mL of toluene. The solution was degassed and cooled to -78 ºC. $^{15}NH_3$ (3 eq.) was added and condensed using a liquid $N_2$ bath. The frozen solution with frozen $^{15}NH_3$ was allowed to melt using an isopropanol bath and was stirred at room temperature for 2 h. The solvent and excess $^{15}NH_3$ were removed *in vacuo*. The brown solid was washed with 5 mL of pentane and dried to afford 99 mg (96%) of $\mathbf{1_{Tol}}$-$^{15}$**NH$_3$** as a brown solid. Crystals suitable for X-ray diffraction were grown by slow diffusion of pentane into a saturated solution of $\mathbf{1_{Tol}}$-$^{14}$**NH$_3$** in benzene. **$^1$H NMR** (500 MHz, $C_6D_6$) δ 9.00 (4H, s), 8.33 (2H, d, $^3J_{HH}$ = 7.5 Hz), 8.23 (4H, d, $^3J_{HH}$ = 7.5 Hz), 7.35 (8H, m), 7.25 (4H, m), 6.60 (1H, s), 2.73 (3H, d, $^1J_{15N\text{-}1H}$ = 62.4 Hz, $^{15}$N**H3**), 2.40 (6H, s, -C**H3**). **$^{11}$B NMR** (161 MHz, $C_6D_6$) δ -1.6 (s). $^{15}$N signal was not observed. **Elemental Analysis** for $C_{31}H_{32}B_2{}^{15}NFeN_9$,$C_6H_6$: C, 63.46; H, 5.57; N, 20.00. Found (%): C, 63.75; H, 5.68; N, 19.46. IR (KBr) ($cm^{-1}$) for $\mathbf{1_{Tol}}$-$^{14}$**NH$_3$**: 3638; 3570. IR (KBr) ($cm^{-1}$) for $\mathbf{1_{Tol}}$-$^{15}$**NH$_3$**: 3642; 3566. The same procedure was used to make $\mathbf{1_{Tol}}$-$^{14}$**NH$_3$** using $^{14}NH_3$; $^{57}\mathbf{1_{Tol}}$-$^{15}$**NH$_3$** using $^{57}\mathbf{1_{Tol}}$ and $\mathbf{1_{Ph}}$-$^{15}$**NH$_3$** using $\mathbf{1_{Ph}}$.




**Synthesis of $\mathbf{2_{Ph}}$-$^{15}$N.**

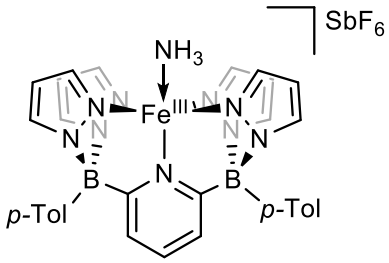
A two neck 100 mL round bottom flask equipped with a Y-joint and a Teflon cap, and a 14/20 septum was charged with $\mathbf{1_{Ph}}$-$^{15}$**NH$_3$** (0.10 g, 1 eq, 0.17 mmol) dissolved in 20 mL of toluene. A solution of **ArO·** (0.22 g, 5 eq, 0.84 mmol) in 10 mL of toluene was added to the RBF through

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 **$2_{Ph}$-$^{15}$N** as a green solid. **$^{1}$H NMR** (500 MHz, $C_6D_6$) δ 17.82 (1H, d, $^{1}J_{15N\text{-}1H}$ = 66.6 Hz, $^{15}$N**H**), 8.19 (2H, s), 8.00 (2H, s), 7.86 (2H, s), 7.77 (2H, s), 7.65 (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, *o*-$^{t}$Bu), 0.83 (9H, *p*-$^{t}$Bu). **$^{11}$B NMR** (161 MHz, $C_6D_6$) no signal. **$^{15}$N{$^{1}$H} NMR** (61 MHz, $C_6D_6$) δ +351.59. **Elemental Analysis** for $C_{43}H_{46}B_2ON_{10}Fe$: 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 $C_{43}H_{46}B_2{}^{15}NON_9Fe$: 797.3345 ($M^{*+}$) m/z found: 797.3356 ($M^{*+}$). The same protocol was repeated with **$1_{Ph}$-$^{14}$NH$_3$**. The same protocol was repeated with **$1_{Tol}$-$^{15}$NH$_3$** and the solid mixture was dissolved in 15 mL of pentane and put in the freezer (-40 ºC). Xray quality crystals of **$2_{Tol}$** were obtained after three weeks left in the freezer in the dark.




**Synthesis of $3_{Tol}$-NH$_3^+$.**

A 100 mL round bottom flask equipped with a Y-joint and a Teflon cap was charged with **$1_{Tol}$-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 **$3_{Tol}$-NH$_3^+$**. Crystals suitable for X-ray diffraction were grown by slow diffusion of pentane into a saturated solution of **$3_{Tol}$-NH$_3^+$** in benzene. **$^{1}$H NMR** (500 MHz, $C_6D_6$) δ 76.9, 12.1, 9.14, 7.4, 4.8, 3.6, 1.4, 0.5, -3.4, -18.8, -34.0. **$^{11}$B NMR** (161 MHz, $C_6D_6$) +7.0 (s). **Elemental Analysis** for $C_{31}H_{32}B_2N_{10}SbF_6Fe$: 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, $C_6D_6$; Standard, $Si_2OMe_6$ (6%); $\mu_{eff}$ = 1.80; s = 1/2, n = 1. The same protocol was used to make **$3_{Tol}$-$^{15}$NH$_3^+$** using **$1_{Tol}$-$^{15}$NH$_3$**.

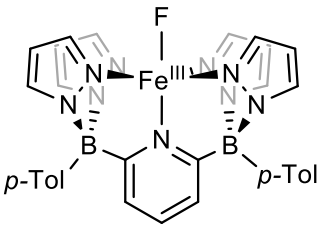



**Synthesis of $3_{Tol}$-Br.**

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. 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

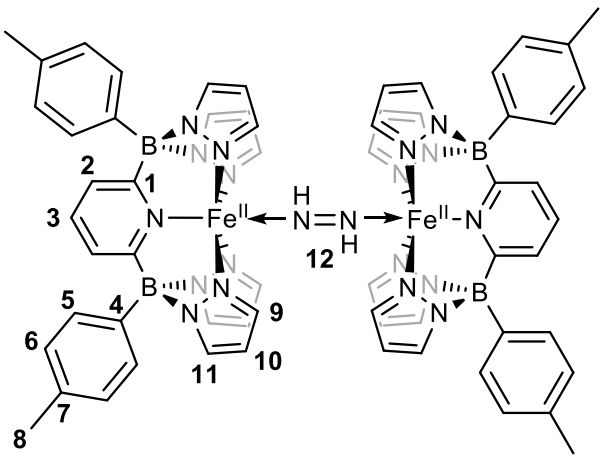
15 mL of hexanes and dried *in vacuo* to afford 0.11 g (95%) of **$3_{Tol}$-Br**. Crystals suitable for X-ray diffraction were grown by slow diffusion of pentane into a saturated solution of **$3_{Tol}$-Br** in benzene. **$^{1}$H NMR** (500 MHz, $C_6D_6$) δ 107.7, 86.3, 55.8, 30.3, 2.6. **$^{11}$B NMR** (161 MHz, $C_6D_6$) no signal. **Elemental Analysis** for $C_{31}H_{29}B_2FeN_9Br$,$C_6H_6$: 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 $C_{31}H_{29}B_2FeN_9Br$: 685.1338 $(M+H)^+$ m/z found: 685.1338 $(M+H)^+$. **Evans Method**: Sample mass, 5.0 mg; Solvent, $C_6D_6$; Standard, $Si_2OMe_6$ (6%); $\mu_{eff}$ = 5.73; s = 5/2, n = 5.

**Synthesis of $3_{Tol}$-F.**




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 **$3_{Tol}$-F**. Crystals suitable for X-ray diffraction were grown by slow diffusion of pentane into a saturated solution of **$3_{Tol}$-F** in benzene. **$^{1}$H NMR** (500 MHz, $C_6D_6$) δ 106.8, 85.8, 59.6, 55.8, 29.8, 20.4, 2.6. **$^{11}$B NMR** (161 MHz, $C_6D_6$) no signal. **$^{19}$F{$^{1}$H} NMR** (471 MHz, $C_6D_6$) no signal. **Elemental Analysis** for $C_{31}H_{29}B_2FeN_9F$: 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 $C_{31}H_{29}B_2FeN_9F$: 625.2070 $(M+H)^+$ m/z found: 625.2097 $(M+H)^+$. **Evans Method**: Sample mass, 5.0 mg; Solvent, $C_6D_6$; Standard, $Si_2OMe_6$ (6%); $\mu_{eff}$ = 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 $Et_2O$ 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. **$^1$H NMR** (500 MHz, $C_6D_6$) 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). **$^{13}$C{$^1$H} NMR** (151 MHz, $C_6D_6$) 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. **$^{11}$B NMR** (161 MHz, $C_6D_6$) no signal. **Elemental Analysis** for $C_{62}H_{60}B_4N_{20}Fe,C_6H_6$: C, 61.95; H, 5.05; N, 21.25. Found (%): C, 61.61; H, 4.86; N, 20.72. **UV-vis** ($C_6H_6$) [$\lambda_{max}$]: 723, 388 nm. **rRaman** (1064 nm, cm$^{-1}$): 1321; 1248. **$4_{Tol}$-($^{15}$N)$_2$** was made via the same protocol using $^{15}N_2H_4$. **$^{15}$N{$^1$H} NMR** (61 MHz, $C_6D_6$) δ +476.44. **rRaman** (1064 nm, cm$^{-1}$): 1279; 1206.

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**Figures S1-S32:**

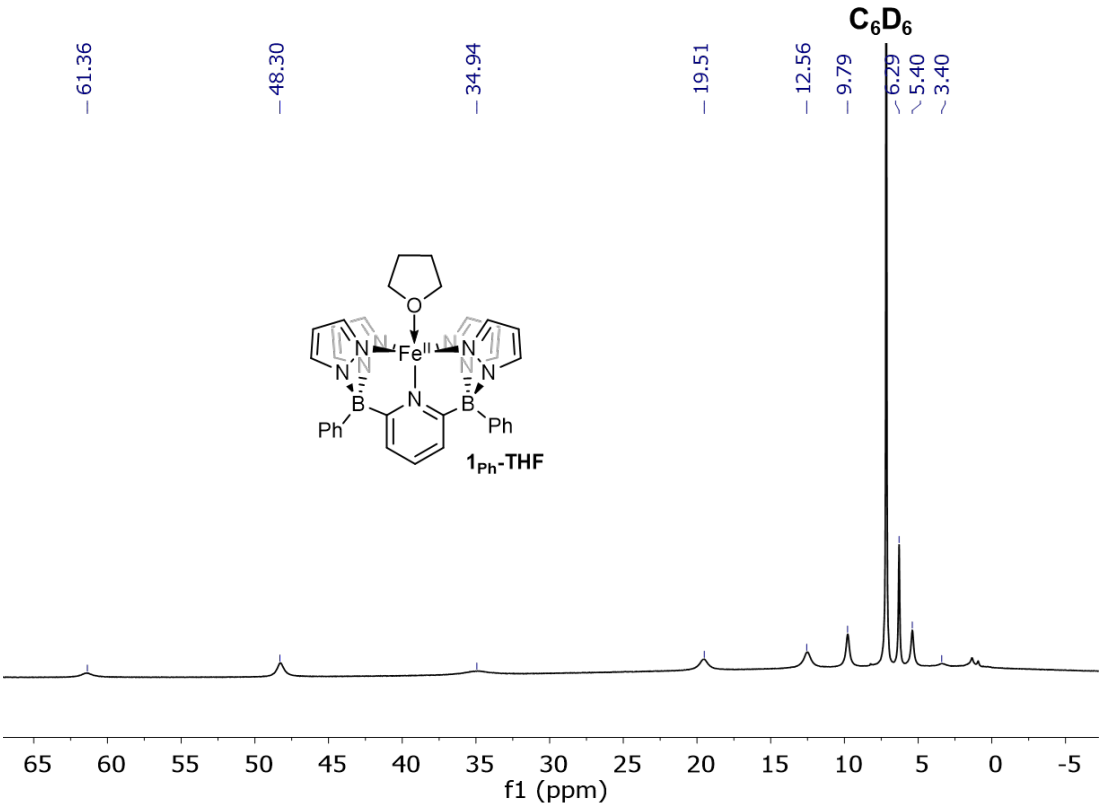



**Figure S1**. $^{1}$H NMR spectrum of **$1_{Ph}$-THF** in $C_6D_6$.

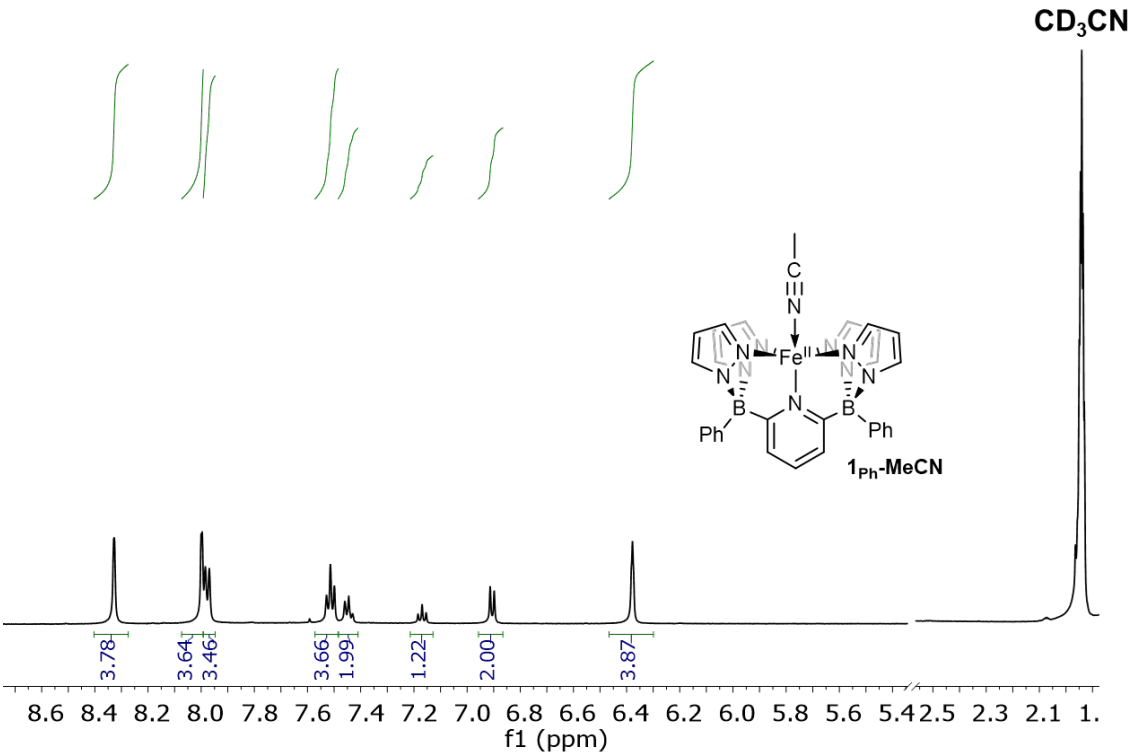
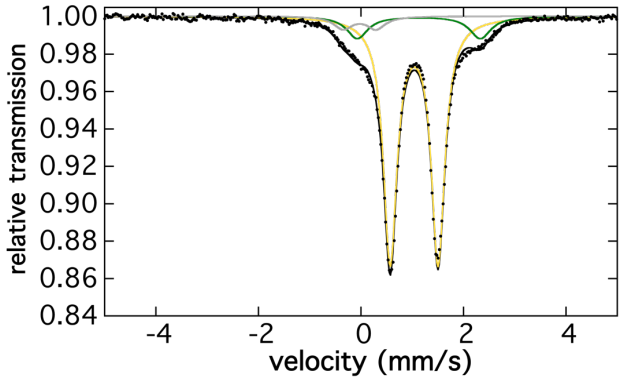
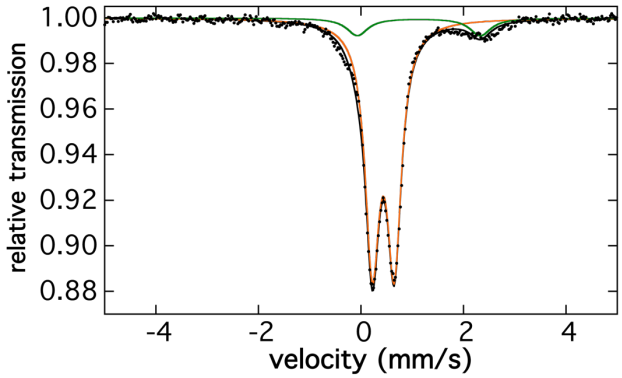



**Figure S2**. $^{1}$H NMR spectrum of **$1_{Ph}$-MeCN** in $CD_3CN$.




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

**Figure S3**. Mössbauer spectrum of a solid sample of $\mathbf{1_{Tol}}$ collected at 80 K. The species in green corresponds to leftover $\mathbf{1_{Tol}}$**-THF** as the parameters match the ones already reported for $\mathbf{1_{Ph}}$**-THF**.[1]




| | | |
|---|---|---|
| δ (mm/s) | 0.44 | 1.13 |
| $\Delta E_Q$ (mm/s) | 0.43 | 2.40 |
| % | 90 | 10 |

**Figure S4**. Mössbauer spectrum of a benzene solution of $\mathbf{1_{Tol}}$ 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 diazene adduct, complex $\mathbf{4_{Tol}}$ (Figure S29). The species in green corresponds to leftover $\mathbf{1_{Tol}}$**-THF** as the parameters match the ones already reported for $\mathbf{1_{Ph}}$**-THF**.[1]

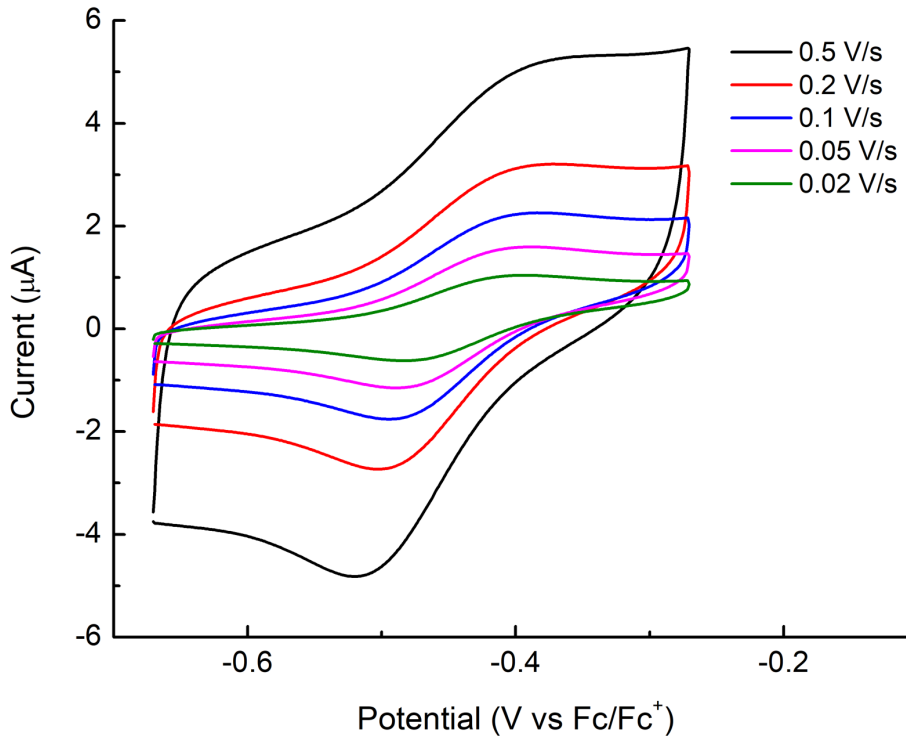



**Figure S5.** Cyclic voltammograms of $\mathbf{1}_{\mathbf{Tol}}$ in THF at different scan rates (0.02 to 0.5 V/s) under argon. Reversible Fe(II)/Fe(III) redox couple at -0.44 V vs Fc/Fc+. Concentration of $\mathbf{1}_{\mathbf{Tol}}$: 0.1 mM.

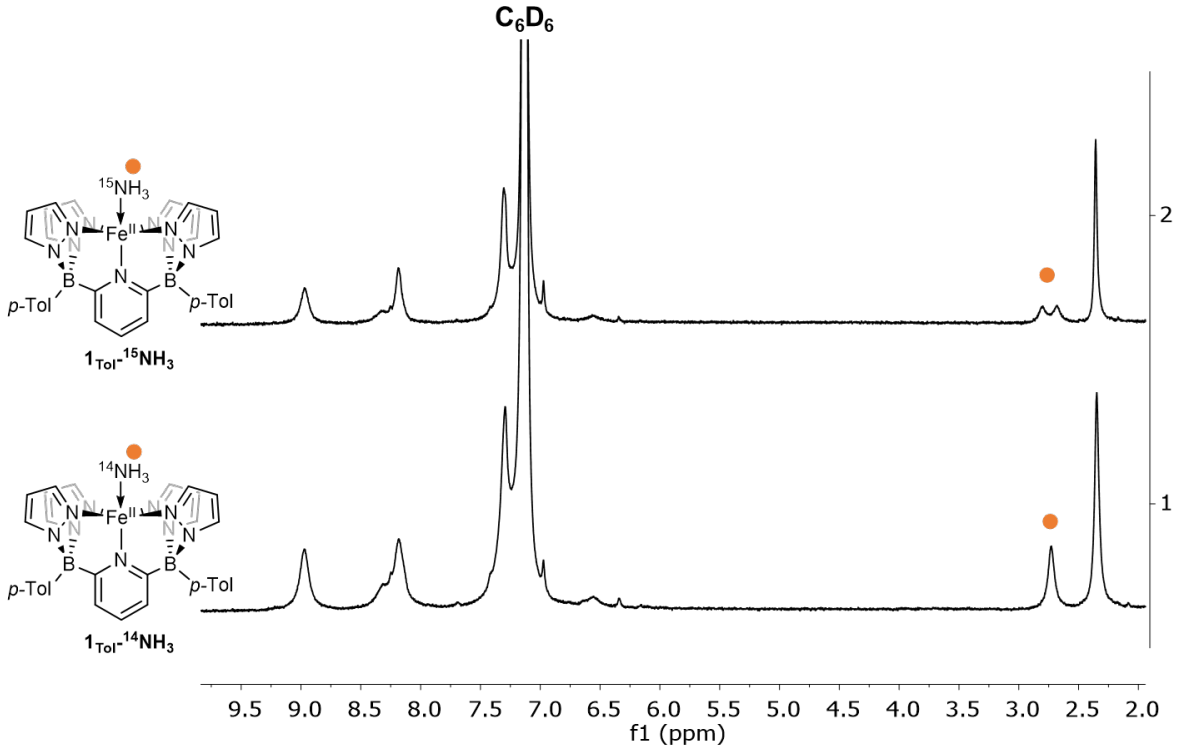
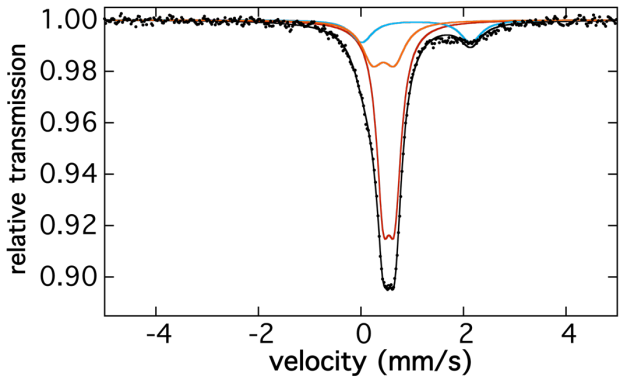



**Figure S6**. Stack $^{1}$H NMR spectra of $\mathbf{1}_{\mathbf{Tol}}$-$^{14}\mathbf{NH_3}$ (spectrum 1) and $\mathbf{1}_{\mathbf{Tol}}$-$^{15}\mathbf{NH_3}$ (spectrum 2) in $C_6D_6$ with the proton assignments of the $NH_3$ ligand.




| | | | |
|---|---|---|---|
| δ (mm/s) | 0.55 | 0.44 | 1.08 |
| $\Delta E_Q$ (mm/s) | 0.22 | 0.43 | 2.13 |
| % | 63 | 23 | 14 |

**Figure S7**. Mössbauer spectrum of a benzene solution of $\mathbf{1_{Tol}}$-$^{15}\mathbf{NH_3}$ collected at 80 K under a dinitrogen atmosphere. The major species (red) corresponds to $\mathbf{1_{Tol}}$-$^{15}\mathbf{NH_3}$ (LS) and the parameters for the species in orange match the dinitrogen adduct reported in Figure S4. The species in blue corresponds to leftover $\mathbf{1_{Tol}}$-**THF** as the parameters match the ones already reported for $\mathbf{1_{Ph}}$-**THF**.[1]

**Procedure for the reactivity of $\mathbf{1_{Ph}}$-$^{n}\mathbf{NH_3}$ with ArO· to isolate $\mathbf{2_{Ph}}$-$^{n}\mathbf{N}$**

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 $\mathbf{1_{Ph}}$-$^{n}\mathbf{NH_3}$ (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.

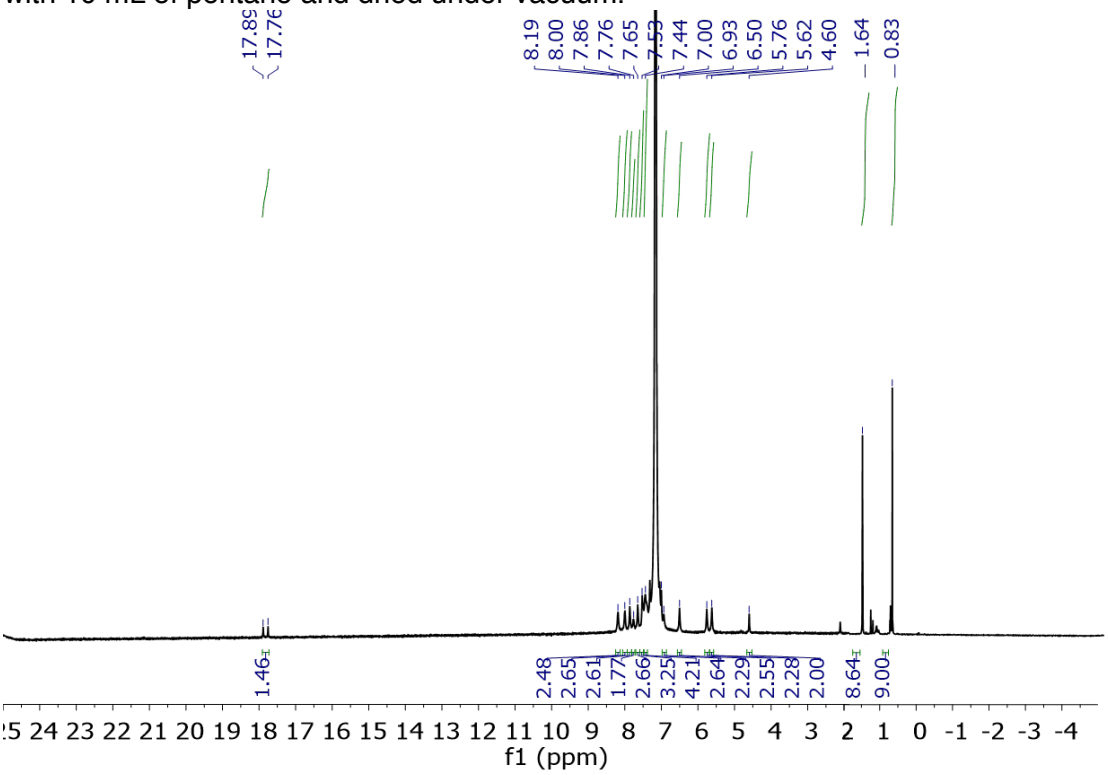



**Figure S8**. $^{1}$H NMR spectrum of $\mathbf{2_{Ph}}$-$^{15}\mathbf{N}$ in $C_6D_6$.

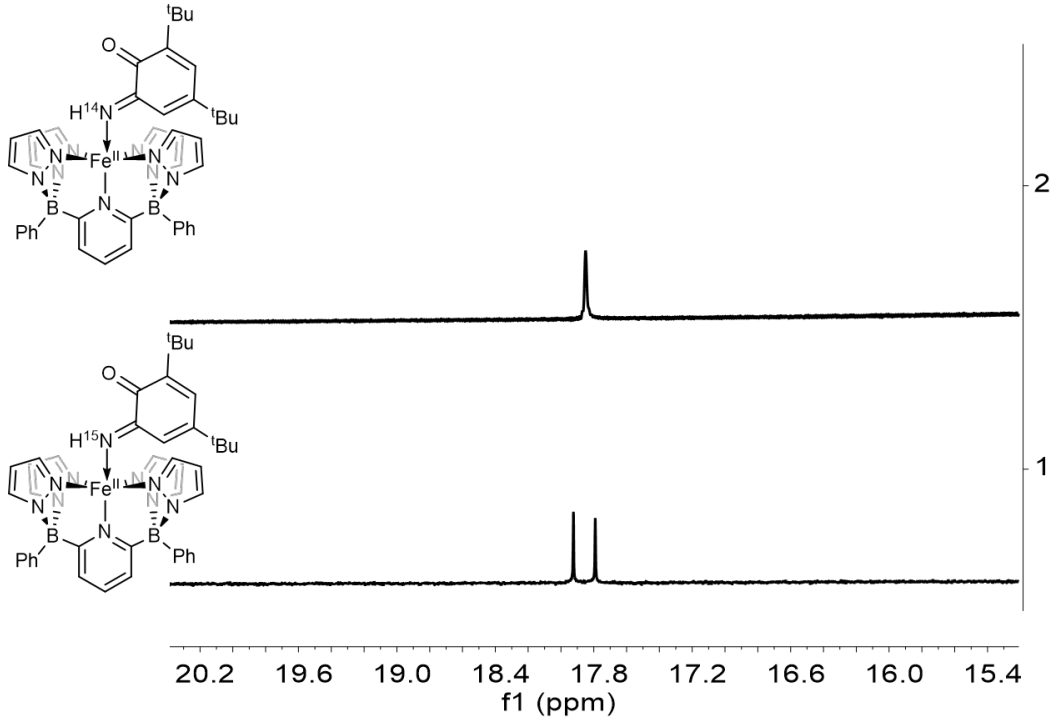
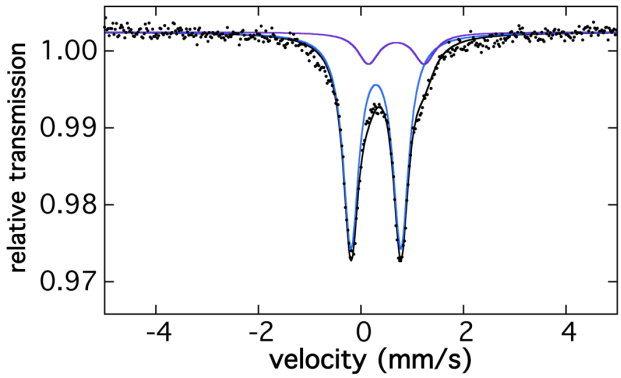


**Figure S9**. Zoomed $^{1}$H NMR stack spectra of $\mathbf{2_{Ph}}$-$^{15}$**N** (spectrum 1) and $\mathbf{2_{Ph}}$-$^{14}$**N** (spectrum 2) in $C_6D_6$.




| | | |
|---|---|---|
| δ (mm/s) | 0.29 | 0.69 |
| $\Delta E_Q$ (mm/s) | 0.97 | 1.09 |
| % | 83 | 17 |

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

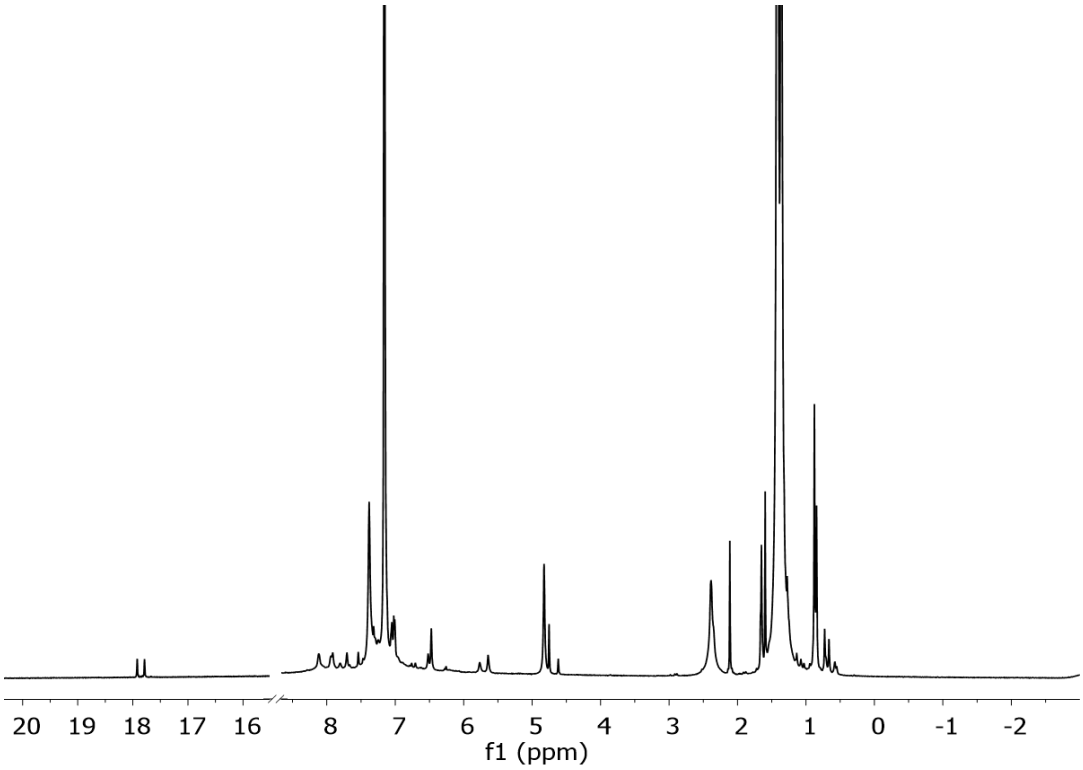



**Figure S11**. $^{1}$H NMR spectrum of the reaction between $\mathbf{1_{Tol}}$-$^{15}\mathbf{NH_3}$ and ArO· after 16 h at room temperature in $C_6D_6$. $\mathbf{2_{Tol}}$-$^{15}$**N** is present, as well as ArOH.

**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 $C_6D_6$. 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.

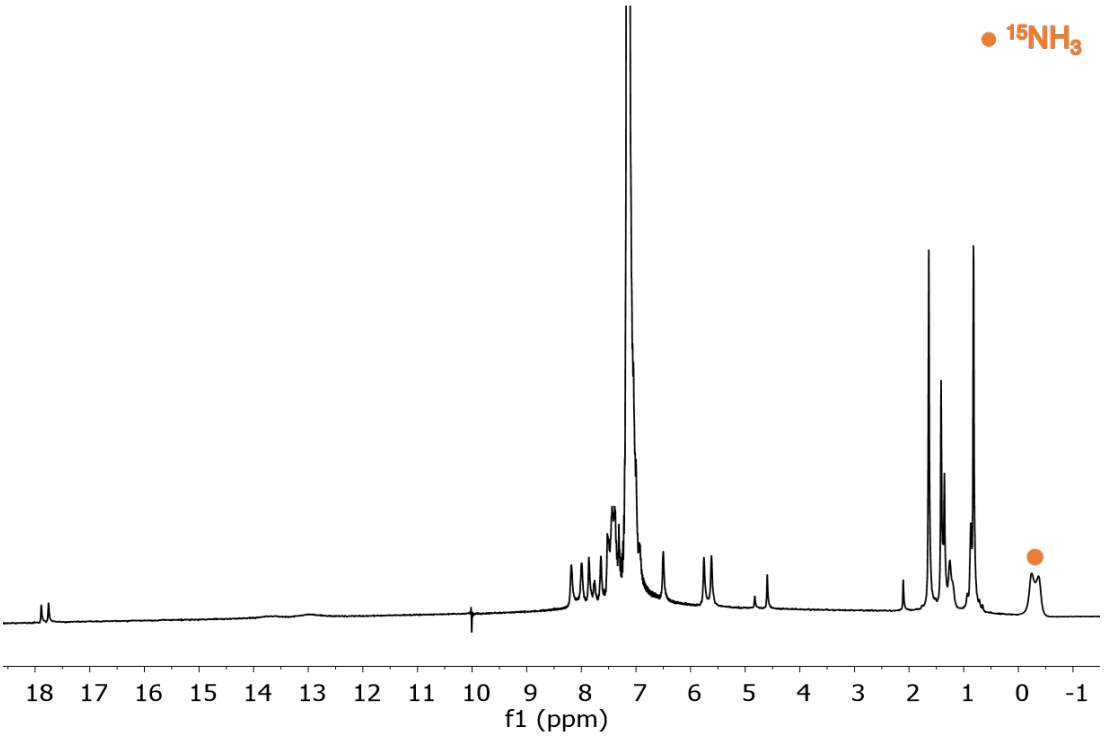



**Figure S12**. $^1H$ NMR spectrum of **$2_{Ph}$-$^{15}N$** + ArO· and $^{15}NH_3$ in $C_6D_6$.

**Procedure for the reactivity of $\mathbf{1_{Ph}}$-$^{n}\mathbf{NH_3}$ with ArO·**

A J-Young tube equipped with a Teflon cap was charged with 20 mg of $\mathbf{1_{Ph}}$-$^{n}\mathbf{NH_3}$ (1 eq, 0.034 mmol) in ~0.5 mL of $C_6D_6$. 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.

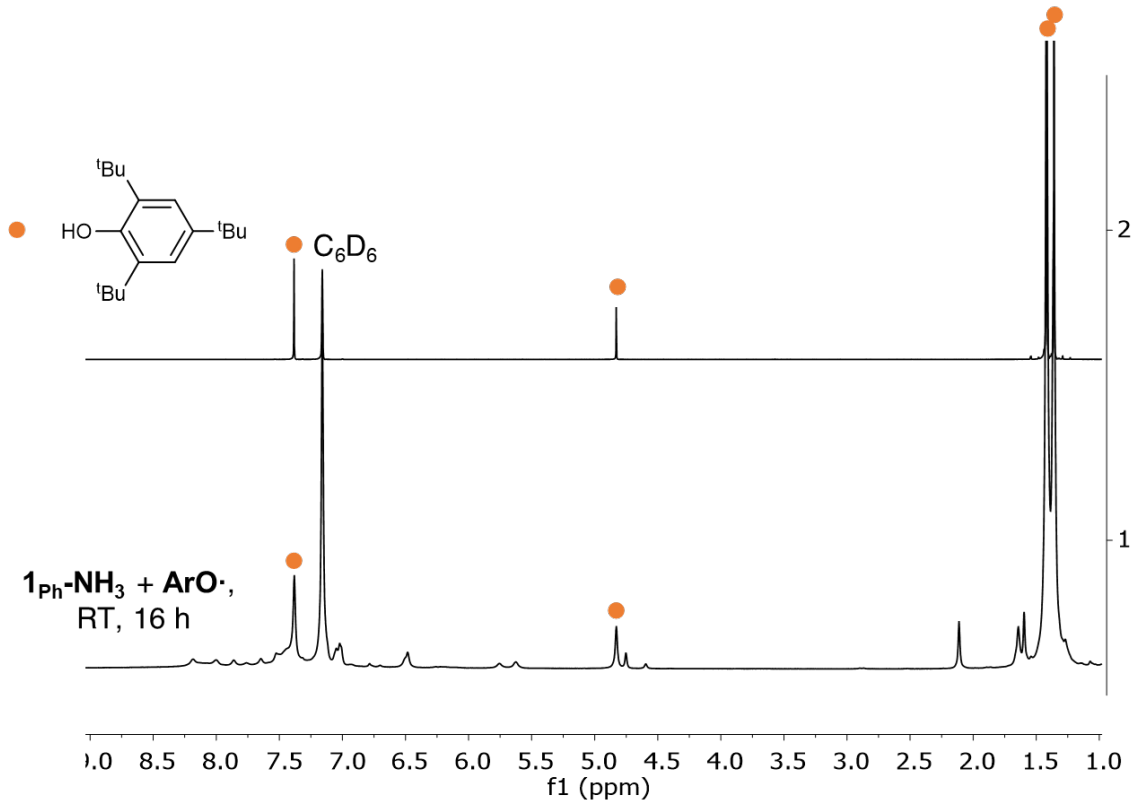



**Figure S13**. Stack $^{1}$H NMR spectra of $\mathbf{1_{Ph}}$-$\mathbf{NH_3}$ + **ArO·** (spectrum 1) and ArOH (spectrum 2) in $C_6D_6$.

**Procedure for the analysis of the headspace of the reaction between $\mathbf{1_{Ph}}$-$^{n}\mathbf{NH_3}$ and 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 $\mathbf{1_{Ph}}$-$^{n}\mathbf{NH_3}$ (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 headspace of the reaction was taken through the 14/20 septum using a 500 µL syringe. The headspace sample was analyzed by GC-MS.

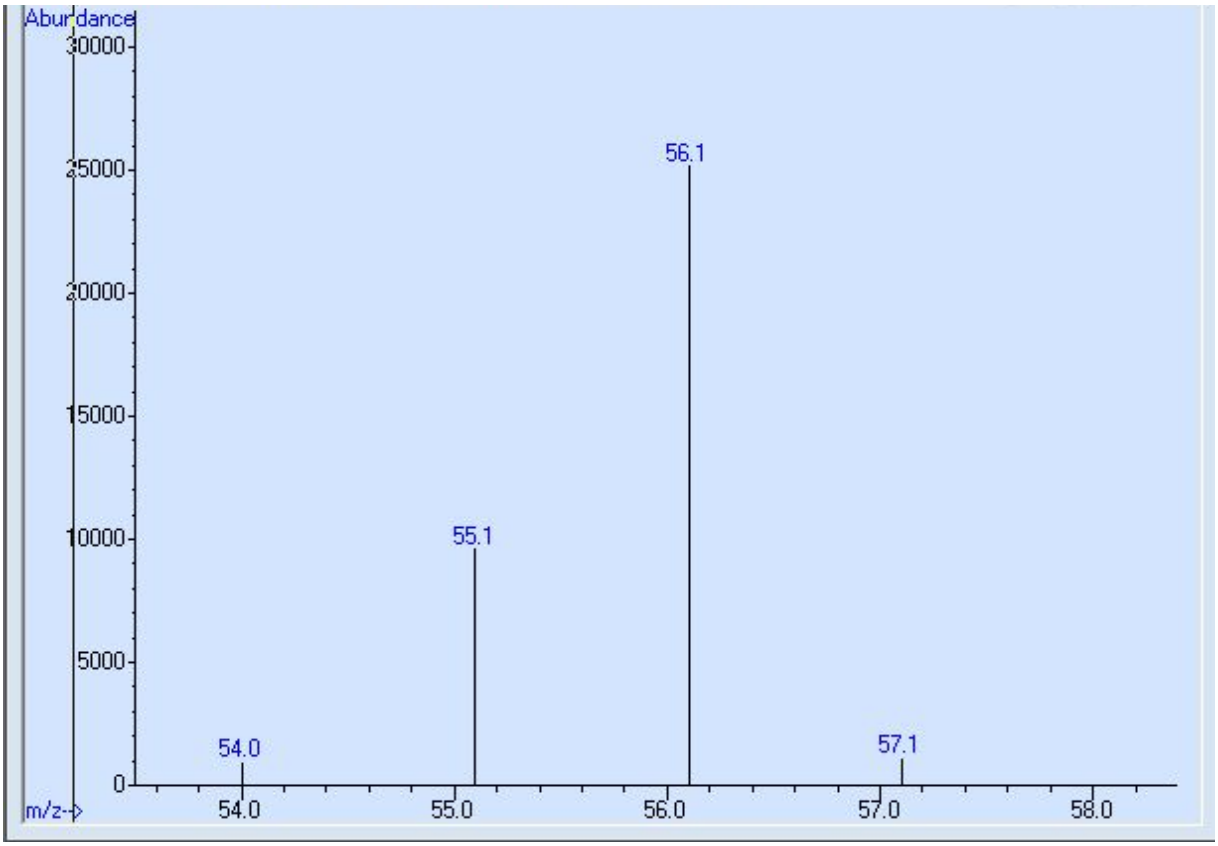



**Figure S14**. GC-MS analysis of the headspace of the reaction between $\mathbf{1_{Ph}}$-$\mathbf{NH_3}$ and ArO· in toluene. The peak at m/z 56.1 corresponds to the formation of isobutene. Notably, no isobutane is observed at m/z 58.

**Procedure for the reaction between $3_{Tol}$-$NH_3^+$ and DBU**

A J-Young tube equipped with a septum screw cap was charged with 10 mg of **$3_{Tol}$-$NH_3^+$** (1 eq, 0.012 mmol) in ~0.5 mL of $C_6D_6$. A $^1$H NMR spectrum was recorded. DBU (stock solution, 1 eq) was added through the septum screw cap. Another $^1$H NMR spectrum was recorded.

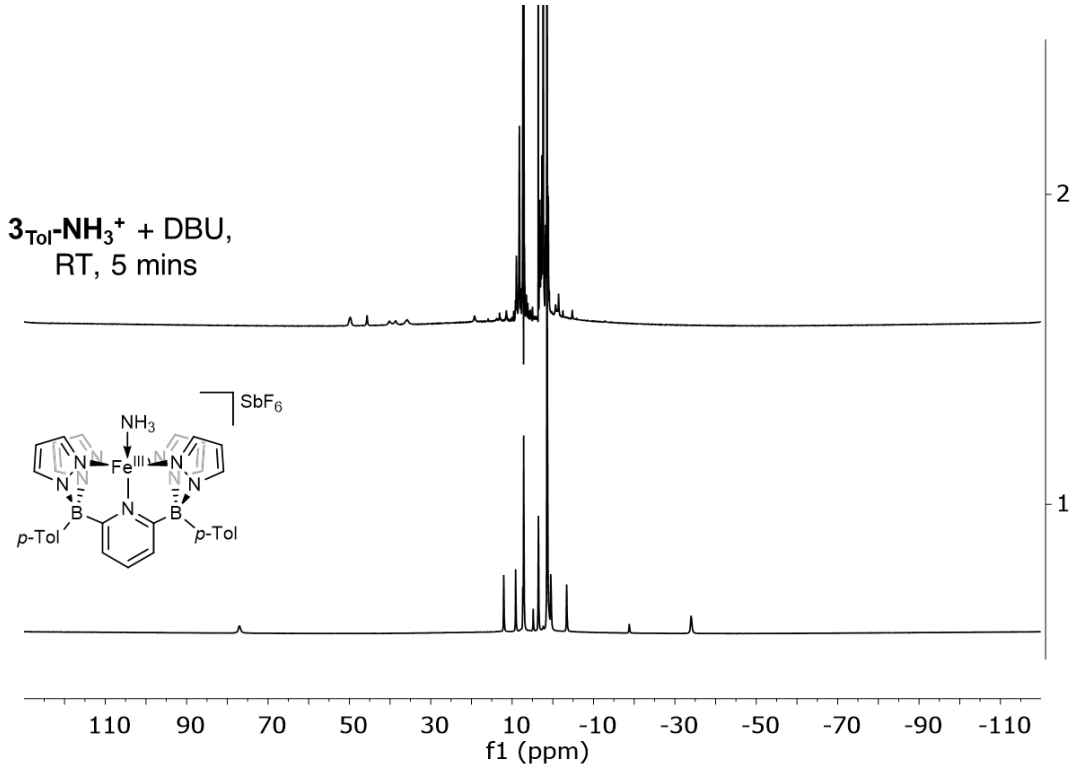



**Figure S15.** Stack $^1$H NMR spectra of **$3_{Tol}$-$NH_3^+$** (spectrum 1) and **$3_{Tol}$-$NH_3^+$** + DBU (spectrum 2) in $C_6D_6$. Large window.

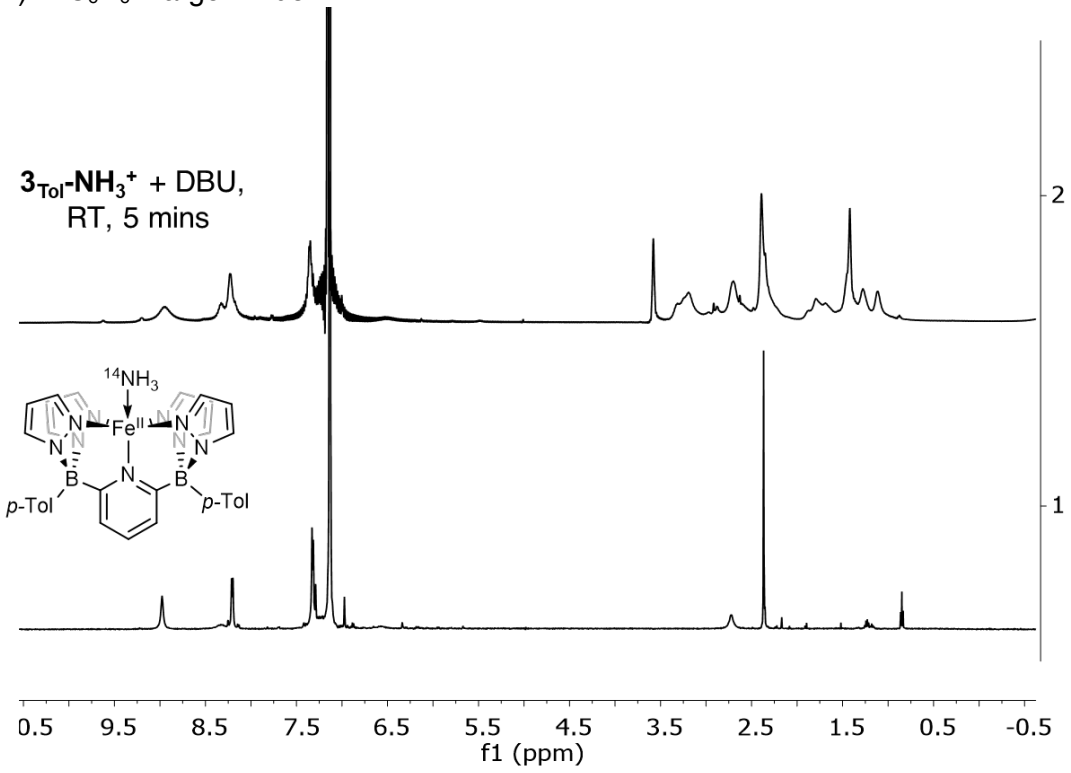


**Figure S16.** Stack $^1$H NMR spectra of $\mathbf{1_{Tol}\text{-}NH_3}$ (spectrum 1) and $\mathbf{3_{Tol}\text{-}NH_3^+}$ + DBU (spectrum 2) in $C_6D_6$.

**Procedure for the reaction between $\mathbf{3_{Tol}\text{-}^{15}NH_3^+}$, ArO· and DBU**

A J-Young tube equipped with a septum screw cap was charged with 10 mg of $\mathbf{3_{Tol}\text{-}^{15}NH_3^+}$ (1 eq, 0.012 mmol) and ArO· (15 mg, 5 eq, 0.058 mmol) in ~0.5 mL of $C_6D_6$. 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.

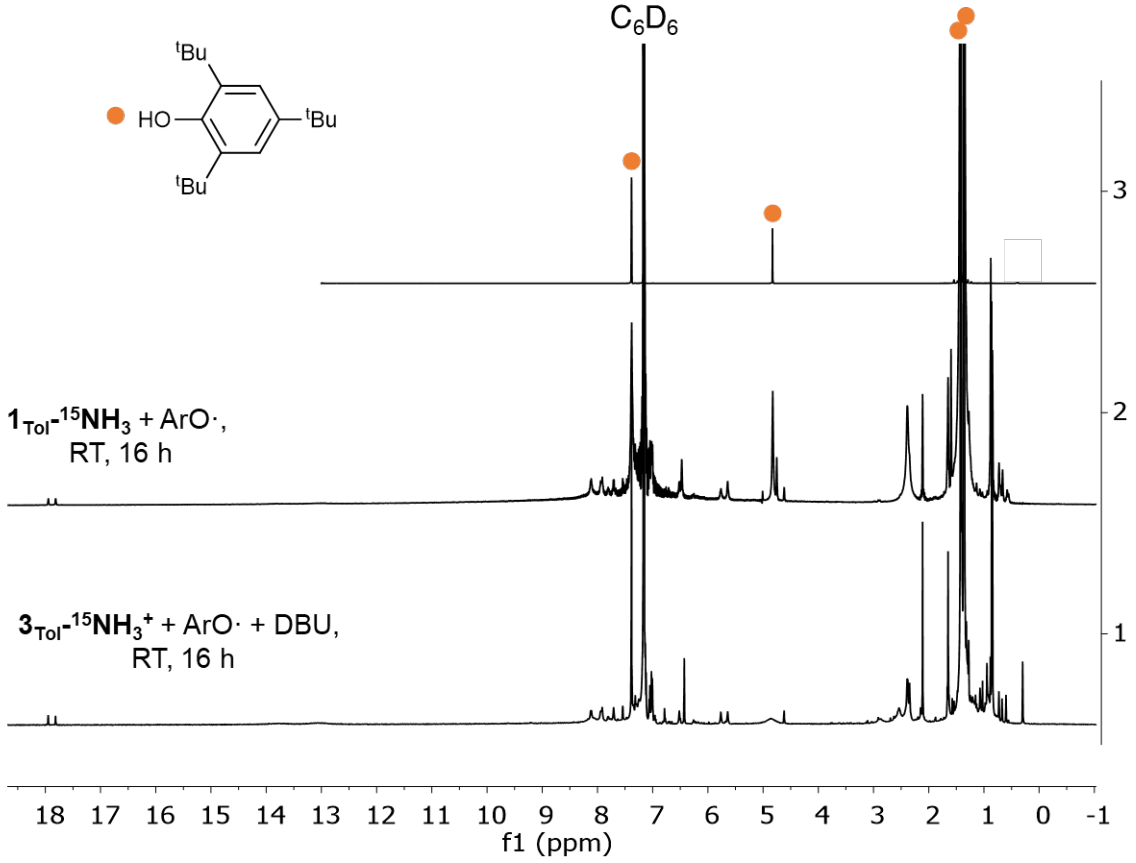



**Figure S17.** Stack $^1$H NMR spectra of $\mathbf{3_{Tol}\text{-}^{15}NH_3^+}$ + ArO· + DBU (spectrum 1), $\mathbf{1_{Tol}\text{-}^{15}NH_3}$ + ArO· (spectrum 2) and ArOH (spectrum 3) in $C_6D_6$.

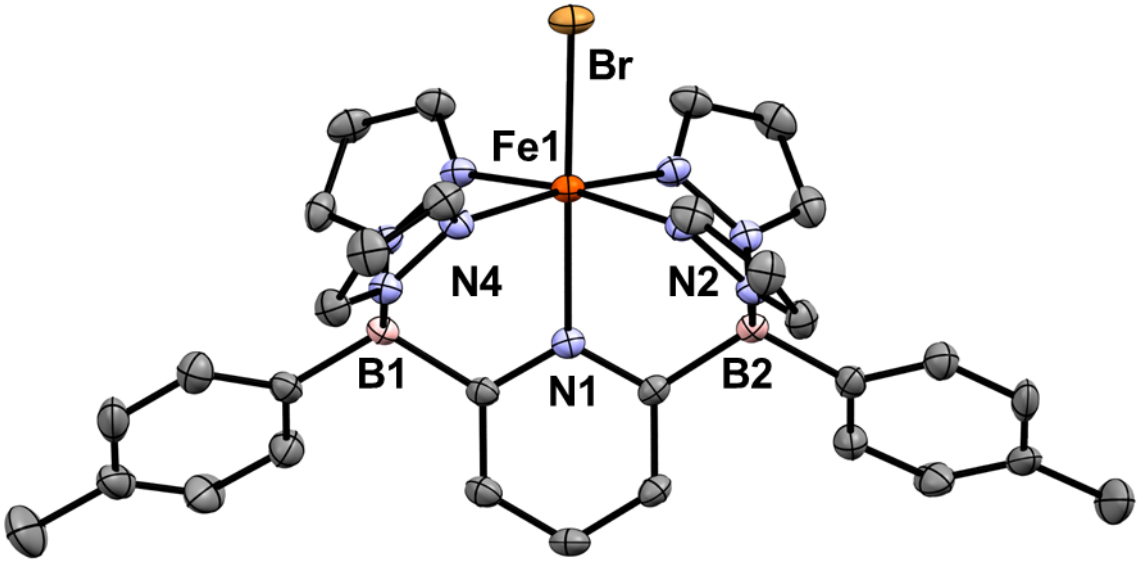



**Figure S18.** ORTEP diagrams for **$3_{Tol}$-Br**. Hydrogen, boron, carbon, nitrogen, bromine and iron atoms are white, pink, grey, light blue, gold and orange respectively. Thermal ellipsoids are shown at the 50% probability level. Calculated hydrogen atoms and the molecule of solvent are omitted 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.

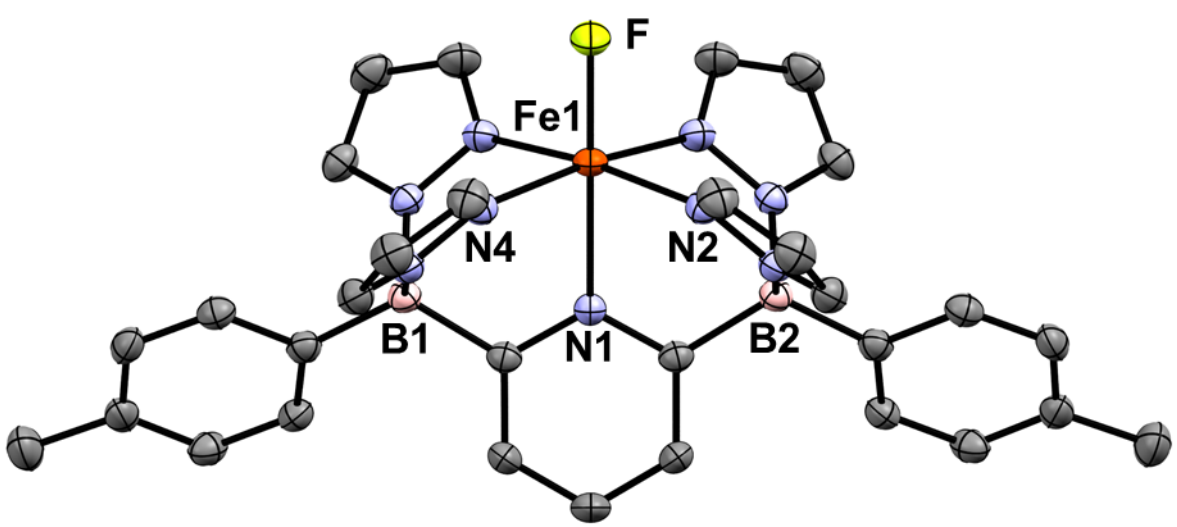



**Figure S19.** ORTEP diagrams for **$3_{Tol}$-F**. Hydrogen, boron, carbon, nitrogen, fluorine and iron atoms are white, pink, grey, light blue, bright yellow and orange respectively. Thermal ellipsoids are shown at the 50% probability level. Calculated hydrogen atoms and the molecule of solvent are 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-Fe1-F, 179.54(8). Selected metrical data are given in Table S2.

**Procedure for the reaction between $3_{Tol}$-Br and $LiNH_2$**

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 $^1$H NMR spectrum was recorded. $LiNH_2$ (1.2 eq, 0.018 mmol) was added as a solid. Another $^1$H NMR spectrum was recorded.

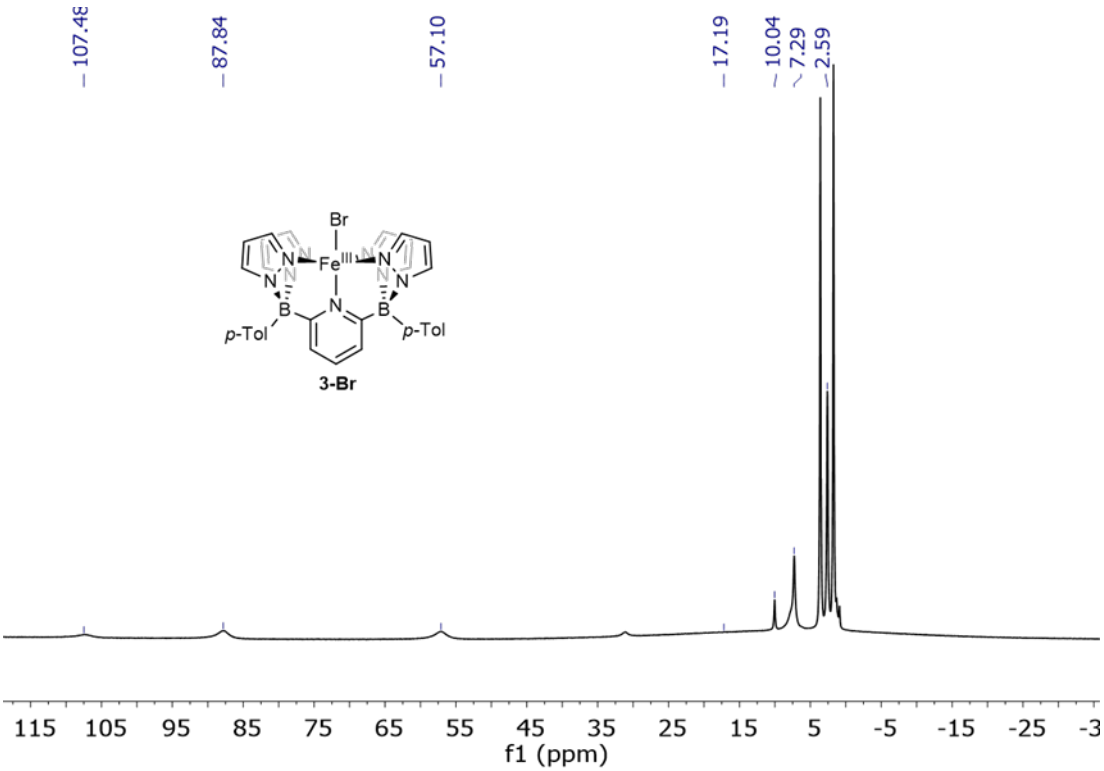



**Figure S20.** $^1$H NMR spectrum of **$3_{Tol}$-Br** in THF-*d8*.

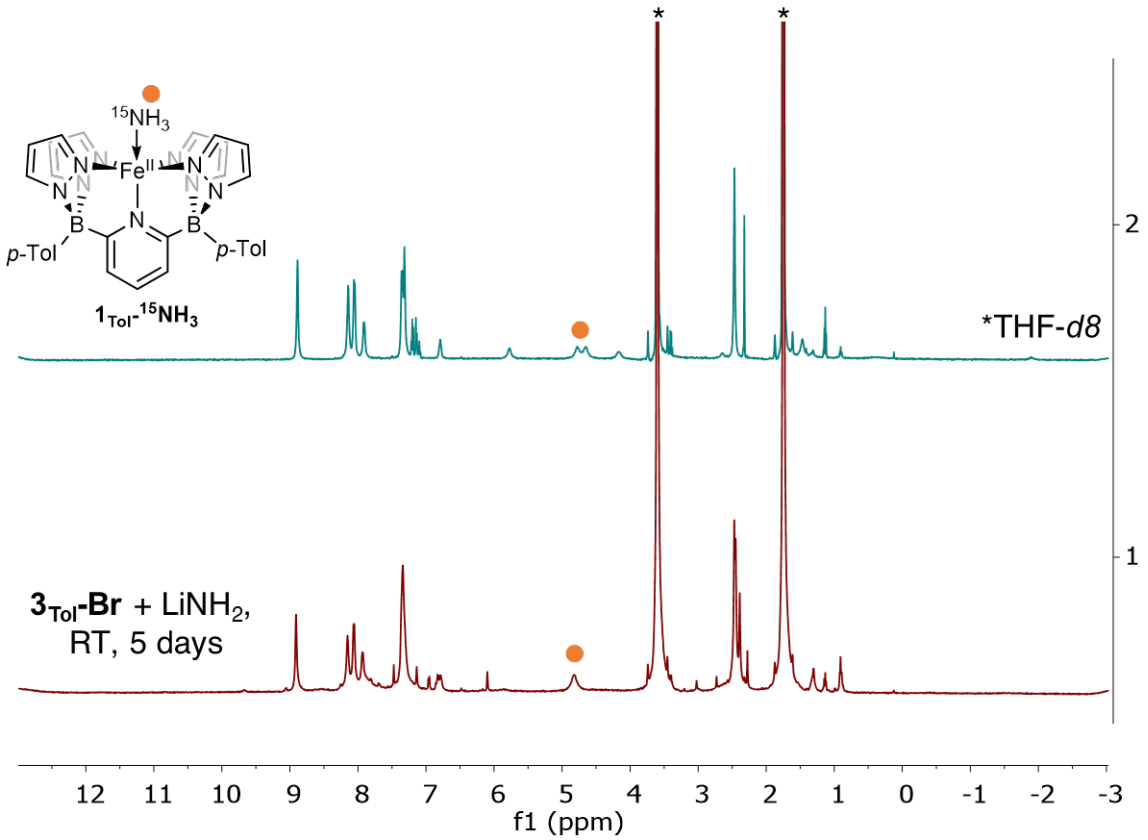



**Figure S21.** Stack $^1$H NMR spectra of $\mathbf{3_{Tol}}$-**Br** + $LiNH_2$ (spectrum 1) and $\mathbf{1_{Tol}}$-$^{15}$**NH$_3$** (spectrum 2) in THF-*d8*.

**Procedure for the reaction between $3_{Tol}$-Br, ArO· and $LiNH_2$**

A J-Young tube equipped with a Teflon cap was charged with 10 mg of **$3_{Tol}$-Br** (1 eq, 0.015 mmol) and ArO· (5 eq, 19 mg, 0.073 mmol) in ~0.5 mL of THF-*d8*. $LiNH_2$ (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.

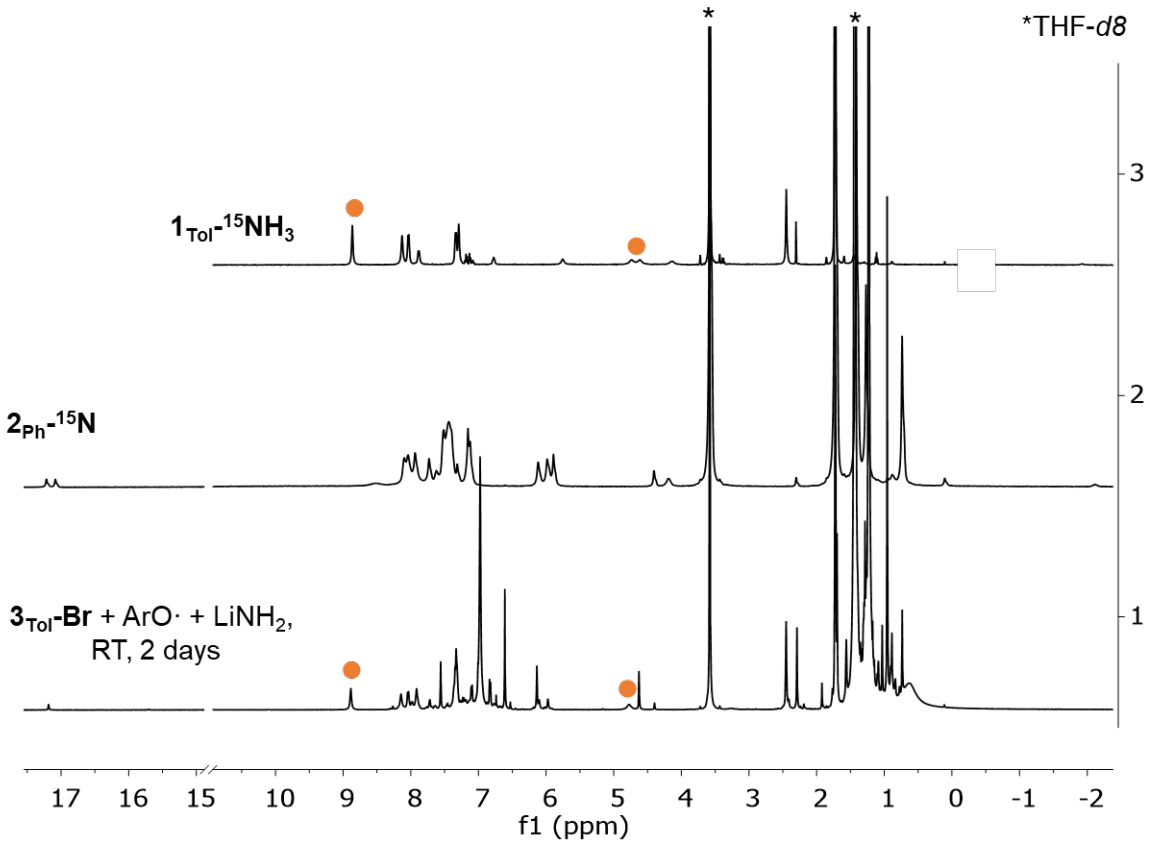



**Figure S22.** Stack $^1$H NMR spectra of **$3_{Tol}$-Br** + ArO· + $LiNH_2$ (spectrum 1), **$2_{Ph}$-$^{15}$N** (spectrum 2) and **$1_{Tol}$-$^{15}NH_3$** (spectrum 3) in THF-*d8*. Based on the $^1$H integration in spectrum 1 between the peaks corresponding to **$2_{Tol}$** and the peaks corresponding to **$1_{Tol}$-$NH_3$**, a 30% NMR yield is found for the formation of **$2_{Tol}$**.

**Procedure for the reaction between $3_{Tol}$-F, ArO· and $LiNH_2$**

A J-Young tube equipped with a Teflon cap was charged with 10 mg of **$3_{Tol}$-F** (1 eq, 0.016 mmol) and ArO· (5 eq, 21 mg, 0.080 mmol) in ~0.5 mL of THF-*d8*. $LiNH_2$ (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.

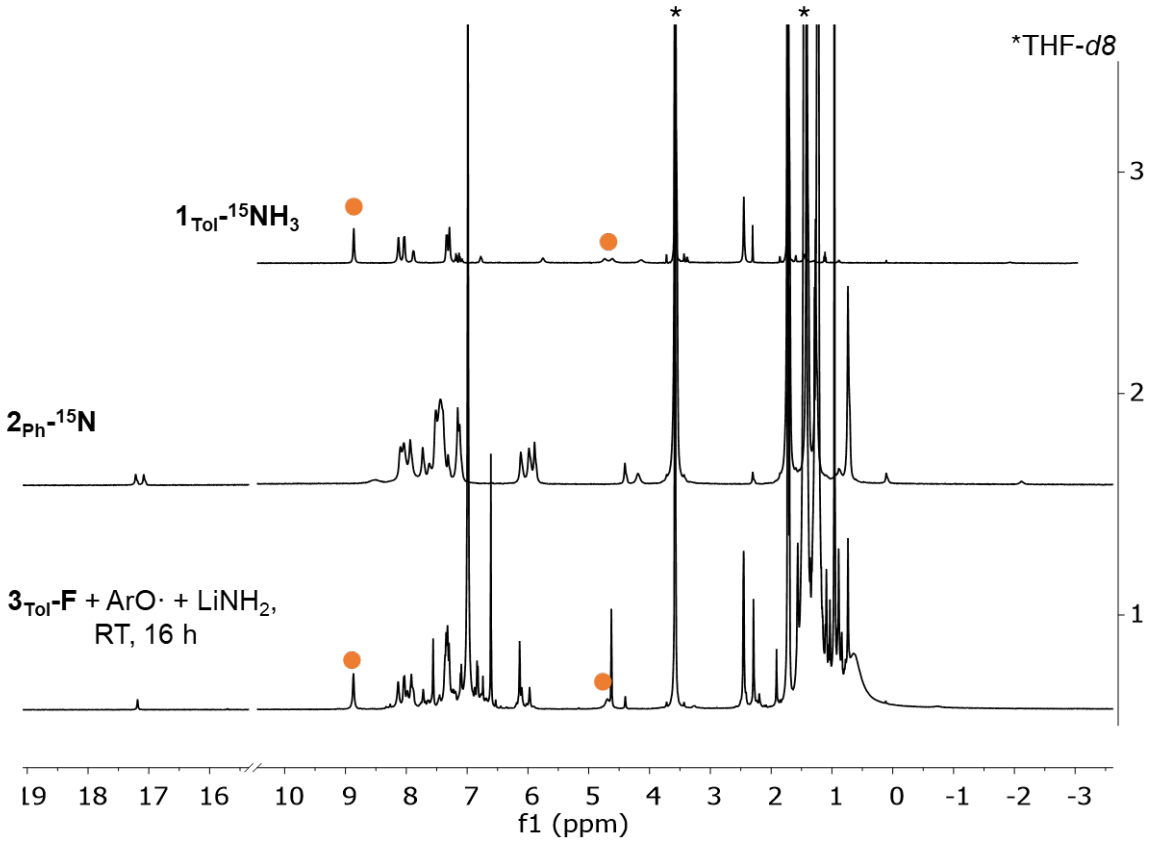



**Figure S23.** Stack $^1$H NMR spectra of **$3_{Tol}$-F** + ArO· + $LiNH_2$ (spectrum 1), **$2_{Ph}$-$^{15}$N** (spectrum 2) and **$1_{Tol}$-$^{15}NH_3$** (spectrum 3) in THF-*d8*. Based on the $^1$H integration in spectrum 1 between the peaks corresponding to **$2_{Tol}$** and the peaks corresponding to **$1_{Tol}$-$NH_3$**, a 40% NMR yield is found for the formation of **$2_{Tol}$**.

**Procedure for the reaction between $\mathbf{1_{Tol}}$ and $^{n}N_2H_4$**

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

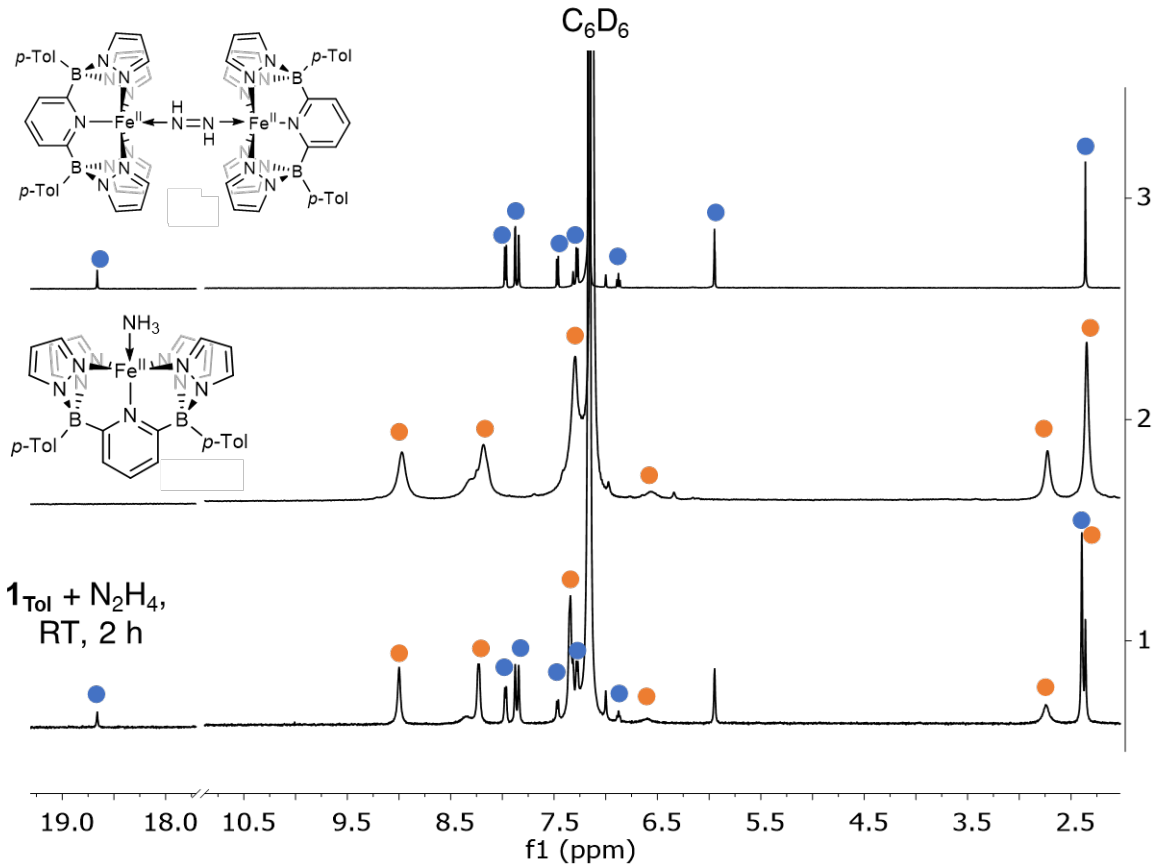



**Figure S24.** Stack $^{1}H$ NMR spectra of $\mathbf{1_{Tol}}$ + $^{14}N_2H_4$ (spectrum 1), $\mathbf{1_{Tol}}$-$^{14}\mathbf{NH_3}$ (spectrum 2) and $\mathbf{4_{Tol}}$ (spectrum 3) in $C_6D_6$.

**Procedure for the reaction between $\mathbf{1_{Tol}}$ and $^{n}N_2H_4$ at low temperature**

A J-Young tube equipped with a Teflon cap was charged with 10 mg of $\mathbf{1_{Tol}}$ (1 eq, 0.017 mmol) in ~0.5 mL of tol-*d8*. Neat anhydrous $^{n}H_2H_4$ (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.

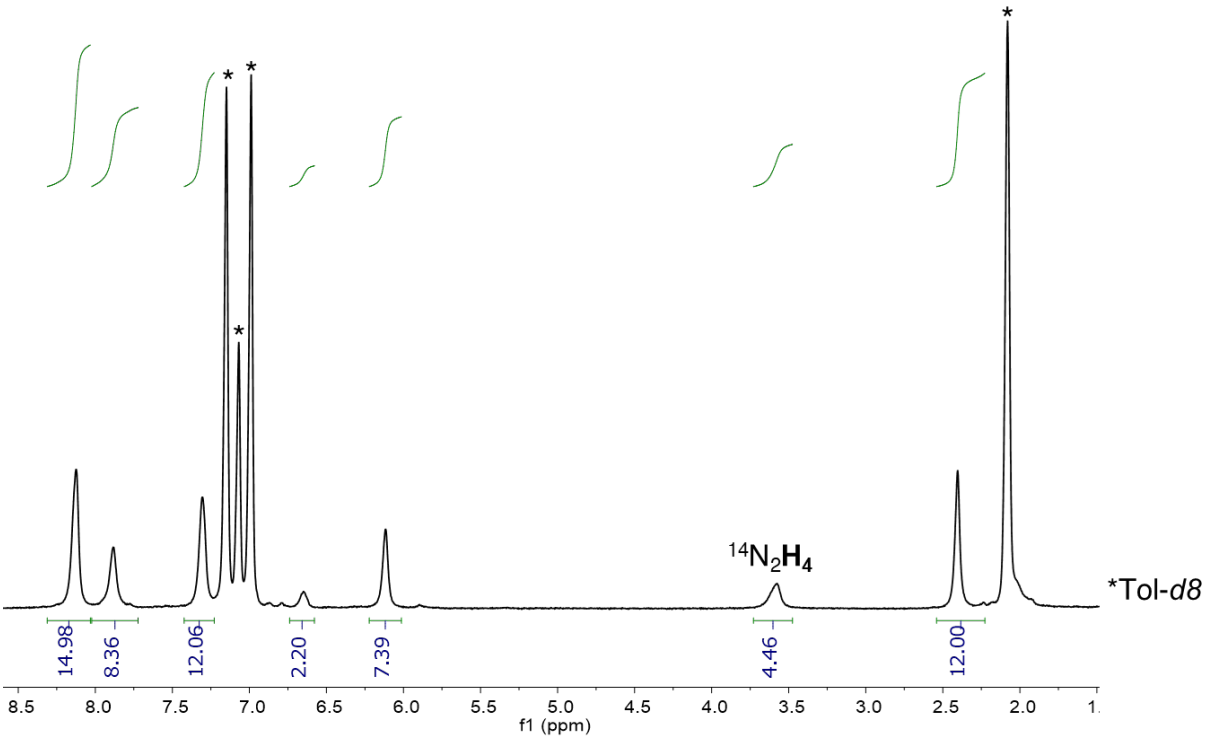



**Figure S25.** $^{1}H$ NMR spectrum of $\mathbf{1_{Tol}}$ + $^{14}N_2H_4$ at 210 K in Tol-*d8*.

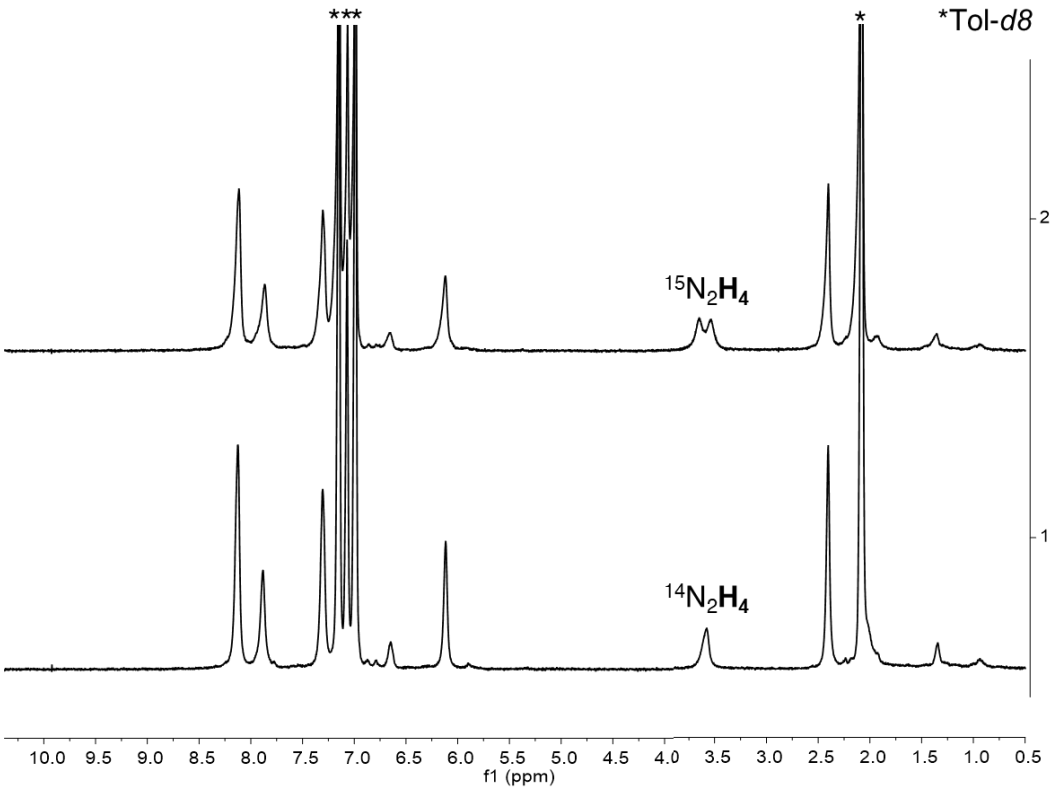



**Figure S26.** Stack $^1$H NMR spectra of $\mathbf{1_{Tol}}$ + $^{14}N_2H_4$ (spectrum 1) and of $\mathbf{1_{Tol}}$ + $^{15}N_2H_4$ (spectrum 2) at 210 K in Tol-*d8*.

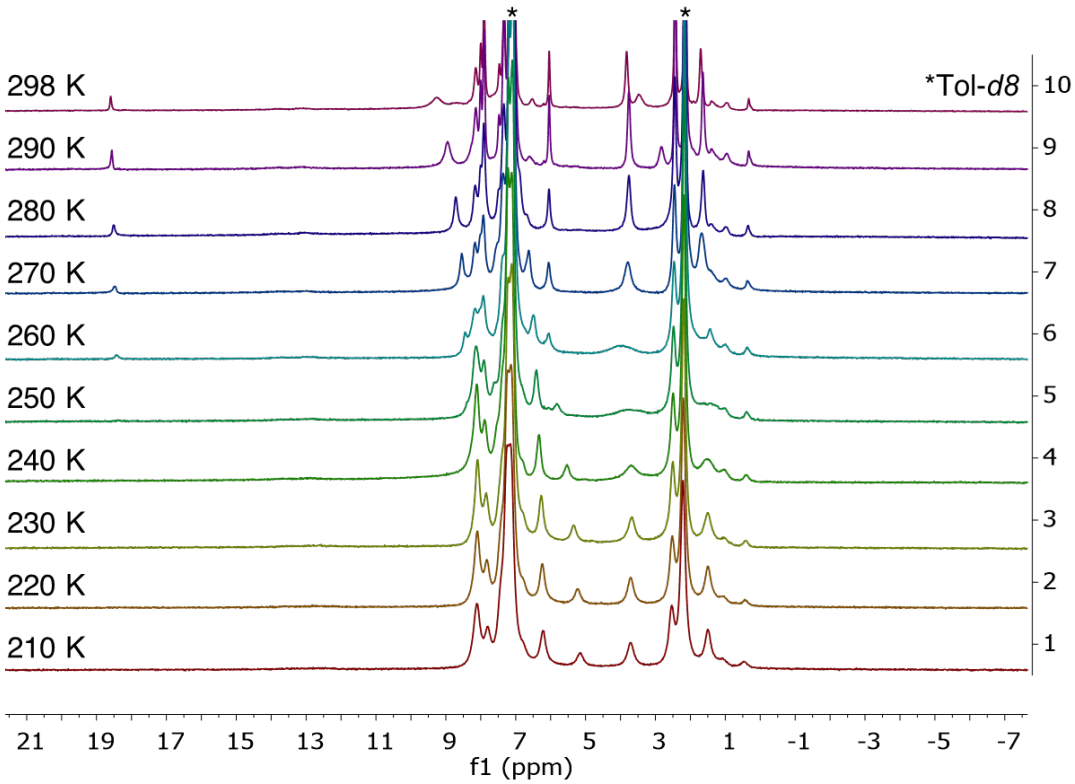



**Figure S27.** Stack $^1$H NMR spectra of $\mathbf{1_{Tol}}$ + $^{14}N_2H_4$ at different temperatures (starting at 210 K) in Tol-*d8*.

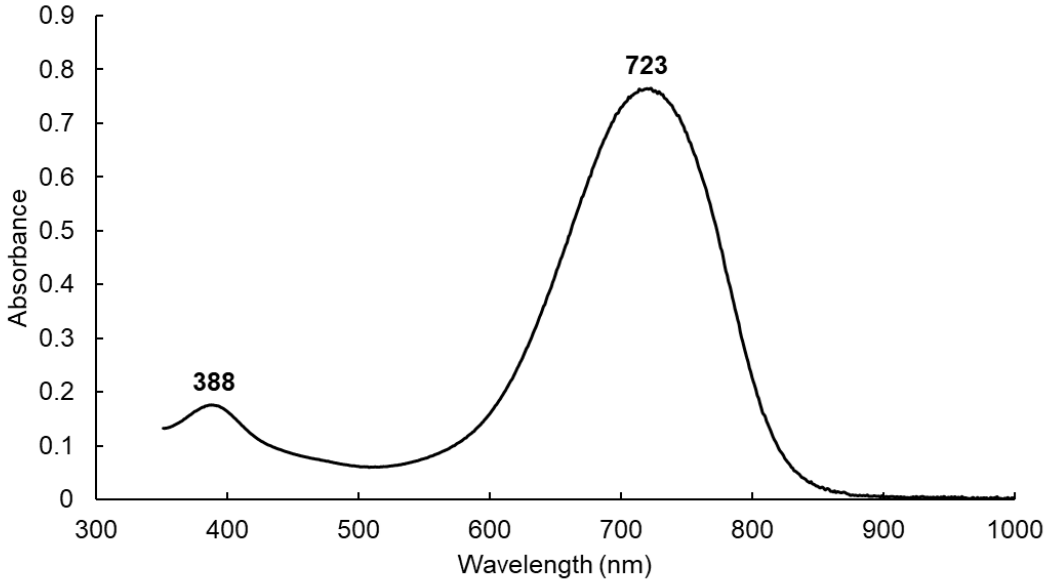
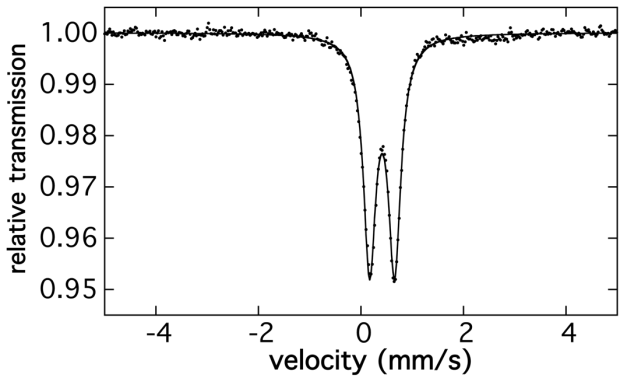



**Figure S28.** UV-vis spectrum of $\mathbf{4_{Tol}}$ in $C_6H_6$.




| | |
|---|---|
| δ (mm/s) | 0.41 |
| $\Delta E_Q$ (mm/s) | 0.49 |

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

## IR spectra

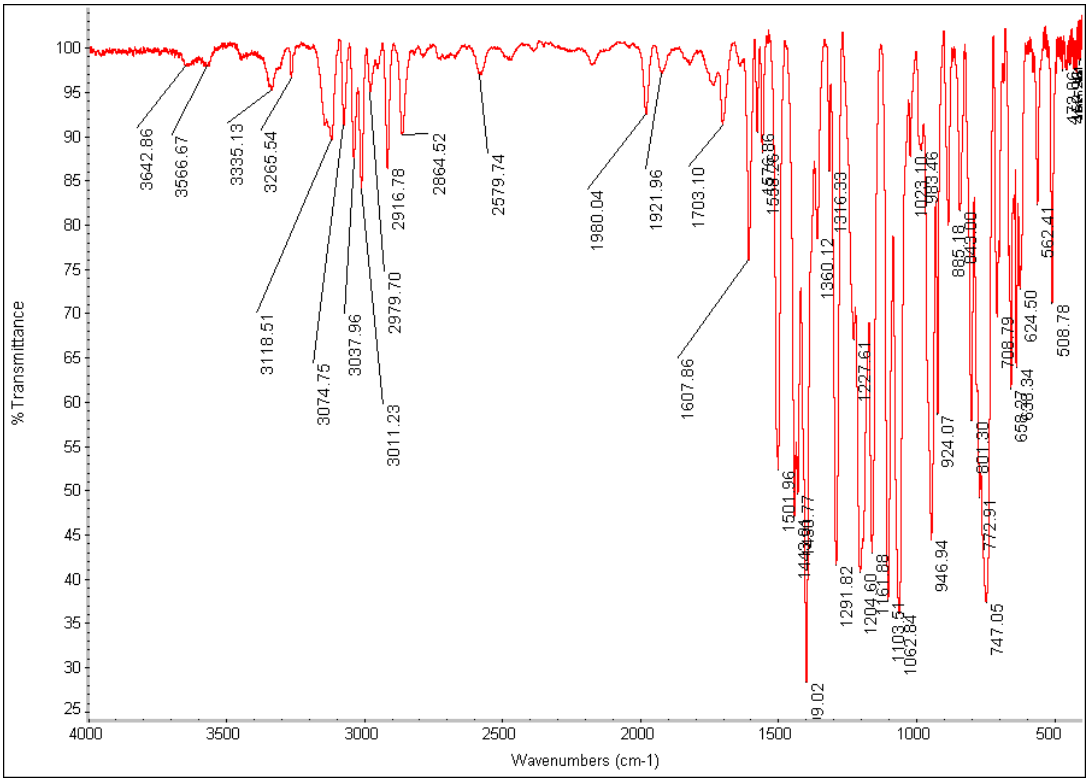



**Figure S30**. IR (KBr pallet) spectrum of $\mathbf{1_{Tol}}$-$^{15}\mathbf{NH_3}$.

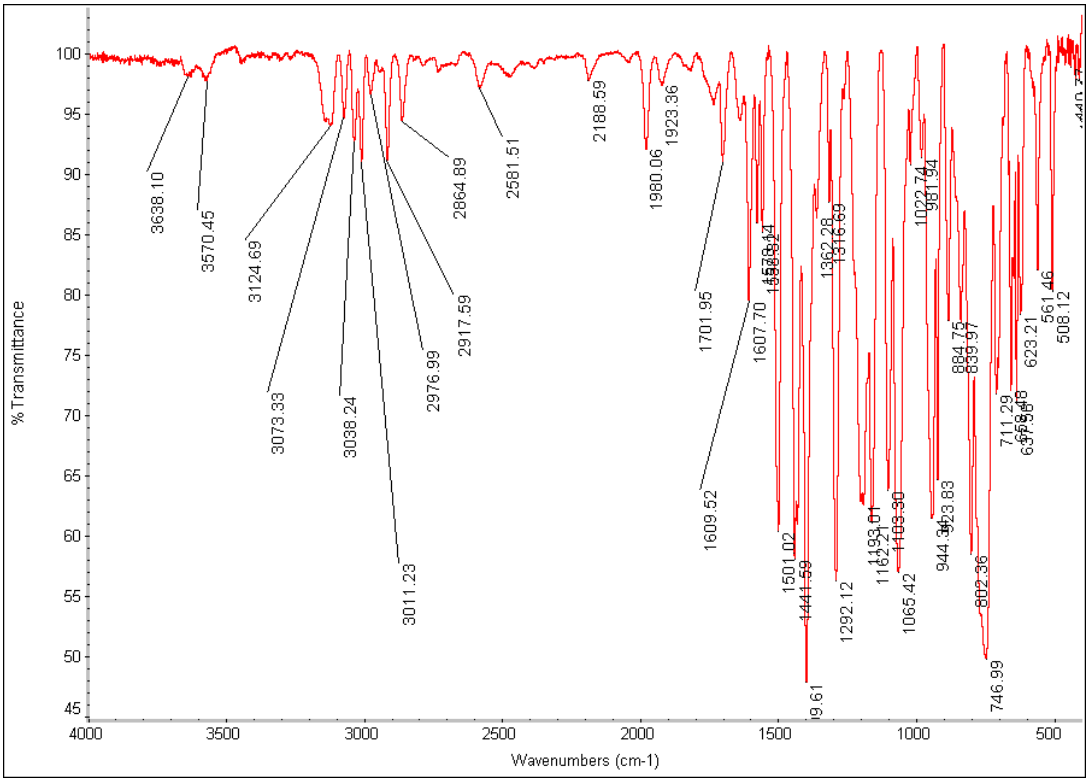


**Figure S31**. IR (KBr pallet) spectrum of $\mathbf{1_{Tol}}$-$^{14}\mathbf{NH_3}$.

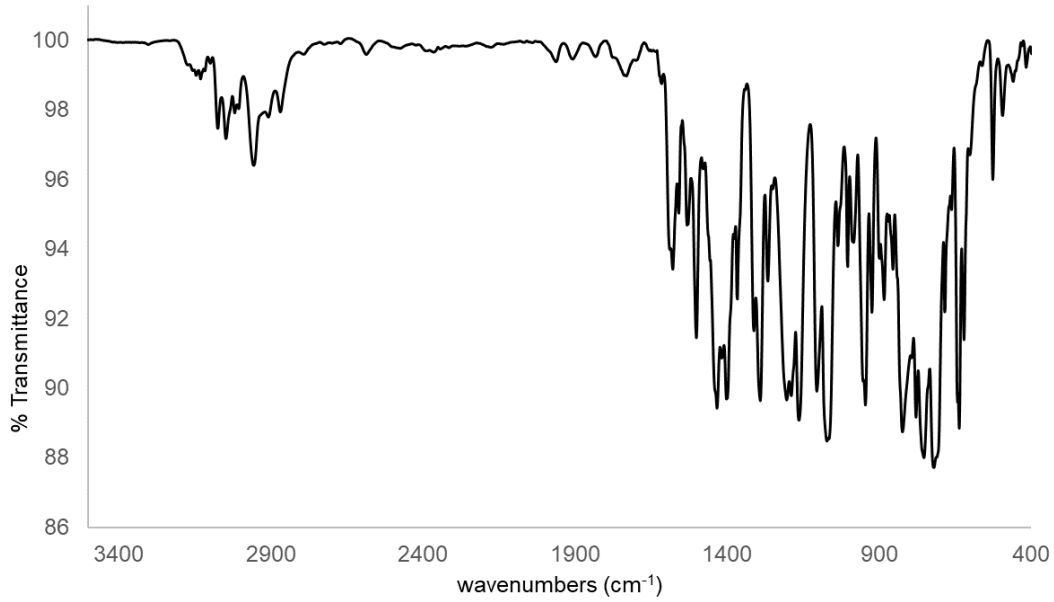



**Figure S32**. IR (KBr pallet) spectrum of $\mathbf{2_{Ph}}$-$^{15}\mathbf{N}$.

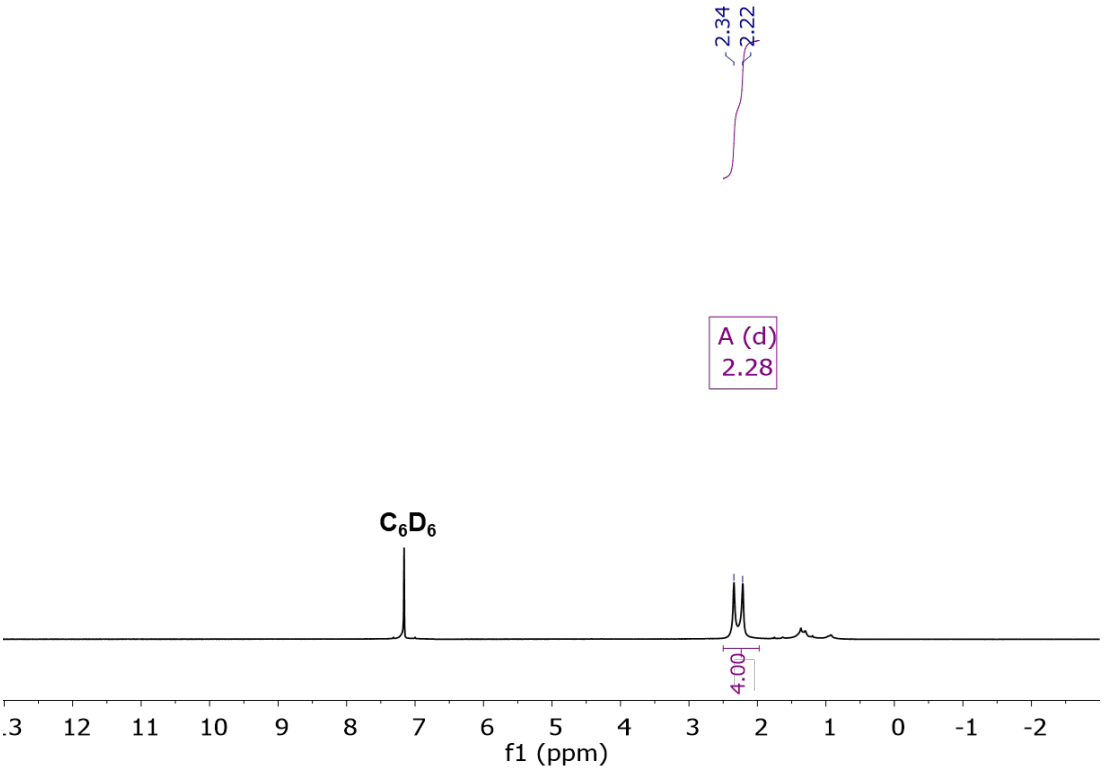



**Figure S33.** $^{1}H$ NMR spectrum of $^{15}N_2H_4$ in $C_6D_6$.

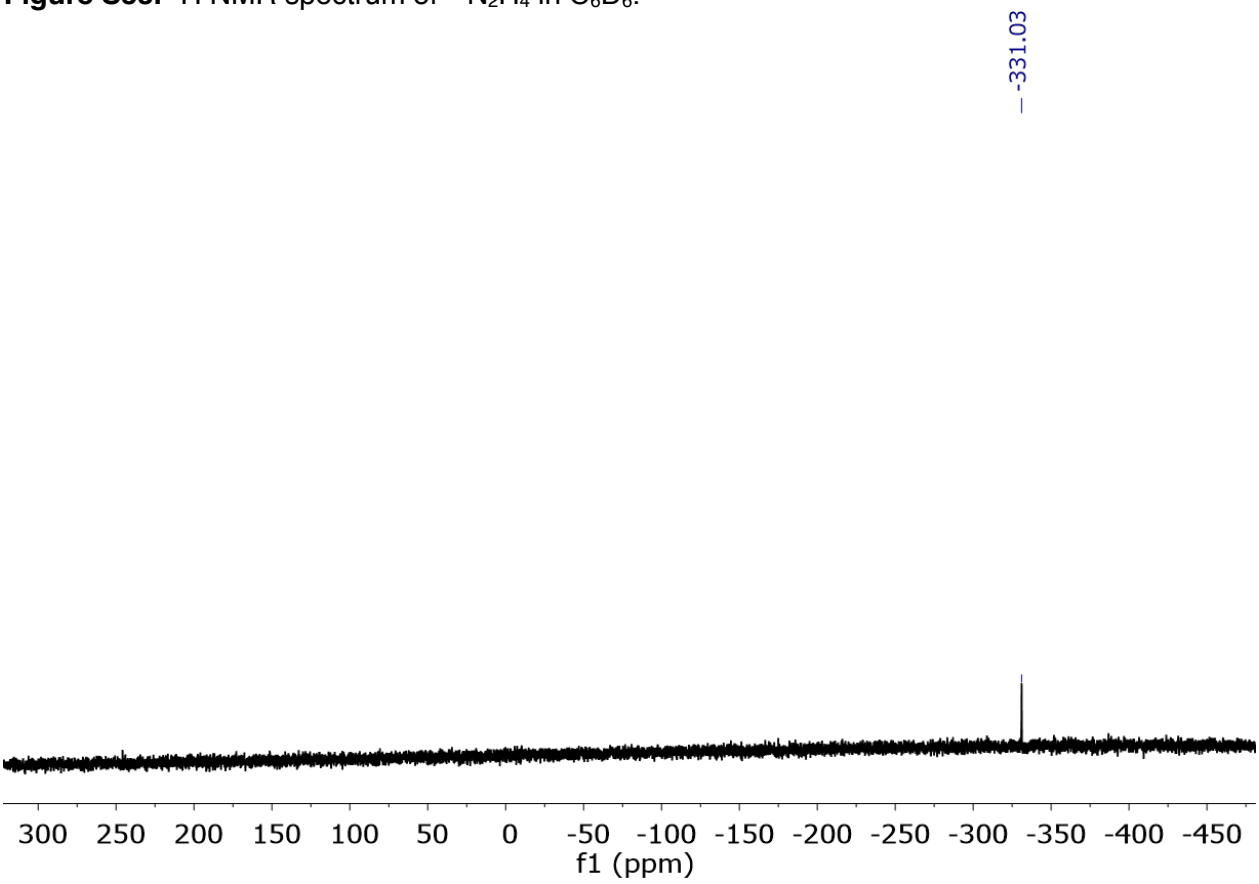



**Figure S34.** $^{15}N\{^{1}H\}$ NMR spectrum of $^{15}N_2H_4$ in $C_6D_6$.

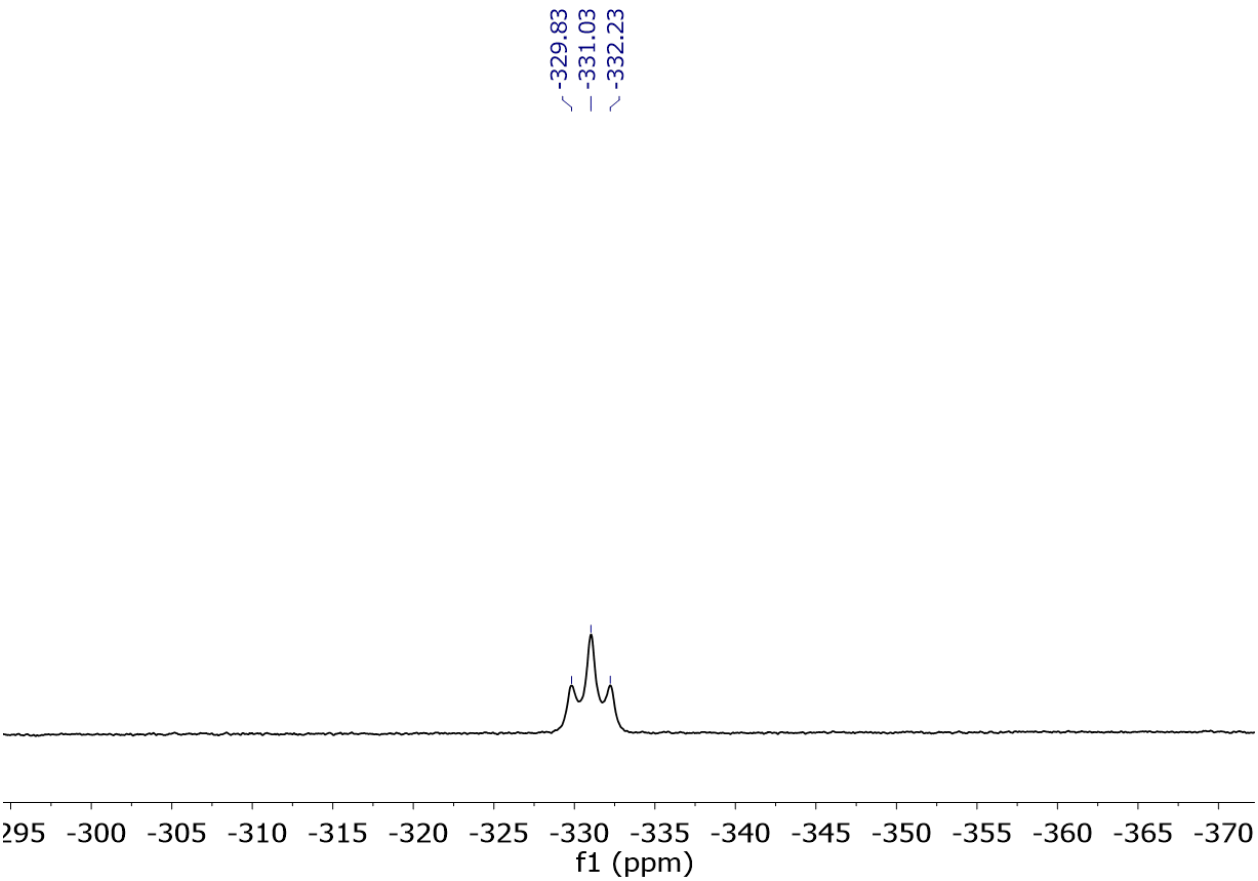



**Figure S35.** $^{15}N$ NMR spectrum of $^{15}N_2H_4$ in $C_6D_6$.

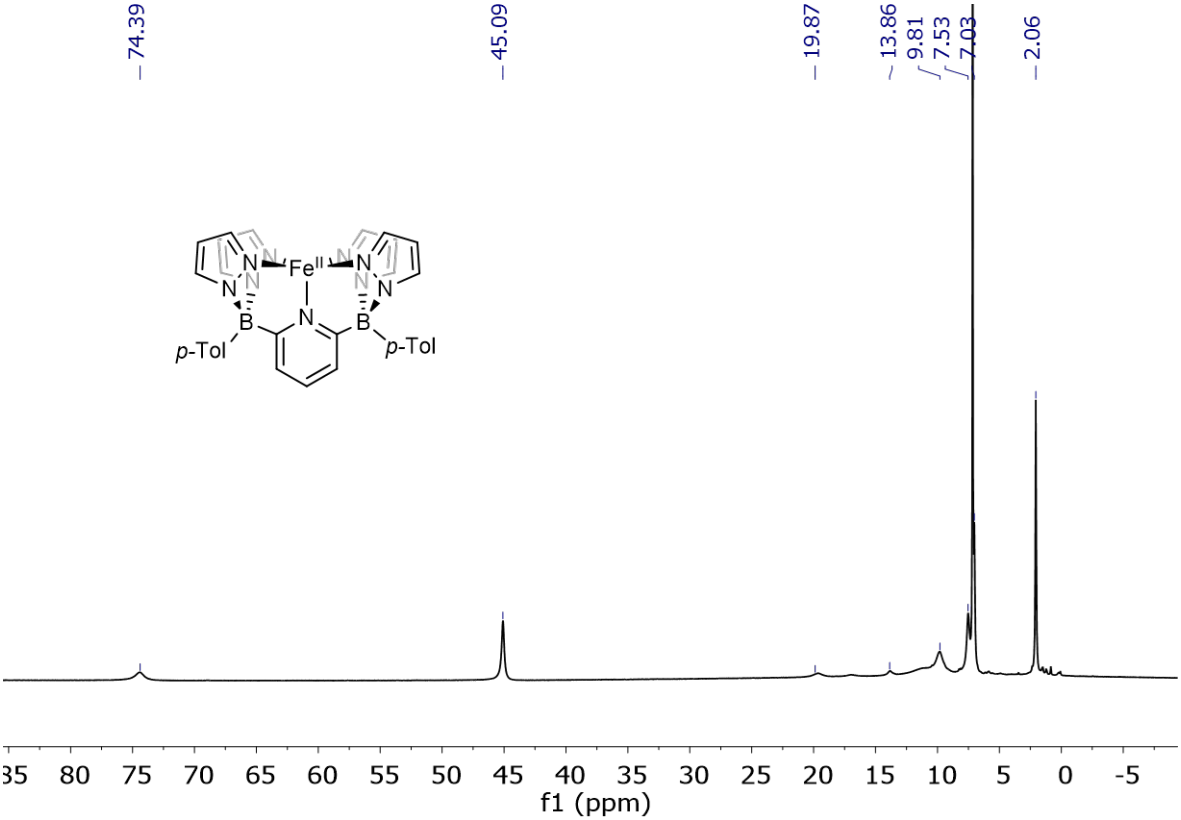



**Figure S36.** $^{1}$H NMR spectrum of $\mathbf{1_{Tol}}$ in $C_6D_6$.

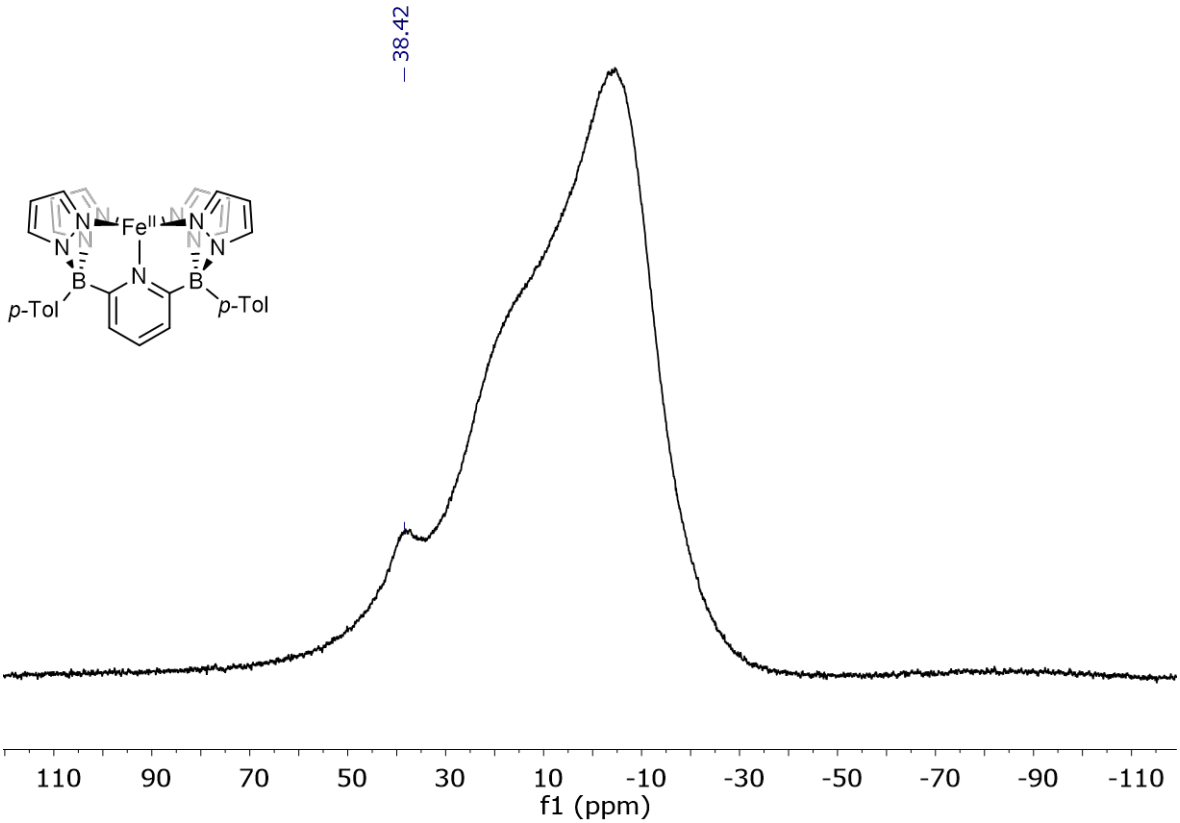



**Figure S37.** $^{11}$B NMR spectrum of $\mathbf{1_{Tol}}$ in $C_6D_6$.

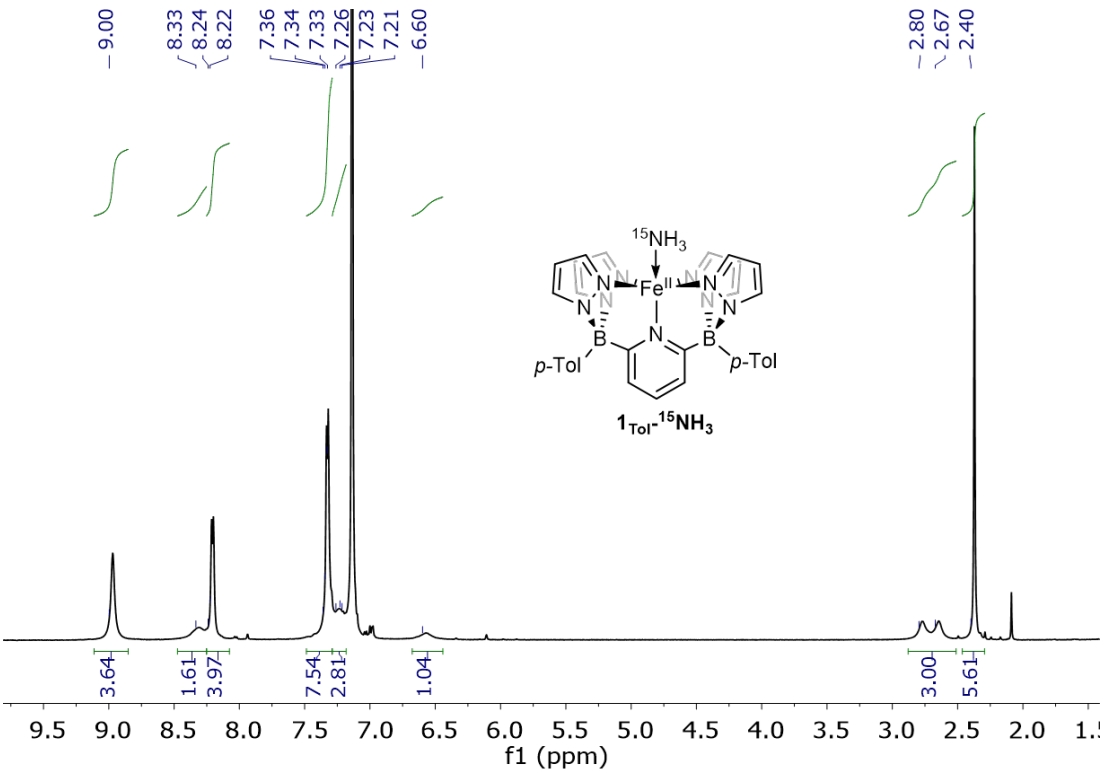



**Figure S38.** $^{1}$H NMR spectrum of $\mathbf{1_{Tol}}$-$^{15}\mathbf{NH_3}$ in $C_6D_6$.

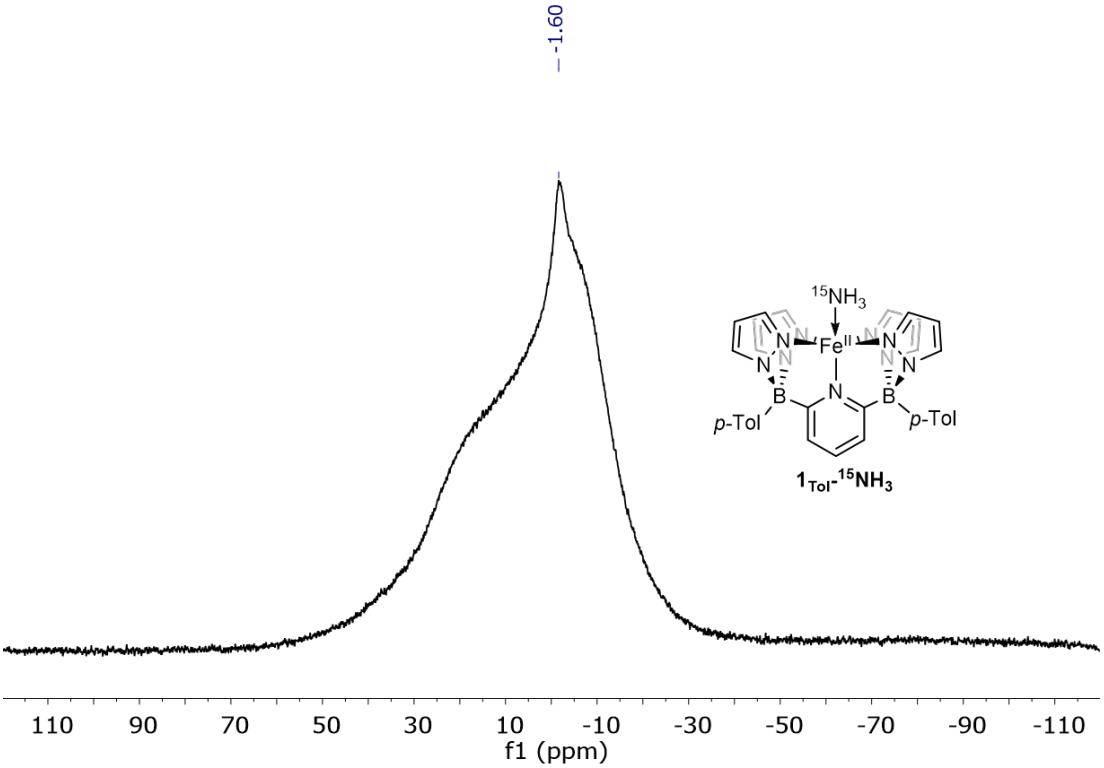



**Figure S39.** $^{11}$B NMR spectrum of $\mathbf{1_{Tol}}$-$^{15}\mathbf{NH_3}$ in $C_6D_6$.

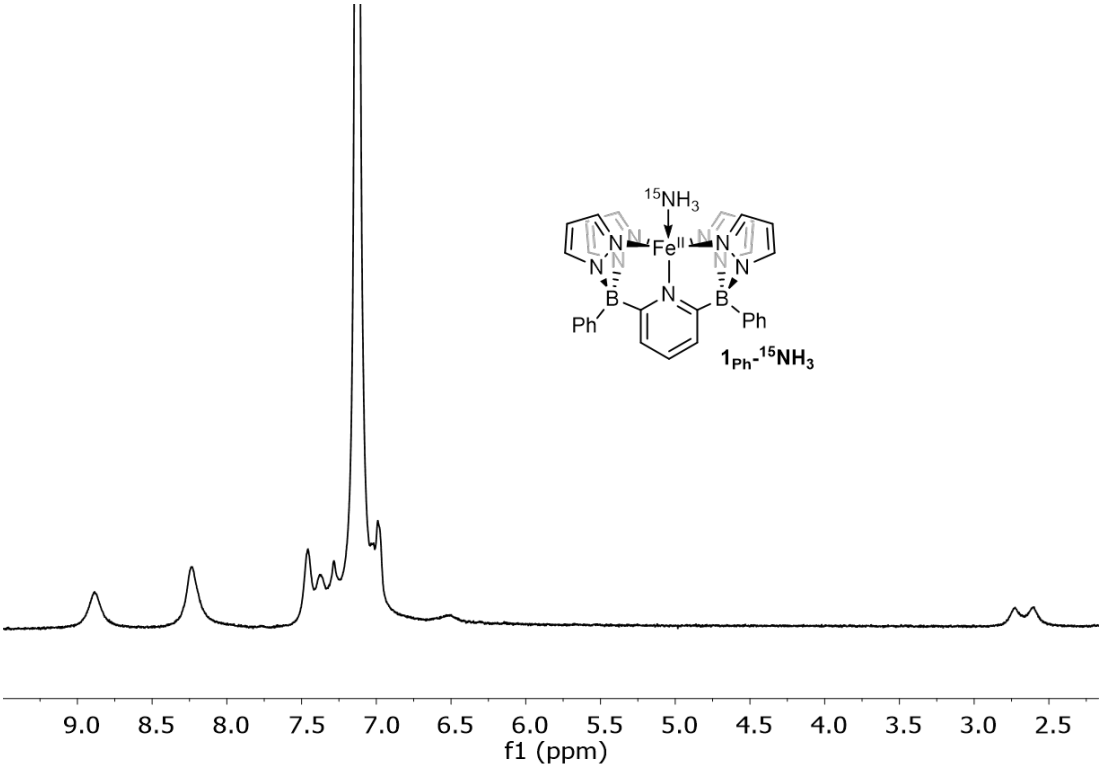



**Figure S40.** $^{1}$H NMR spectrum of $\mathbf{1_{Ph}}$-$^{15}$**NH$_3$** in $C_6D_6$.

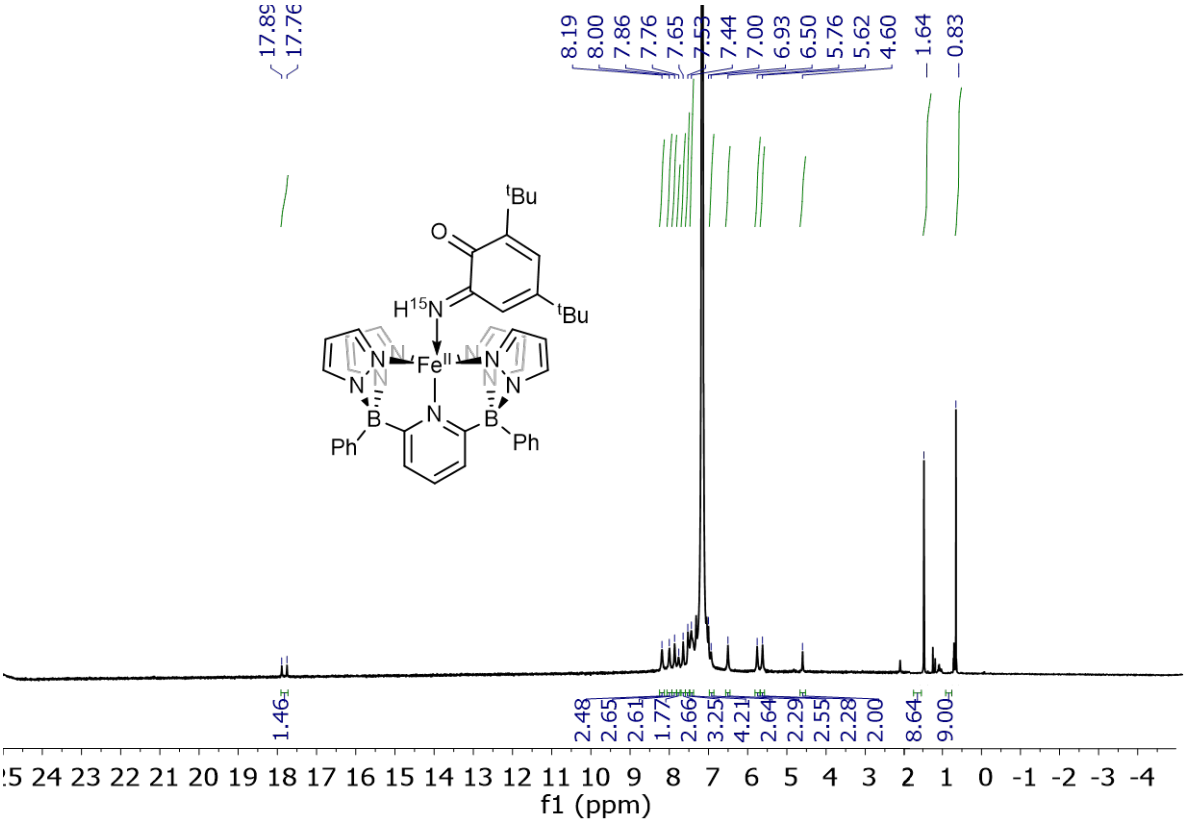



**Figure S41.** $^{1}$H NMR spectrum of $\mathbf{2_{Ph}}$-$^{15}$**N** in $C_6D_6$.

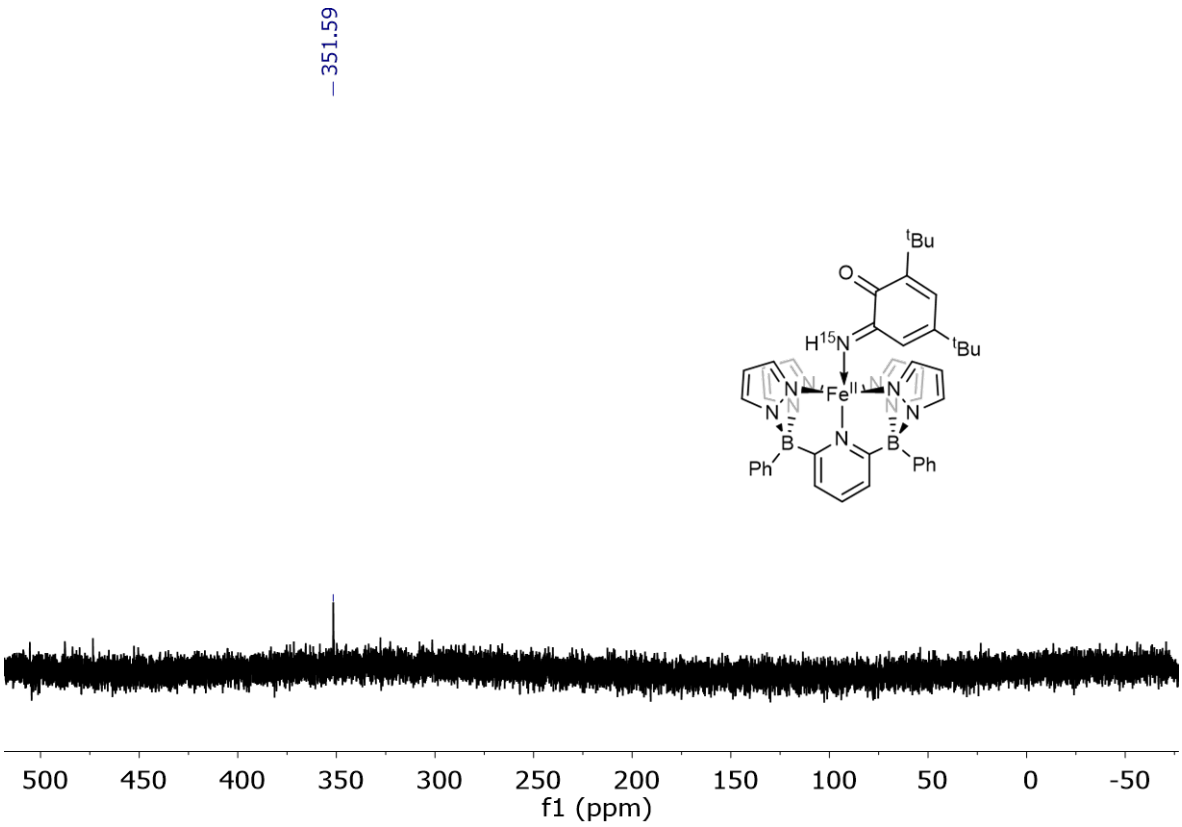



**Figure S42.** $^{15}N\{^{1}H\}$ NMR spectrum of $\mathbf{2_{Ph}}$-$^{15}$**N** in $C_6D_6$.

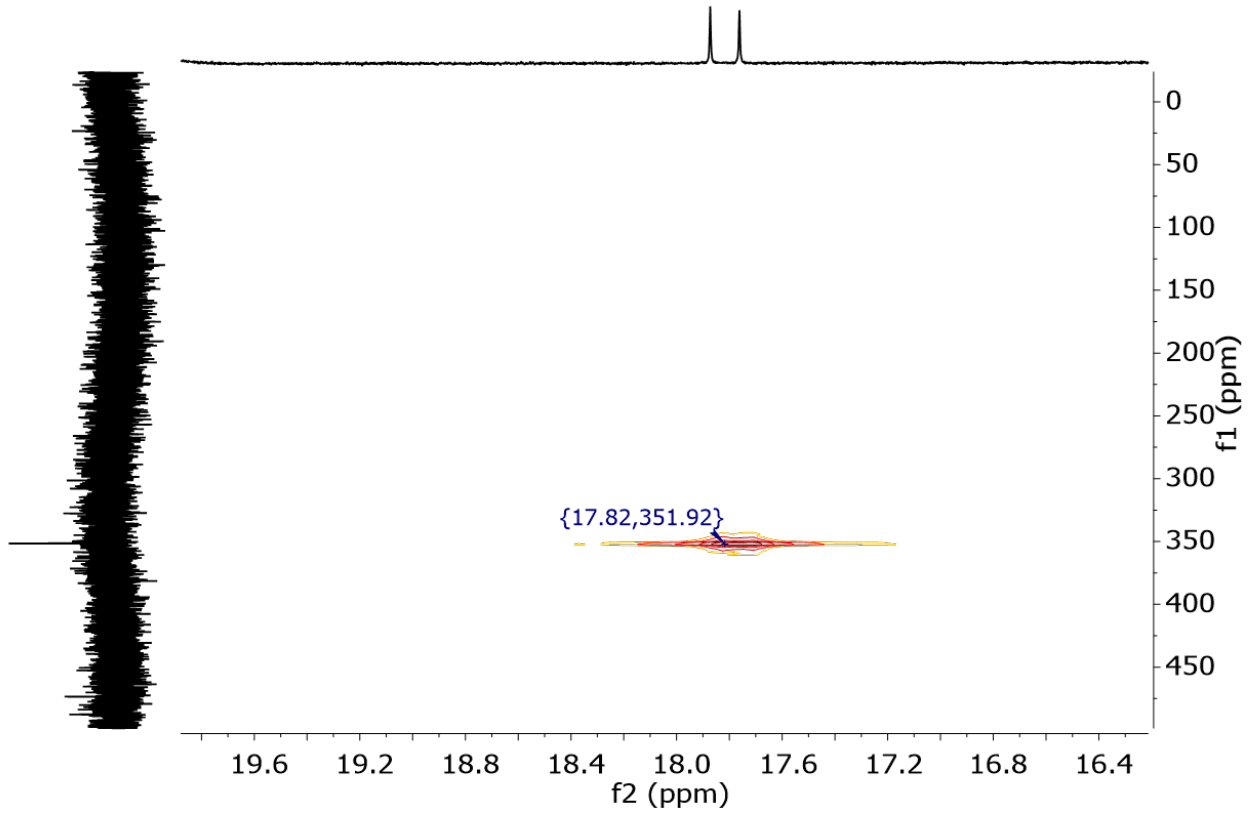



**Figure S43.** $^{15}N$-$^{1}H$ HMBC of $\mathbf{2_{Ph}}$-$^{15}$**N** in $C_6D_6$.

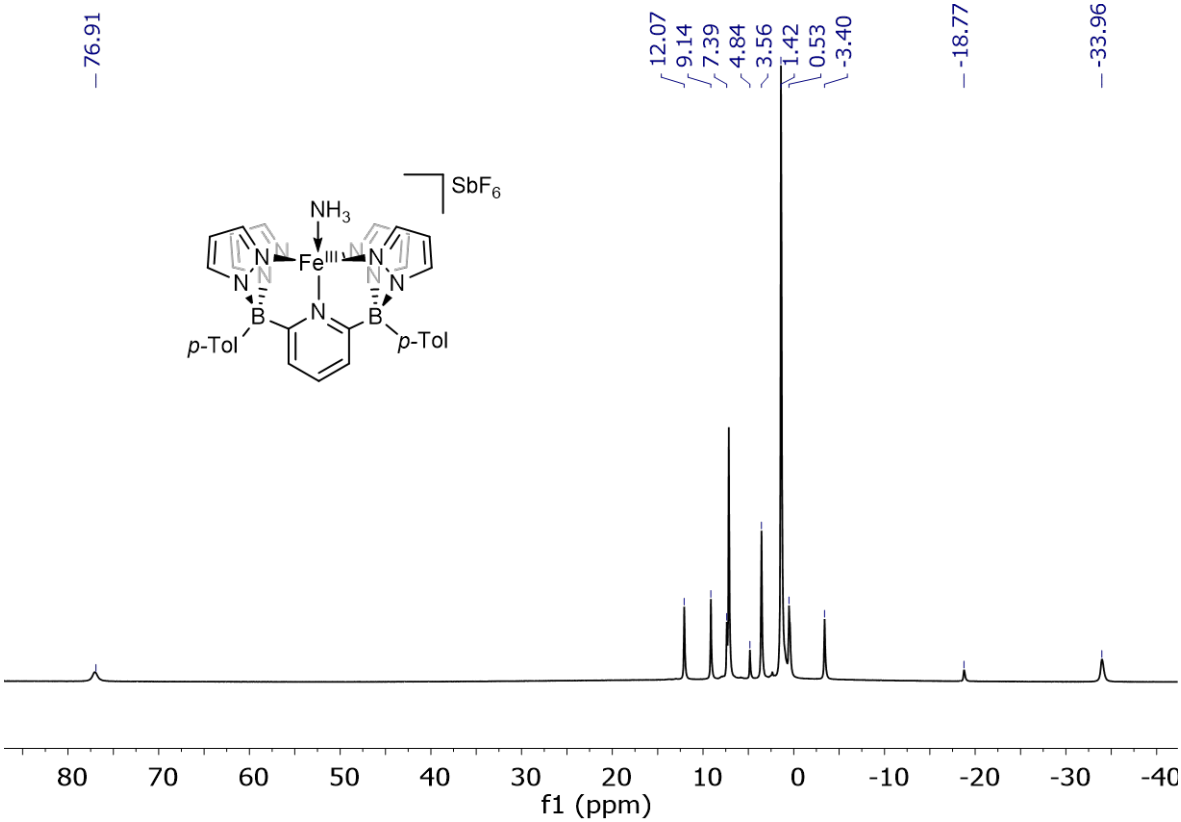



**Figure S44.** $^{1}$H NMR spectrum of $\mathbf{3_{Tol}\text{-}NH_3^+}$ in $C_6D_6$.

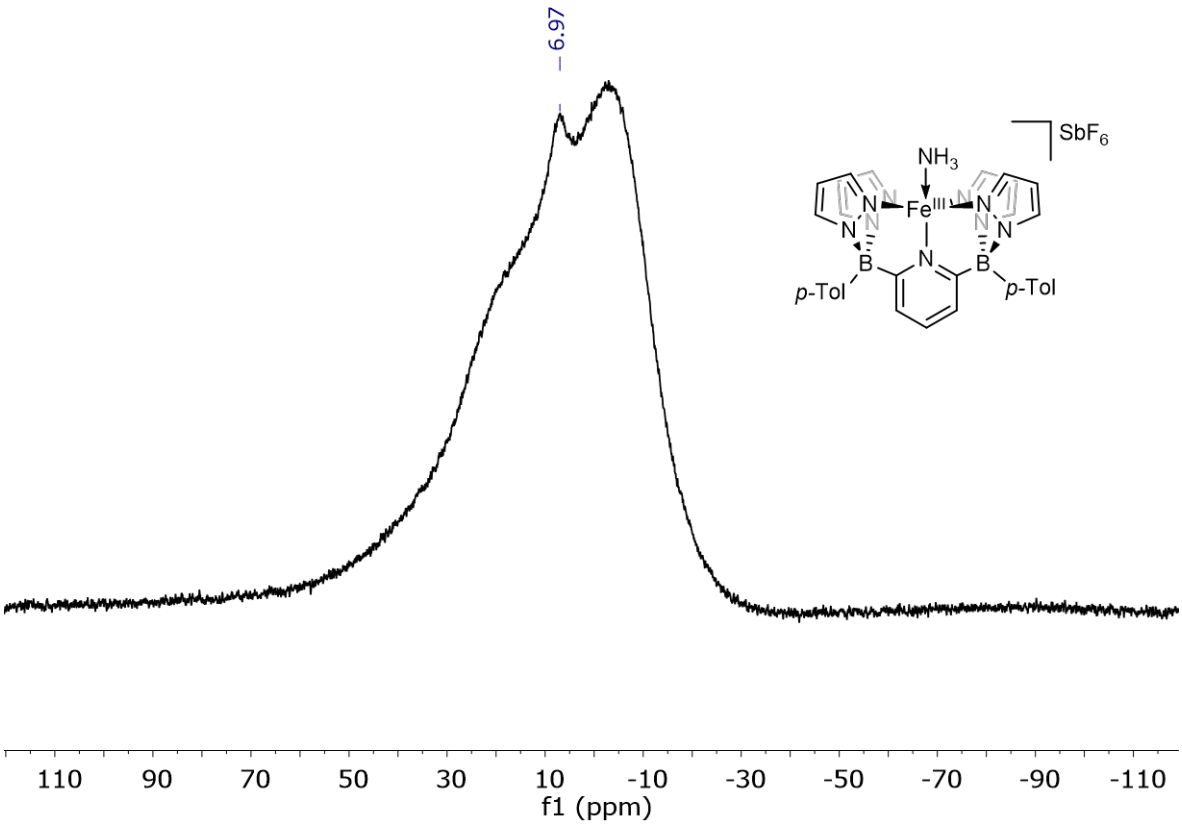



**Figure S45.** $^{11}$B NMR spectrum of $\mathbf{3_{Tol}\text{-}NH_3^+}$ in $C_6D_6$.

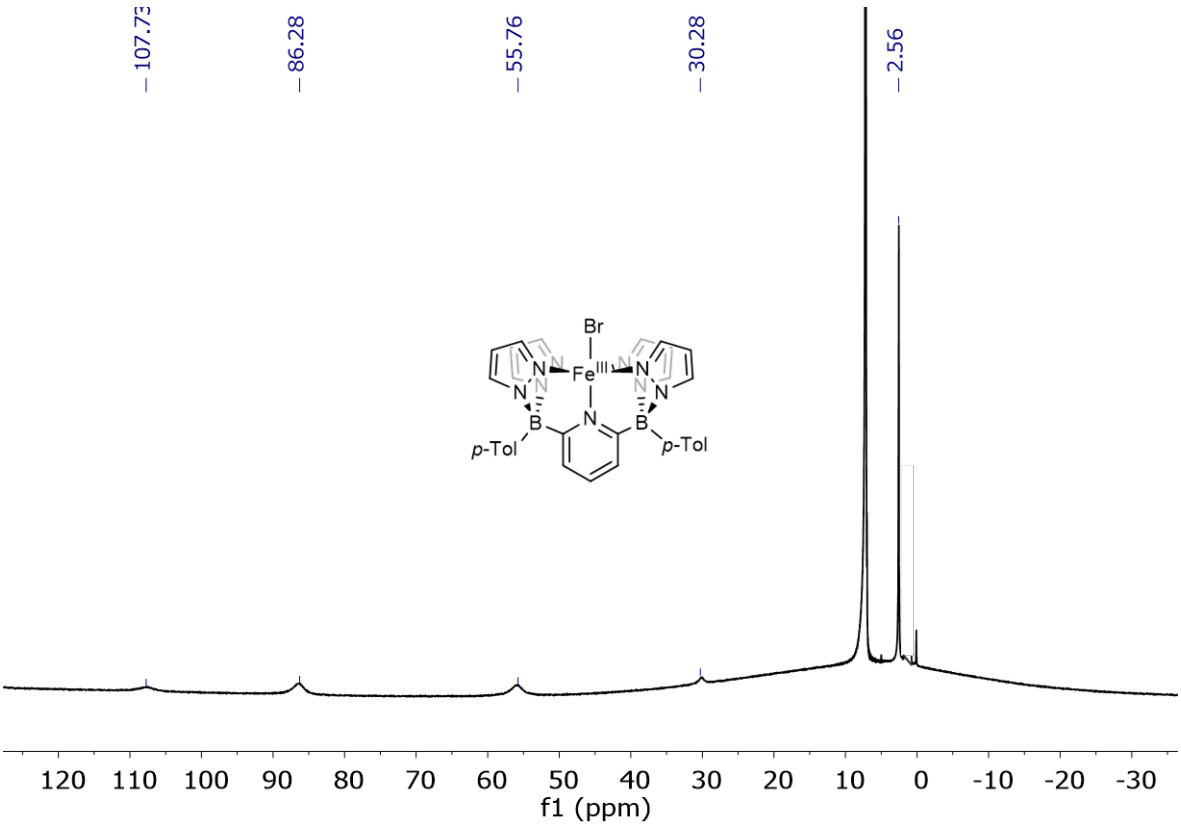



**Figure S46.** $^{1}$H NMR spectrum of $\mathbf{3_{Tol}}$**-Br** in $C_6D_6$.

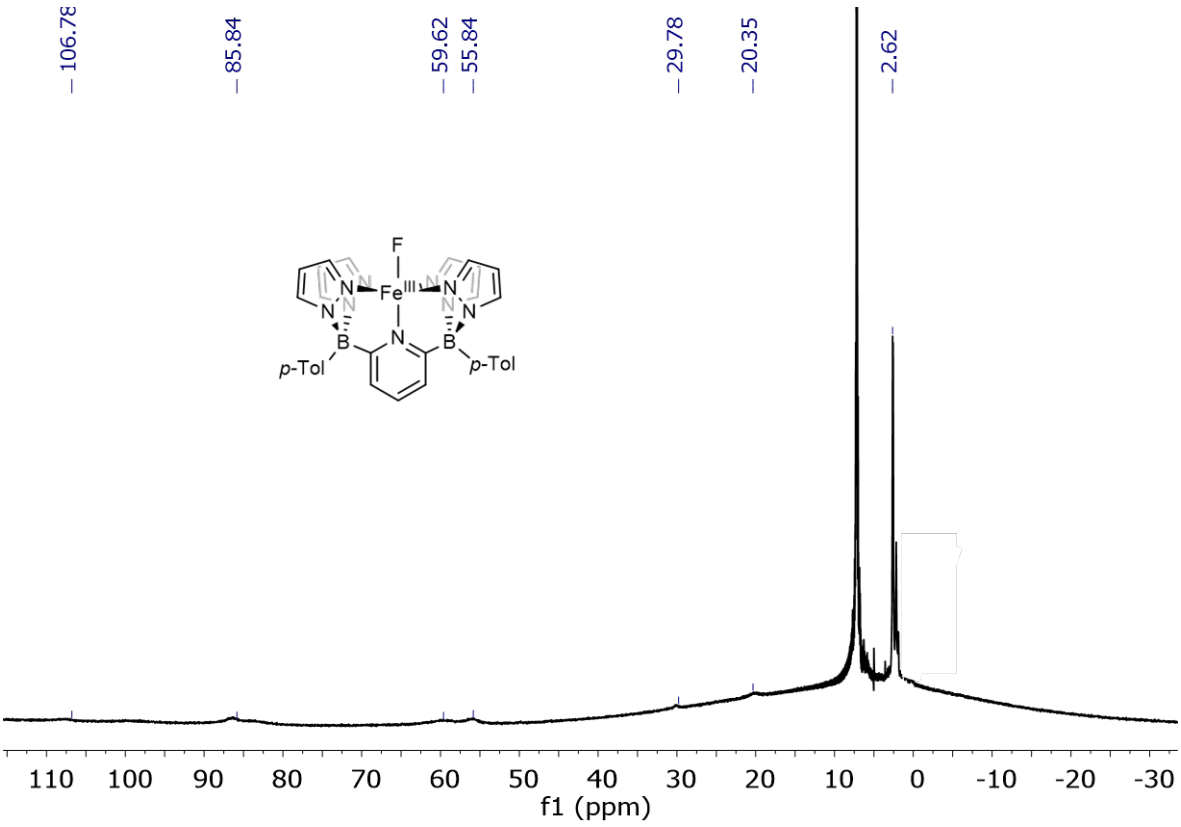



**Figure S47.** $^{1}$H NMR spectrum of $\mathbf{3_{Tol}}$**-F** in $C_6D_6$.

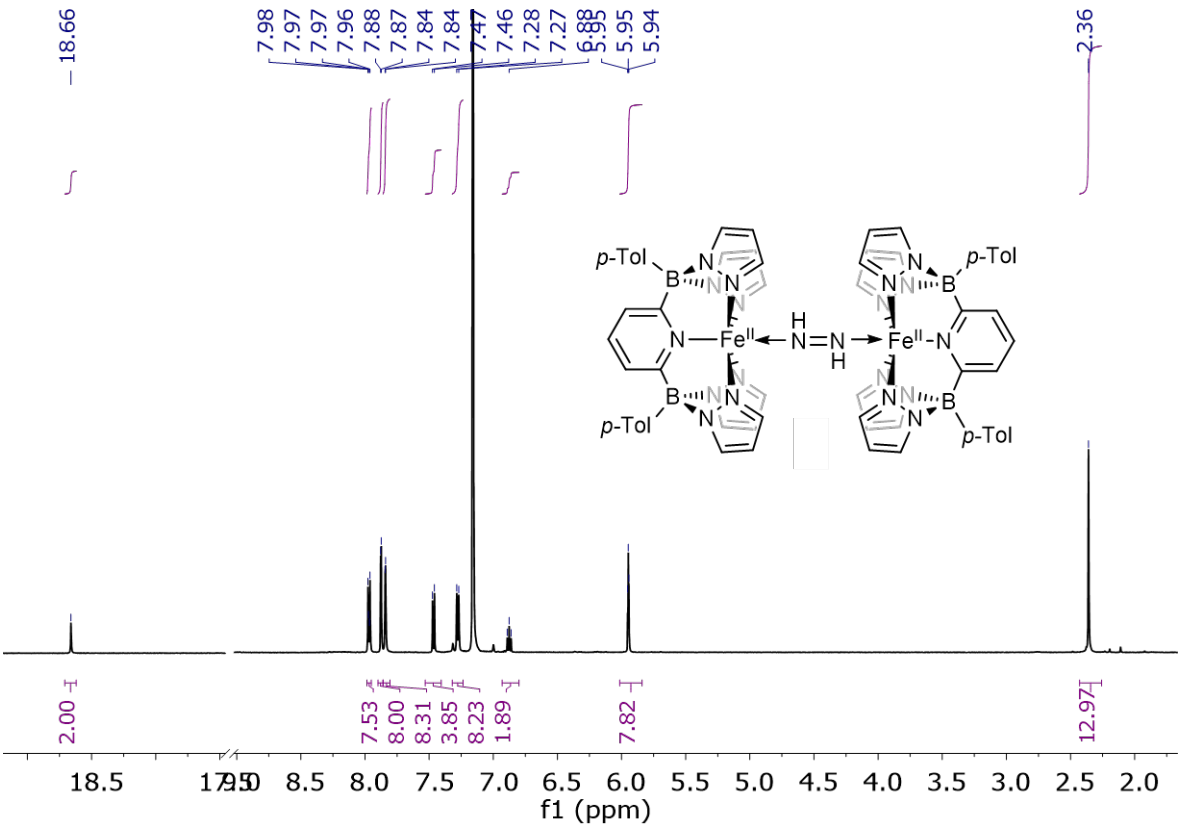



**Figure S48.** $^{1}$H NMR spectrum of $\mathbf{4_{Tol}}$ in $C_6D_6$.

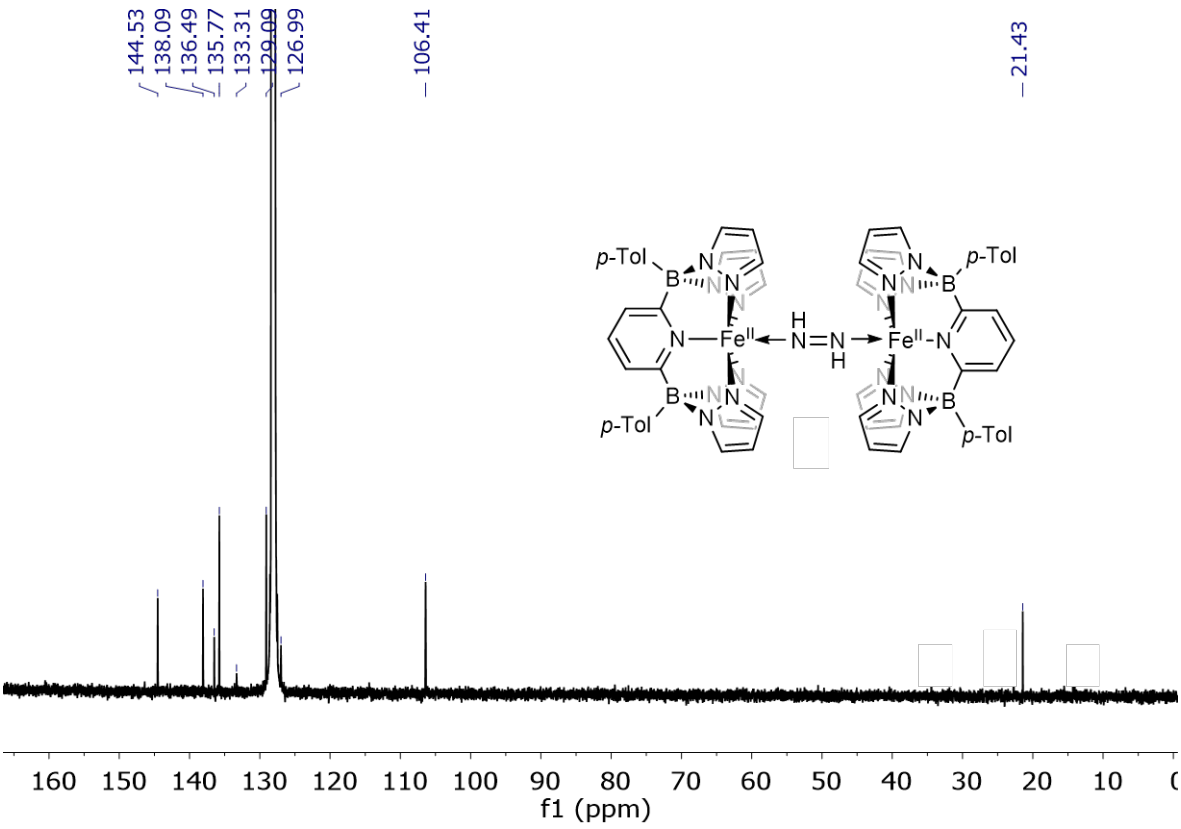



**Figure S49.** $^{13}$C{$^{1}$H} NMR spectrum of $\mathbf{4_{Tol}}$ in $C_6D_6$.

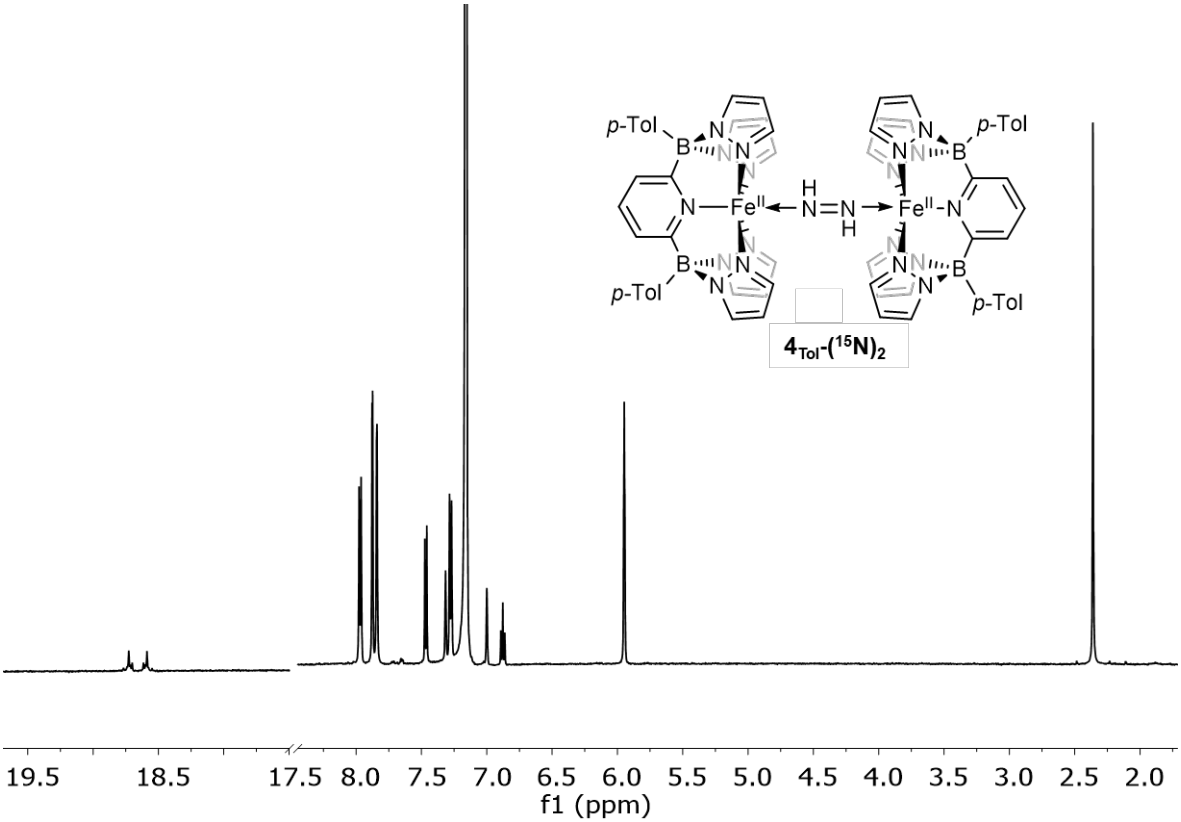



**Figure S50.** $^{1}H$ NMR spectrum of $\mathbf{4_{Tol}\text{-}(^{15}N)_2}$ in $C_6D_6$.

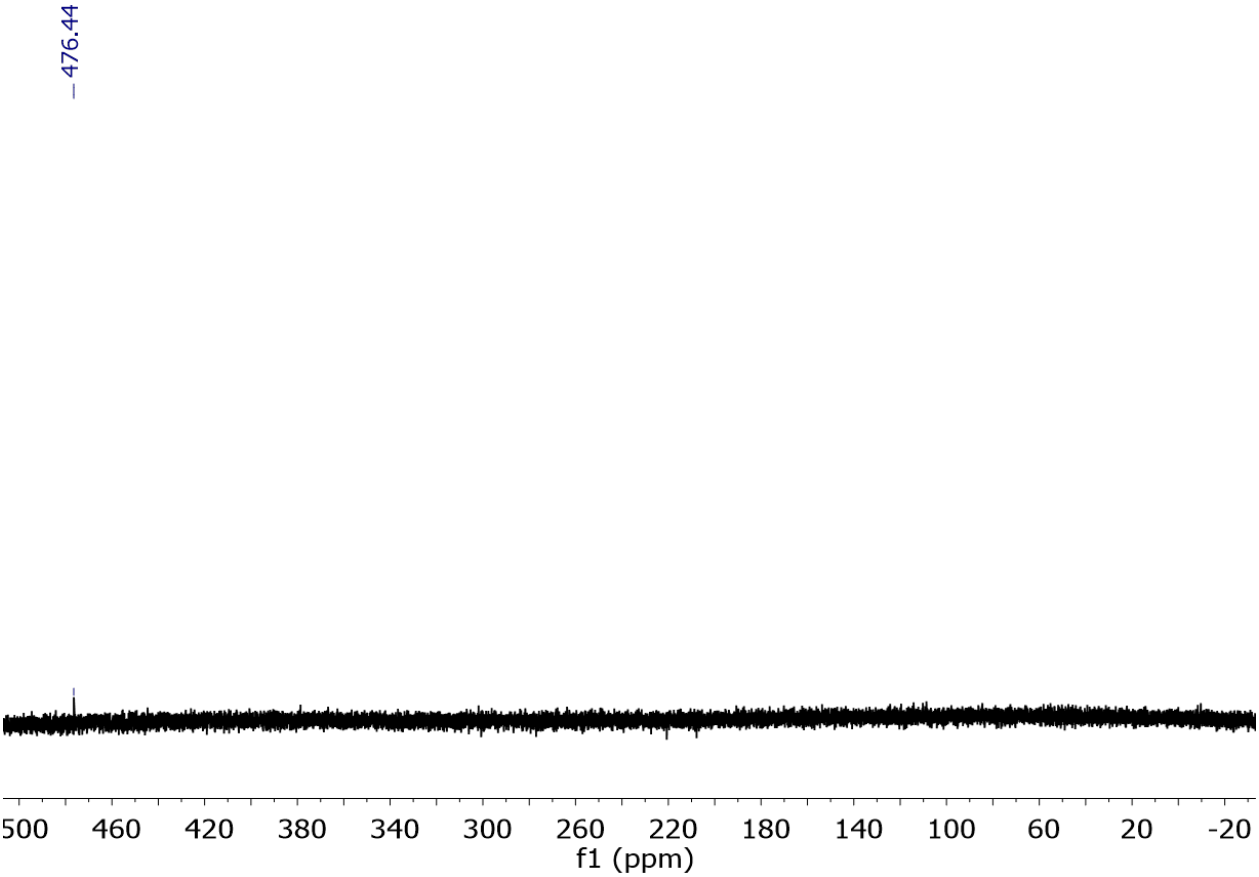



**Figure S51.** $^{15}N\{^{1}H\}$ NMR spectrum of $\mathbf{4_{Tol}\text{-}(^{15}N)_2}$ in $C_6D_6$.

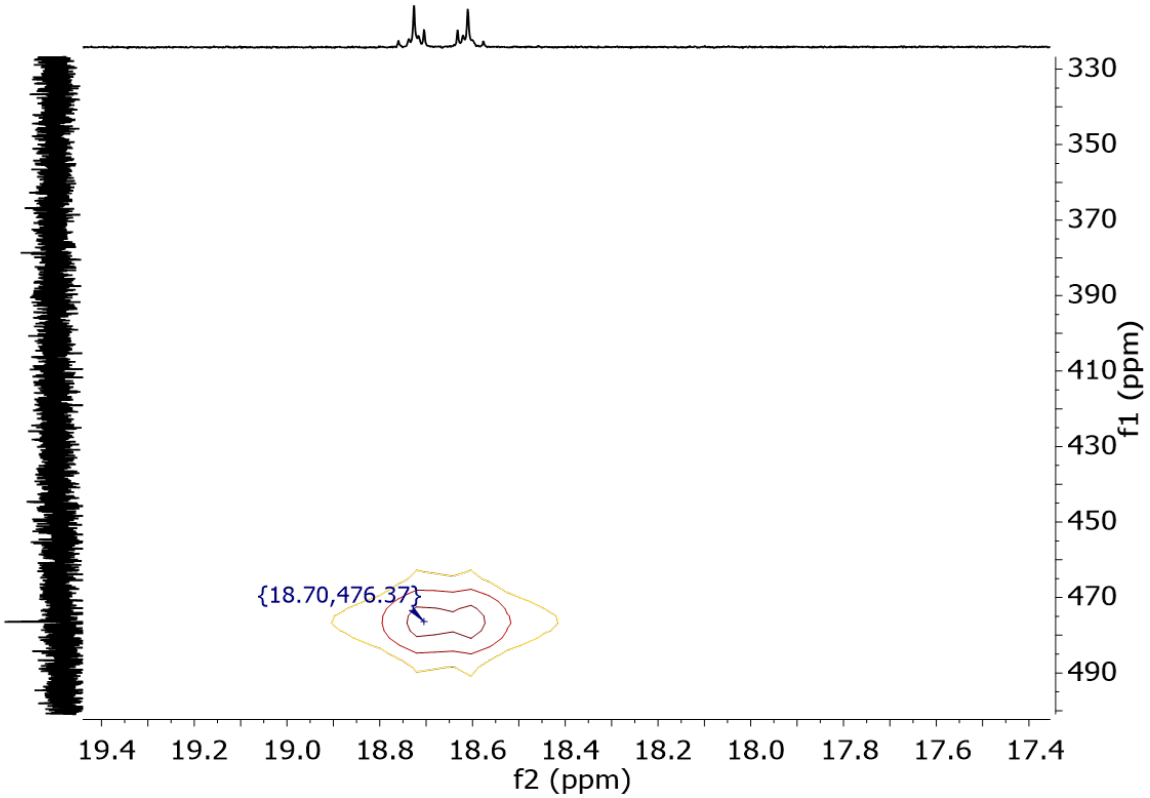



**Figure S52.** $^{15}N$-$^{1}H$ HMBC of **$4_{Tol}$-($^{15}N$)$_2$** in $C_6D_6$.

**Table S1**

| | $\mathbf{1_{Tol}\text{-}NH_3}$ | $\mathbf{2_{Tol}}$ | $\mathbf{3_{Tol}\text{-}NH_3^+}$ |
|---|---|---|---|
| **chemical formula** | $C_{37}H_{38}B_2N_{10}Fe$ | $C_{45}H_{50}B_2N_{10}OFe$ | $C_{37}H_{38}B_2F_6N_{10}SbFe$ |
| **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 | $P2_1/n$ |
| ***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* (Å$^3$)** | 6753.7(10) | 10570.5(7) | 3984.29(14) |
| **$\rho_{calcd}$ (g·cm$^{-3}$)** | 1.377 | 1.036 | 1.560 |
| **$\mu$ (mm$^{-1}$)** | 3.928 | 2.588 | 8.900 |
| **θ range (deg); completeness** | 7.48 to 136.582; 98.9% | 3.656 to 136.696; 98.4% | 7.024 to 140.13; 99.8% |
| **collected reflections; $R_\sigma$** | 18406; 0.0778 | 19096; 0.0660 | 28060; 0.0373 |
| **unique reflections; $R_{int}$** | 6138; 0.0545 | 19096; 0.0704 | 7559; 0.0422 |
| **R1[a]; wR2[b] [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] $R_1=\Sigma(||F_o|-|F_c||)/\Sigma|F_o|$

[b] $wR_2=\{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$

**Table S2**

| | $3_{Tol}$-Br | $3_{Tol}$-F | $4_{Tol}$ |
|---|---|---|---|
| **chemical formula** | $C_{43}H_{41}B_2BrN_9Fe$ | $C_{31}H_{29}B_2FFeN_9$ | $C_{65}H_{63}B_4Fe_2N_{20}$ |
| **crystal colour** | Red | yellow | blue |
| ***Fw*; *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) |
| **α (deg)** | 104.192(5) | 90 | 98.128(5) |
| **β (deg)** | 92.618(5) | 90 | 100.359(5) |
| **γ (deg)** | 112.901(5) | 90 | 115.218(5) |
| ***Z*** | 2 | 4 | 2 |
| ***V* (Å$^3$)** | 2000.3(15) | 2876.3(2) | 3053.3(4) |
| **$\rho_{calcd}$ (g·cm$^{-3}$)** | 1.397 | 1.441 | 1.391 |
| ***μ* (mm$^{-1}$)** | 1.420 | 0.571 | 4.291 |
| **θ 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; $R_{int}$** | 7875; 0.1088 | 3656; 0.0420 | 10913; 0.0678 |
| **R1[a]; wR2[b] [I > 2σ(I)]** | 0.0521; 0.0779 | 0.0432; 0.1125 | 0.0546; 0.1325 |
| **R1; wR2 [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] $R_1=\Sigma(||F_o|-|F_c||)/\Sigma|F_o|$

[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**

$\mathbf{1}_{\mathbf{Tol}}$ (HS)

| | | | |
|---|---|---|---|
| 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 | 8.15499600 | 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 | 21.84988300 |
| H | 2.89971200 | 11.79097000 | 22.17982200 |
| 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 |

| | | | |
|---|---|---|---|
| H | 9.55763600 | 8.58790700 | 20.05501500 |
| C | 7.61149000 | 13.66822600 | 17.76836800 |
| H | 7.09596600 | 14.01763700 | 16.88686200 |
| C | 8.57254900 | 14.32091800 | 18.53779200 |
| H | 8.98913000 | 15.30645500 | 18.38978900 |
| C | 8.87333400 | 13.41356200 | 19.54374700 |
| H | 9.54412800 | 13.49749200 | 20.38527600 |
| C | 9.24797400 | 10.81070300 | 21.28727200 |
| C | 10.56551200 | 11.16002200 | 20.93853300 |
| H | 10.75851400 | 11.65267000 | 19.98828000 |
| C | 11.65709400 | 10.86345200 | 21.75314400 |
| H | 12.65660000 | 11.15838000 | 21.43683800 |
| C | 11.49359700 | 10.17907200 | 22.96154300 |
| C | 10.19767100 | 9.78024400 | 23.30227100 |
| H | 10.03558100 | 9.21436100 | 24.21845700 |
| C | 9.11059100 | 10.08553300 | 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 |
| H | 13.59234700 | 9.76921500 | 23.28901500 |
| B | 3.00276200 | 11.36765400 | 19.35785700 |
| B | 7.99001200 | 11.02250200 | 20.28952700 |

**$1_{Tol}$-$NH_3$** (LS)

| | | | |
|---|---|---|---|
| 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 | 8.03353900 | 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 | 13.70060900 | 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 | 16.33492100 |
| C | 2.14865700 | 9.28014500 | 17.90927100 |
| 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 |

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|---|---|---|---|
| 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 | 11.78295800 | 22.10189700 |
| C | 5.01134800 | 11.75463400 | 22.66667000 |
| H | 4.82691600 | 11.99246100 | 23.71234100 |
| C | 6.30402000 | 11.55075000 | 22.20340200 |
| H | 7.14820100 | 11.64261200 | 22.87755800 |
| C | 6.53359100 | 11.24250200 | 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 | 10.17286900 | 22.99935300 |
| C | 10.16123800 | 9.77297200 | 23.30479700 |
| H | 9.97627300 | 9.19868300 | 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 |

**$1_{Tol}$-$NH_3$** (HS)

| | | | |
|---|---|---|---|
| Fe | 5.80658200 | 10.98431900 | 17.96800300 |

| | | | |
|---|---|---|---|
| N | 4.44568400 | 12.41768400 | 17.64145900 |
| N | 3.23279100 | 12.35474300 | 18.23076400 |
| N | 4.06718700 | 9.45603800 | 17.83366200 |
| N | 2.91387800 | 9.90880100 | 18.37088800 |
| N | 5.50053100 | 11.09712700 | 19.92094600 |
| N | 7.19498800 | 9.61301300 | 18.27897700 |
| N | 8.16592800 | 9.85786600 | 19.17909000 |
| N | 7.68903600 | 12.49712500 | 18.08683200 |
| N | 8.24281100 | 12.39931600 | 19.31671900 |
| N | 6.17744200 | 10.88961100 | 15.93416600 |
| 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 | 1.38283700 | 13.34628100 | 17.98502400 |
| C | 3.73365500 | 8.48888700 | 16.97537600 |
| H | 4.50195600 | 7.94683900 | 16.43772200 |
| C | 2.34413500 | 8.31480800 | 16.92992400 |
| H | 1.77384200 | 7.60830600 | 16.34373100 |
| C | 1.86246100 | 9.25259200 | 17.82716000 |
| H | 0.84923900 | 9.49630700 | 18.10877300 |
| C | 1.55734100 | 11.42828900 | 20.06523900 |
| C | 0.78938900 | 10.35585000 | 20.55320700 |
| H | 1.09733500 | 9.33461700 | 20.34133800 |
| C | -0.34663100 | 10.54716900 | 21.33912800 |
| H | -0.90530900 | 9.68079100 | 21.69036300 |
| C | -0.77428700 | 11.82950900 | 21.69456300 |
| C | 0.00259400 | 12.90717400 | 21.25808200 |
| H | -0.27755800 | 13.91963600 | 21.54545500 |
| C | 1.13751600 | 12.70757900 | 20.47425500 |
| H | 1.72903900 | 13.57920500 | 20.20281200 |
| C | -2.02243000 | 12.04279200 | 22.51023400 |
| H | -2.22482700 | 11.18890200 | 23.16606000 |
| 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 |
| H | 2.93179300 | 11.28891900 | 22.06422600 |
| C | 5.00574100 | 11.36501700 | 22.61662100 |
| H | 4.80737200 | 11.48578500 | 23.67973700 |
| C | 6.30897700 | 11.32243200 | 22.14215300 |
| H | 7.14663200 | 11.42362700 | 22.82333500 |
| C | 6.55565100 | 11.14393600 | 20.77772000 |
| C | 7.50575800 | 8.47028600 | 17.65758800 |
| H | 6.84529000 | 8.05611400 | 16.90749500 |
| C | 8.70743800 | 7.95907000 | 18.15687500 |
| H | 9.21578100 | 7.05012800 | 17.86979600 |
| C | 9.09082800 | 8.87511900 | 19.12254700 |
| H | 9.94782600 | 8.89107100 | 19.77762300 |
| C | 7.83666200 | 13.77430600 | 17.71286900 |
| H | 7.48859400 | 14.10043200 | 16.74059400 |
| C | 8.46776300 | 14.52540200 | 18.70954800 |

| | | | |
|---|---|---|---|
| H | 8.72614000 | 15.57469800 | 18.70026100 |
| C | 8.69351200 | 13.60595300 | 19.72217900 |
| H | 9.14025400 | 13.73118400 | 20.69775200 |
| C | 9.27442900 | 10.88577600 | 21.23884700 |
| C | 10.54673600 | 11.46177900 | 21.08832600 |
| H | 10.73842200 | 12.13116400 | 20.25327800 |
| C | 11.59985600 | 11.18502500 | 21.96154000 |
| H | 12.56648900 | 11.66040400 | 21.80096600 |
| C | 11.44031300 | 10.30000300 | 23.03032800 |
| C | 10.19168700 | 9.68399400 | 23.17318800 |
| H | 10.03831300 | 8.96537300 | 23.97713000 |
| C | 9.14526800 | 9.96802100 | 22.29935500 |
| H | 8.20418900 | 9.43923200 | 22.43618900 |
| C | 12.56223800 | 10.02276300 | 23.99648100 |
| H | 12.45913100 | 10.62526200 | 24.90908000 |
| H | 12.57687200 | 8.97125800 | 24.30538800 |
| H | 13.53751700 | 10.26016000 | 23.55813800 |
| B | 2.95074300 | 11.19651800 | 19.26990500 |
| B | 8.07577000 | 11.08268000 | 20.16069600 |
| H | 5.48109000 | 11.37885800 | 15.37475200 |
| H | 7.08652600 | 11.32922200 | 15.79559800 |
| H | 6.24535500 | 9.93766200 | 15.58016500 |

**$3_{Tol}$-$NH_2$** (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 | 18.42877700 |
| 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 | 2.37073400 | 13.38996000 | 17.68503100 |
| H | 1.34447000 | 13.47818400 | 18.00547100 |
| C | 4.06000700 | 8.89668600 | 16.90783100 |
| H | 4.85376200 | 8.56667400 | 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 | 20.51502500 |
| C | -0.21690700 | 10.36982500 | 21.41007400 |
| H | -0.63649700 | 9.44888600 | 21.81225400 |

| | | | |
|---|---|---|---|
| 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 | 20.42444000 |
| 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 |
| H | -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 |
| H | 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 | 12.39591200 | 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***

| | | | |
|---|---|---|---|
| Fe | 6.68269800 | 11.19368800 | 18.74487200 |
| N | 5.56386100 | 12.75091900 | 18.14250400 |
| N | 4.26325300 | 12.82249500 | 18.50898100 |

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|---|---|---|---|
| N | 5.13551900 | 10.08164400 | 18.13316600 |
| N | 3.88617600 | 10.41716800 | 18.53380700 |
| N | 5.90017600 | 11.20305000 | 20.69718400 |
| N | 7.85073500 | 9.64530700 | 19.10650300 |
| N | 8.40870200 | 9.56861700 | 20.33390700 |
| N | 8.21344500 | 12.32882900 | 19.37557900 |
| N | 8.78012300 | 12.03664800 | 20.57174800 |
| N | 5.52069400 | 11.31838500 | 14.44235100 |
| C | 5.75576000 | 13.65235000 | 17.17284800 |
| H | 6.72605100 | 13.75763200 | 16.70824500 |
| C | 4.56111000 | 14.31899600 | 16.88648000 |
| H | 4.39263300 | 15.10890300 | 16.16893200 |
| C | 3.63957900 | 13.74845500 | 17.75153100 |
| H | 2.58342800 | 13.93510900 | 17.86534500 |
| C | 5.01387300 | 9.09334400 | 17.23937700 |
| H | 5.88941700 | 8.65558900 | 16.78413200 |
| C | 3.66623600 | 8.78922900 | 17.03073000 |
| H | 3.24516800 | 8.04164600 | 16.37454700 |
| C | 2.98848300 | 9.66218500 | 17.86711100 |
| H | 1.92984100 | 9.79869800 | 18.02274400 |
| C | 2.14262000 | 11.92091900 | 19.87796500 |
| C | 1.31688300 | 10.84274700 | 20.24787500 |
| H | 1.70140900 | 9.82682000 | 20.19205600 |
| C | 0.02243300 | 11.02229800 | 20.73149100 |
| H | -0.57294200 | 10.15072400 | 20.99918900 |
| C | -0.51904600 | 12.30113900 | 20.89505800 |
| C | 0.30629900 | 13.38689600 | 20.59063700 |
| H | -0.06272900 | 14.39957100 | 20.74607800 |
| C | 1.60026100 | 13.19842200 | 20.10523000 |
| H | 2.21107500 | 14.08284200 | 19.94059600 |
| C | -1.93070400 | 12.49890000 | 21.38079700 |
| H | -2.04486100 | 13.45325700 | 21.90631100 |
| H | -2.64213800 | 12.50166200 | 20.54392300 |
| H | -2.23703300 | 11.69798600 | 22.06270300 |
| C | 4.60674400 | 11.57005000 | 20.81556200 |
| C | 4.10655800 | 11.86565600 | 22.09003300 |
| H | 3.06855700 | 12.15501300 | 22.20905600 |
| C | 4.95317600 | 11.81096600 | 23.19181100 |
| H | 4.58041800 | 12.06933300 | 24.18111200 |
| C | 6.28064700 | 11.43076800 | 23.02151100 |
| H | 6.95713700 | 11.40926400 | 23.86923800 |
| C | 6.74746700 | 11.09831100 | 21.74550100 |
| C | 8.21812200 | 8.55218800 | 18.42969900 |
| H | 7.91035800 | 8.41206200 | 17.40339300 |
| 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 | 10.08383200 | 13.03185500 | 21.90158900 |
| C | 9.28606600 | 10.37018100 | 22.60070000 |
| C | 10.67670700 | 10.58080700 | 22.56285100 |
| H | 11.12336800 | 11.07661000 | 21.70400600 |
| C | 11.52615500 | 10.14056500 | 23.57644200 |
| H | 12.59538300 | 10.33247600 | 23.49951400 |
| C | 11.03183600 | 9.44177300 | 24.68239700 |
| C | 9.65924500 | 9.17834800 | 24.71340400 |
| H | 9.24299600 | 8.60580800 | 25.54093200 |
| C | 8.81539800 | 9.62825400 | 23.69875400 |
| H | 7.76168200 | 9.36614800 | 23.75563900 |
| C | 11.94065200 | 8.99520000 | 25.79727000 |
| H | 12.02605600 | 9.76817700 | 26.57297700 |
| H | 11.56419600 | 8.08869400 | 26.28364300 |
| H | 12.95313000 | 8.78917900 | 25.43302100 |
| 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 | 3.66171700 | 11.36398000 | 12.85457000 |
| C | 4.69048000 | 8.79014800 | 12.15339000 |
| C | 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 |

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|---|---|---|---|
| C | 0.92995700 | 12.16580300 | 12.86772500 |
| 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 |
| H | 0.99863400 | 9.83542400 | 10.31772000 |
| H | -0.24470800 | 11.03846700 | 10.72267500 |
| H | 1.37181600 | 11.57067300 | 10.22603600 |
| C | 0.45857200 | 9.73293300 | 13.04449800 |
| H | 0.60562500 | 8.73588400 | 12.62540600 |
| H | 0.75190500 | 9.71721100 | 14.10150800 |
| H | -0.61090300 | 9.97325200 | 12.99732400 |
| H | 6.53735600 | 9.46473800 | 12.92100800 |
| O | 2.50757800 | 8.37075200 | 11.31936300 |

**C-N*ortho***

| | | | |
|---|---|---|---|
| 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 | 20.24855800 |
| 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 | 1.37522900 | 13.79662600 | 20.43720700 |
| C | -1.85351500 | 12.18931500 | 23.39237600 |
| H | -1.84738900 | 11.45072400 | 24.20152400 |

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|---|---|---|---|
| H | -1.85945700 | 13.18708900 | 23.84490400 |
| H | -2.80359600 | 12.07209100 | 22.85350500 |
| C | 4.17500700 | 11.54447900 | 20.71622300 |
| C | 4.05235600 | 11.98127400 | 22.04155500 |
| H | 3.07480100 | 12.22981300 | 22.43693000 |
| C | 5.18259400 | 12.12145200 | 22.83714200 |
| H | 5.09351600 | 12.49415700 | 23.85586400 |
| C | 6.42581500 | 11.78283200 | 22.31932500 |
| H | 7.32044300 | 11.90435600 | 22.92007700 |
| C | 6.53017100 | 11.30147200 | 21.00937400 |
| C | 7.34749900 | 8.31862900 | 17.84644200 |
| H | 6.79807200 | 7.95771900 | 16.98620300 |
| C | 8.38167400 | 7.69086900 | 18.54169400 |
| H | 8.81468200 | 6.71793800 | 18.36026200 |
| C | 8.73502100 | 8.60500600 | 19.52070100 |
| H | 9.49141000 | 8.54841200 | 20.28734300 |
| C | 7.50486600 | 13.69117300 | 17.84969400 |
| H | 6.93373600 | 14.06945300 | 17.01399300 |
| C | 8.47752100 | 14.33781100 | 18.61361400 |
| H | 8.85485400 | 15.34430800 | 18.50511000 |
| C | 8.85063800 | 13.38891000 | 19.55319900 |
| H | 9.55317800 | 13.45268800 | 20.37027100 |
| C | 9.24636000 | 10.82358700 | 21.28905100 |
| C | 10.56223600 | 11.13091000 | 20.89804600 |
| H | 10.74274600 | 11.57174500 | 19.92009000 |
| C | 11.66489000 | 10.85768000 | 21.70626100 |
| H | 12.66286100 | 11.11794600 | 21.35628400 |
| C | 11.51390900 | 10.23976300 | 22.95140800 |
| C | 10.21790600 | 9.88476900 | 23.33834900 |
| H | 10.06423300 | 9.37208300 | 24.28683400 |
| C | 9.12019700 | 10.16708600 | 22.52657200 |
| H | 8.13815800 | 9.84005500 | 22.86062900 |
| C | 12.69824200 | 9.97224100 | 23.84279600 |
| H | 13.61591700 | 9.83259100 | 23.26085400 |
| H | 12.87484600 | 10.80971000 | 24.53136500 |
| H | 12.54596300 | 9.07677300 | 24.45545500 |
| B | 2.84731500 | 11.44506400 | 19.73959100 |
| B | 7.97823900 | 11.00420700 | 20.29042800 |
| H | 4.44877700 | 10.25330300 | 15.85541000 |
| H | 5.89623100 | 9.52788600 | 15.92347200 |
| C | 5.58819100 | 10.45809200 | 14.18323800 |
| C | 5.48157200 | 9.00903400 | 13.64823800 |
| C | 4.52670100 | 11.35972500 | 13.63001600 |
| C | 4.77416400 | 8.75199200 | 12.37790700 |
| C | 3.77397700 | 11.04772300 | 12.55839100 |
| H | 4.39369400 | 12.29886200 | 14.15559400 |
| C | 3.97363000 | 9.74777000 | 11.91734600 |
| H | 3.39273600 | 9.56112800 | 11.01949400 |
| C | 7.04061400 | 11.02904300 | 13.81485300 |
| C | 7.32741700 | 10.87079700 | 12.31507600 |
| H | 8.25763400 | 11.39586400 | 12.06722400 |
| H | 7.45927700 | 9.82188100 | 12.02924500 |
| H | 6.52833200 | 11.29816300 | 11.69963600 |

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|---|---|---|---|
| C | 8.12568800 | 10.29474800 | 14.61494600 |
| H | 8.03034600 | 10.48030700 | 15.68911900 |
| H | 8.11015200 | 9.21427800 | 14.44565000 |
| H | 9.10849900 | 10.66828200 | 14.30211400 |
| C | 7.10556300 | 12.51933400 | 14.17475400 |
| H | 6.48278500 | 13.13248500 | 13.51375600 |
| H | 6.79424700 | 12.67808700 | 15.21038100 |
| H | 8.13889400 | 12.87253300 | 14.07936900 |
| C | 2.69690800 | 11.96760100 | 11.97659300 |
| C | 4.86074300 | 7.37144400 | 11.71831500 |
| C | 4.14245200 | 7.34704300 | 10.36125400 |
| H | 4.27435700 | 6.36148600 | 9.90061200 |
| H | 3.06320400 | 7.51517200 | 10.46006600 |
| H | 4.54831500 | 8.09376300 | 9.66772000 |
| C | 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 | 13.85454300 | 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 | 11.44933900 |
| H | 1.05455800 | 11.00773800 | 13.05673500 |
| H | 0.55197400 | 11.89521100 | 11.60430600 |
| O | 5.98134200 | 8.10677000 | 14.32016900 |

**$(1_{Tol})_2$-$NH_2NH_2$** (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 | 4.69145900 | 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 |

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|---|---|---|---|
| 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 |
| N | 8.87829100 | 5.14750100 | 11.25178900 |
| N | 6.60988400 | 1.52910600 | 13.92757400 |
| 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 | 1.94000300 | 10.27961400 |
| H | 10.69945500 | 2.31259500 | 9.72795900 |
| C | 7.06806400 | 1.17079500 | 15.14407800 |
| H | 7.11946500 | 0.13118900 | 15.42849600 |
| C | 6.15245200 | -0.91168400 | 12.96684100 |
| C | 8.74384300 | 0.23538600 | 11.53290000 |
| H | 8.72754700 | -0.75205000 | 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 | 7.35396200 | 17.05545300 |
| 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 |
| H | 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 |

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|---|---|---|---|
| H | 7.69900500 | 5.46453300 | 7.46734800 |
| C | -3.13588000 | 4.14400500 | 18.19626200 |
| H | -4.14632900 | 4.00603900 | 17.81419100 |
| C | 5.45454000 | -1.33986200 | 14.11128500 |
| H | 5.10508600 | -0.60678900 | 14.83528200 |
| C | 3.10930200 | 1.28659500 | 10.89746300 |
| H | 2.16285800 | 1.03567000 | 10.44120000 |
| C | 2.63540000 | 10.47544800 | 14.21108500 |
| C | -2.08523500 | 4.33067700 | 17.29870600 |
| H | -2.32496500 | 4.36939700 | 16.23869800 |
| C | 1.79121600 | 11.12210900 | 13.28979700 |
| H | 1.20052100 | 10.53376700 | 12.59256200 |
| C | -0.33303700 | 8.71885200 | 16.81982700 |
| H | -1.03106700 | 9.40231800 | 17.29878200 |
| C | 9.86482100 | 0.67120000 | 10.83912800 |
| H | 10.73870400 | 0.03125600 | 10.73580000 |
| C | 2.54600700 | 8.54180900 | 11.68294900 |
| H | 2.71131600 | 9.58128800 | 11.44759700 |
| C | 3.97691000 | 0.44331700 | 11.56874800 |
| H | 3.91063600 | -0.61141600 | 11.78479100 |
| C | 10.22230100 | 6.00354900 | 8.53935900 |
| H | 9.93381800 | 6.79909300 | 9.22189400 |
| C | 6.15597600 | 8.01037100 | 15.61597000 |
| H | 7.17649500 | 8.17239000 | 15.93162800 |
| C | 1.63281500 | 12.50717000 | 13.26073600 |
| H | 0.96685300 | 12.95226300 | 12.52302300 |
| C | 5.27492500 | 8.94038200 | 15.08848300 |
| H | 5.41575500 | 9.98339900 | 14.85257300 |
| C | -2.91844000 | 4.14596500 | 19.57691600 |
| C | -0.56764900 | 4.56575300 | 19.11334200 |
| H | 0.41734300 | 4.79204200 | 19.51509600 |
| C | -0.04053400 | 2.67152200 | 13.66756100 |
| H | -0.42631600 | 1.85163500 | 13.07970500 |
| C | 5.51795400 | -3.67345200 | 13.43042300 |
| C | 2.29861900 | 13.33259000 | 14.17051100 |
| C | 9.50645200 | 6.49989700 | 12.89768900 |
| H | 10.06057400 | 7.20422100 | 13.50077700 |
| C | 7.43271800 | 2.31373700 | 15.83600600 |
| H | 7.83362200 | 2.38363900 | 16.83674800 |
| C | 10.87062400 | 4.10071200 | 6.64793700 |
| H | 11.09384400 | 3.34172000 | 5.89956800 |
| C | 2.32151200 | 7.45667100 | 10.85162200 |
| H | 2.23756300 | 7.45613500 | 9.77459500 |
| C | -1.61238200 | 4.38055400 | 20.01733200 |
| H | -1.40901600 | 4.43101100 | 21.08608100 |
| C | 3.24701600 | 11.32104000 | 15.15606000 |
| H | 3.83280400 | 10.89142300 | 15.96475400 |
| C | 11.02078500 | 6.34427900 | 7.44845300 |
| H | 11.36233500 | 7.37232200 | 7.33642600 |
| C | 5.15282300 | -2.68078500 | 14.34478700 |
| H | 4.61243200 | -2.95838800 | 15.24854500 |
| C | 11.37624300 | 5.39395700 | 6.48663400 |
| C | 6.46969900 | -1.91956000 | 12.03876300 |

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|---|---|---|---|
| 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 | 12.26256800 |
| 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 |

**$(1_{Tol})_2$-$NH_2NH_2$** (HS)

| | | | |
|---|---|---|---|
| Fe | 6.41219100 | 3.56015000 | 11.86086300 |
| Fe | 2.57717900 | 5.73407300 | 14.68420800 |
| N | 0.80281300 | 4.60669900 | 14.06425900 |
| N | 7.04367200 | 4.39389700 | 9.18201000 |
| N | 2.55056200 | 4.45919000 | 16.46476100 |
| N | 7.81320600 | 2.27407100 | 11.15512200 |
| N | 2.46772700 | 7.09267800 | 12.94016600 |
| N | -0.09929100 | 4.31231000 | 15.02837100 |
| N | 4.05126300 | 4.33021800 | 13.62258500 |
| N | 5.05704600 | 2.11090300 | 11.71313000 |
| N | 4.20275600 | 8.28685100 | 15.22802900 |
| N | 7.80098100 | 5.06501000 | 11.91140900 |
| N | 4.24988700 | 6.95467000 | 15.44282700 |
| N | 5.04810900 | 4.85307700 | 12.69321600 |
| N | 6.87049100 | 2.89344600 | 13.73689700 |
| N | 1.32301100 | 7.08272400 | 15.65904600 |
| N | 5.36155200 | 0.88291800 | 12.17567300 |
| N | 1.34343000 | 4.22374200 | 17.03008300 |
| N | 6.01335600 | 4.21926600 | 10.03444800 |
| N | 8.69233800 | 5.17420400 | 10.89853600 |
| N | 6.97546900 | 1.56709200 | 13.98501600 |

| | | | |
|---|---|---|---|
| N | 2.82402400 | 8.37531000 | 13.16730300 |
| C | 1.56474000 | 8.40862500 | 15.51059600 |
| C | 7.93847700 | 1.05170800 | 11.74137800 |
| C | -1.25008900 | 4.66644400 | 17.39911000 |
| C | 8.75946100 | 2.74022000 | 10.29979000 |
| C | 0.27734100 | 6.58422300 | 16.36021600 |
| C | 3.40794500 | 3.57838800 | 16.99353400 |
| H | 4.45198300 | 3.58381300 | 16.70500100 |
| C | 2.57083500 | 6.88886800 | 11.62086300 |
| 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 | 2.43532400 | 9.48820800 |
| C | 7.47960800 | 1.36761200 | 15.21891600 |
| H | 7.67981700 | 0.37019400 | 15.57838800 |
| C | 6.74959600 | -0.98129200 | 13.22858400 |
| C | 9.11528300 | 0.31773400 | 11.56632000 |
| H | 9.23321900 | -0.62460200 | 12.08961000 |
| C | 0.68350400 | 9.31799500 | 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 | 14.84956100 |
| H | 7.31371700 | 4.59611000 | 14.89204400 |
| C | -0.60646700 | 7.48479300 | 16.97000900 |
| H | -1.44936500 | 7.11209500 | 17.53989500 |
| C | 9.84927300 | 3.65305700 | 7.44000100 |
| H | 9.58966100 | 2.60954900 | 7.60042300 |
| C | 9.46074900 | 4.61710300 | 8.38780000 |
| C | 3.81338100 | 2.03610200 | 11.21707900 |
| H | 3.35261800 | 2.89258900 | 10.75016000 |
| C | 0.53288800 | 3.81295800 | 13.02229400 |
| H | 1.12100700 | 3.88512000 | 12.11660500 |
| C | 5.47639900 | 6.67352700 | 15.89761300 |
| H | 5.72353900 | 5.66216200 | 16.19137600 |
| C | 1.44311800 | 3.17946700 | 17.88016800 |
| H | 0.57577000 | 2.80903500 | 18.40438000 |
| C | 2.75749500 | 2.74073100 | 17.90275800 |
| H | 3.17533200 | 1.93651400 | 18.49088900 |
| C | -0.90268000 | 3.31528600 | 14.60126900 |
| H | -1.66922300 | 2.90985000 | 15.24352100 |
| C | 8.13399800 | 6.00237800 | 12.80980800 |
| H | 7.54569000 | 6.16479800 | 13.70196700 |
| C | 9.60389700 | 6.12371300 | 11.18874400 |
| H | 10.42581300 | 6.32137100 | 10.51860100 |
| C | 6.58421700 | 4.84766700 | 7.99527000 |
| H | 7.26513600 | 5.04709500 | 7.18296200 |
| C | -3.68697100 | 4.55116000 | 17.68081900 |
| H | -4.67368400 | 4.55299100 | 17.21986200 |
| C | 6.17215100 | -1.40134100 | 14.44115600 |
| H | 5.78360400 | -0.66187000 | 15.13803200 |
| C | 3.30082700 | 0.74398700 | 11.36200800 |

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|---|---|---|---|
| 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 | 11.07468900 | 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 | 9.75552400 | 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 | -3.57868000 | 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 | 15.82329100 |
| 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 | 10.68000100 | 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 |

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|---|---|---|---|
| H | 1.89807800 | 15.34030700 | 14.52848400 |
| C | -4.79534200 | 4.28901700 | 19.94366600 |
| H | -5.02249500 | 3.22833600 | 20.11715400 |
| H | -4.65043500 | 4.75310300 | 20.92553800 |
| H | -5.68226300 | 4.73904000 | 19.48427900 |
| B | 8.53305100 | 4.21556600 | 9.65716800 |
| C | 6.98229400 | -3.36032300 | 12.67332000 |
| H | 7.28560900 | -4.11845800 | 11.95285700 |
| B | 6.77483200 | 0.57513200 | 12.77893100 |
| B | 2.87393100 | 8.93341600 | 14.64982900 |
| C | 6.33863700 | -5.21124000 | 14.27797100 |
| H | 5.50722800 | -5.38551600 | 14.96968400 |
| H | 6.18352700 | -5.84200100 | 13.39577300 |
| H | 7.25274300 | -5.56574700 | 14.77317700 |
| B | 0.05022000 | 4.95263000 | 16.47214400 |
| C | 11.64141800 | 5.66990900 | 4.73866400 |
| H | 11.48014900 | 4.94029200 | 3.93762500 |
| H | 11.35893400 | 6.65816300 | 4.35911600 |
| H | 12.72069800 | 5.69700800 | 4.94099000 |
| H | 4.52112600 | 5.38303900 | 11.99399900 |
| H | 4.60328300 | 3.80607600 | 14.30516700 |
| H | 3.57389400 | 3.58474900 | 13.11064000 |
| H | 5.51976400 | 5.59177100 | 13.21918100 |

**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 | 18.68876300 |
| 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 | 10.86838000 | 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 | 19.09697700 |
| C | 3.38470400 | 14.51913800 | 20.66689500 |
| C | 2.30975000 | 13.96222700 | 21.38474600 |
| H | 1.97032000 | 12.95598900 | 21.14879400 |
| C | 1.67650000 | 14.63652100 | 22.42704300 |

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|---|---|---|---|
| H | 0.84812100 | 14.15809600 | 22.94764700 |
| C | 2.09587200 | 15.90924100 | 22.82683400 |
| C | 3.19565200 | 16.45757700 | 22.16149800 |
| H | 3.57730200 | 17.42980600 | 22.46993700 |
| C | 3.82338800 | 15.77647500 | 21.11865500 |
| H | 4.70537900 | 16.23196000 | 20.67456300 |
| C | 1.39071000 | 16.65709100 | 23.92773200 |
| H | 0.97891700 | 15.97330600 | 24.67833000 |
| H | 2.06612500 | 17.35259000 | 24.43781700 |
| H | 0.55269200 | 17.24801200 | 23.53378400 |
| C | 5.32285500 | 12.73102100 | 20.29332300 |
| C | 5.59788000 | 12.87239200 | 21.65894500 |
| H | 5.02243200 | 13.58019000 | 22.24368100 |
| C | 6.61718800 | 12.13924200 | 22.24714500 |
| H | 6.86450000 | 12.27580000 | 23.29787800 |
| C | 7.31541200 | 11.22606000 | 21.46774700 |
| H | 8.12888200 | 10.65128400 | 21.89576800 |
| C | 6.99221000 | 11.05443200 | 20.11990600 |
| C | 4.95585700 | 8.94003600 | 17.14631300 |
| H | 4.05760900 | 9.22013200 | 16.61780700 |
| C | 5.41854500 | 7.66304300 | 17.48282800 |
| H | 4.96894600 | 6.70907600 | 17.24834500 |
| C | 6.57387300 | 7.89972800 | 18.20793800 |
| H | 7.26264500 | 7.21740900 | 18.68110700 |
| C | 8.66018300 | 12.81440900 | 16.95802900 |
| H | 8.29057700 | 13.63827400 | 16.36771600 |
| C | 9.96856300 | 12.55531400 | 17.37519700 |
| H | 10.86305800 | 13.11827700 | 17.15138300 |
| C | 9.85405100 | 11.42009500 | 18.16077200 |
| H | 10.59934800 | 10.87640400 | 18.72057800 |
| C | 8.80301400 | 8.93730800 | 19.79304600 |
| C | 9.89591800 | 8.41349700 | 19.07779400 |
| H | 10.12197400 | 8.79551300 | 18.08469800 |
| C | 10.69402300 | 7.38544300 | 19.57716300 |
| H | 11.52949900 | 7.01930100 | 18.98229100 |
| C | 10.43057100 | 6.80611400 | 20.82185100 |
| C | 9.31651000 | 7.27586800 | 21.52440700 |
| H | 9.05738400 | 6.82286000 | 22.48019200 |
| C | 8.52499100 | 8.30630100 | 21.01892200 |
| H | 7.64853900 | 8.60380700 | 21.58907800 |
| C | 11.31226000 | 5.72247100 | 21.38429700 |
| H | 11.79244100 | 5.14203100 | 20.58895500 |
| H | 12.11274900 | 6.14566500 | 22.00610300 |
| H | 10.74512100 | 5.02920300 | 22.01515900 |
| B | 4.19061200 | 13.65201300 | 19.56349300 |
| B | 7.81043400 | 10.03689800 | 19.13723100 |
| H | 5.85333000 | 12.68173500 | 15.06214200 |
| H | 4.74513400 | 11.54096900 | 15.17827500 |
| Fe | 6.53940300 | 10.82873700 | 12.76954800 |
| N | 8.57948100 | 10.76981600 | 12.72499800 |
| N | 9.19466300 | 9.94122000 | 11.84886600 |
| N | 6.67607800 | 8.81363800 | 12.73624700 |
| N | 7.46927100 | 8.21894300 | 11.81529700 |

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|---|---|---|---|
| N | 6.43753600 | 10.91776600 | 10.78655000 |
| N | 4.56128300 | 10.76312600 | 12.82306300 |
| N | 3.85866900 | 11.67361500 | 12.12209200 |
| N | 6.51043600 | 12.85385000 | 12.75260300 |
| N | 5.59355600 | 13.51883700 | 12.01258600 |
| N | 6.57054600 | 10.85279600 | 14.83616100 |
| C | 9.51551100 | 11.15262700 | 13.60477700 |
| H | 9.28352300 | 11.81907000 | 14.42398000 |
| C | 10.74741400 | 10.56294100 | 13.31168800 |
| H | 11.68377000 | 10.68140500 | 13.83702900 |
| C | 10.49017700 | 9.78826700 | 12.19458400 |
| H | 11.13556000 | 9.12809000 | 11.63658100 |
| C | 6.30846400 | 7.85687100 | 13.59824600 |
| H | 5.67875100 | 8.07562500 | 14.44873600 |
| C | 6.87056700 | 6.62707200 | 13.24632300 |
| H | 6.75712500 | 5.67577100 | 13.74523400 |
| C | 7.61293800 | 6.90988900 | 12.11428900 |
| H | 8.24512200 | 6.27440000 | 11.51404500 |
| C | 9.14968400 | 8.27254600 | 9.76005900 |
| C | 8.60735800 | 7.12838000 | 9.14605200 |
| H | 7.62597600 | 6.76987600 | 9.44907100 |
| C | 9.26260800 | 6.44628400 | 8.12223300 |
| H | 8.79644700 | 5.56492100 | 7.68413700 |
| C | 10.49906300 | 6.88246600 | 7.63665200 |
| C | 11.02988200 | 8.04776400 | 8.19693700 |
| H | 11.97171400 | 8.44267600 | 7.81866300 |
| C | 10.36846400 | 8.72346600 | 9.22186300 |
| H | 10.80598500 | 9.65238800 | 9.58002700 |
| C | 11.22819700 | 6.12812300 | 6.55595800 |
| H | 11.83908300 | 6.79759600 | 5.94039600 |
| H | 11.90316300 | 5.37410500 | 6.98314600 |
| H | 10.53212100 | 5.60125800 | 5.89401900 |
| C | 7.31492900 | 10.17808100 | 10.06653200 |
| C | 7.39057300 | 10.35295900 | 8.67947000 |
| H | 8.09136300 | 9.75516700 | 8.10885300 |
| C | 6.60165300 | 11.30341900 | 8.04954400 |
| H | 6.68647800 | 11.47424000 | 6.97834500 |
| C | 5.69964000 | 12.03167800 | 8.81413500 |
| H | 5.08028100 | 12.79272500 | 8.35303300 |
| C | 5.59416900 | 11.80565500 | 10.18840000 |
| C | 3.66956600 | 9.96787700 | 13.43080100 |
| H | 3.99722500 | 9.12676100 | 14.02198300 |
| C | 2.36549400 | 10.37280000 | 13.12550200 |
| H | 1.43673500 | 9.92807000 | 13.45232700 |
| C | 2.53495600 | 11.46060500 | 12.28625000 |
| H | 1.81152000 | 12.08945200 | 11.79141100 |
| C | 7.40994700 | 13.76299000 | 13.15706800 |
| H | 8.26502500 | 13.46200400 | 13.74214600 |
| C | 7.08701600 | 15.03021600 | 12.66384400 |
| H | 7.62173000 | 15.95776900 | 12.80818400 |
| C | 5.93298800 | 14.82137800 | 11.92624300 |
| H | 5.34425700 | 15.50624100 | 11.33570100 |
| C | 3.42850900 | 13.55583400 | 10.45626500 |

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|---|---|---|---|
| C | 2.88875100 | 14.69749300 | 11.07632500 |
| H | 3.30324500 | 15.04398300 | 12.02040300 |
| C | 1.80218000 | 15.39296800 | 10.54720900 |
| H | 1.42494600 | 16.27228700 | 11.06717400 |
| C | 1.17766400 | 14.97082600 | 9.36979300 |
| C | 1.66713700 | 13.80852200 | 8.76581400 |
| H | 1.18264800 | 13.42813500 | 7.86779500 |
| C | 2.75623100 | 13.12147200 | 9.29919700 |
| H | 3.06883400 | 12.20193500 | 8.81074800 |
| C | 0.02613900 | 15.73778800 | 8.77492600 |
| H | -0.65530600 | 15.07826400 | 8.22638300 |
| H | -0.55259900 | 16.25726700 | 9.54657100 |
| H | 0.38009200 | 16.49941900 | 8.06701900 |
| B | 8.30033500 | 9.13062000 | 10.83779700 |
| B | 4.59086800 | 12.66506900 | 11.14886900 |
| H | 6.35305500 | 9.94429100 | 15.25195200 |
| H | 7.49160800 | 11.05839800 | 15.22926800 |

**TSA**

| | | | |
|---|---|---|---|
| Fe | 5.44756200 | 11.83367500 | 17.73680600 |
| N | 3.70386800 | 12.92387300 | 17.80433100 |
| N | 2.84564600 | 12.76691500 | 18.83803000 |
| N | 4.27216400 | 10.30662500 | 18.27279400 |
| N | 3.39523400 | 10.43335200 | 19.29337700 |
| N | 5.80123700 | 12.32032700 | 19.65577000 |
| N | 7.08114400 | 10.72614600 | 17.77330000 |
| N | 8.21957200 | 11.24646300 | 18.27313700 |
| N | 6.57356500 | 13.43422800 | 17.21293700 |
| N | 7.75065000 | 13.68474400 | 17.82648100 |
| 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 | 16.71664200 |
| 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 | 2.55008500 | 9.37992600 | 19.29646600 |
| H | 1.74980900 | 9.31809100 | 20.01745400 |
| C | 2.24908000 | 11.79251800 | 21.25968700 |
| C | 2.18680800 | 10.68322900 | 22.12377100 |
| H | 2.80145200 | 9.80904000 | 21.92026200 |
| C | 1.38984800 | 10.66832900 | 23.26686700 |
| H | 1.37900800 | 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 |

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|---|---|---|---|
| C | -0.27787700 | 11.75022500 | 24.83670100 |
| H | 0.13807100 | 11.11823900 | 25.62926800 |
| H | -0.42677300 | 12.75458700 | 25.24804200 |
| H | -1.27069000 | 11.34946000 | 24.59082600 |
| C | 4.75689300 | 12.32968100 | 20.52012300 |
| C | 4.93675800 | 12.82447900 | 21.81699300 |
| H | 4.09933400 | 12.82204100 | 22.50445300 |
| C | 6.16219500 | 13.34545200 | 22.20404800 |
| H | 6.29504500 | 13.77575700 | 23.19460400 |
| C | 7.21663400 | 13.30175800 | 21.30240300 |
| H | 8.18455400 | 13.70998300 | 21.57057600 |
| C | 7.03964400 | 12.74276000 | 20.03461100 |
| C | 7.35410100 | 9.47256600 | 17.39926900 |
| H | 6.59128100 | 8.85110100 | 16.96073600 |
| C | 8.69545300 | 9.16924600 | 17.65294700 |
| H | 9.21317100 | 8.23806900 | 17.47278200 |
| C | 9.20724300 | 10.32930000 | 18.21186600 |
| H | 10.19635900 | 10.56137700 | 18.57462800 |
| C | 6.30188000 | 14.50033300 | 16.45132300 |
| H | 5.40641100 | 14.53882900 | 15.85135000 |
| C | 7.29598100 | 15.47221900 | 16.59035200 |
| H | 7.35099800 | 16.44100400 | 16.11558000 |
| C | 8.19060800 | 14.91393300 | 17.48786000 |
| H | 9.09717800 | 15.31357800 | 17.91520600 |
| C | 9.75603200 | 12.93232000 | 19.41763800 |
| C | 10.75322100 | 13.41676600 | 18.55129800 |
| H | 10.49223900 | 13.69156000 | 17.53212300 |
| C | 12.08951300 | 13.52618300 | 18.93386600 |
| H | 12.81976700 | 13.91184300 | 18.22368200 |
| C | 12.51125900 | 13.13597000 | 20.20834100 |
| C | 11.54542900 | 12.60094300 | 21.06599300 |
| H | 11.84236500 | 12.25008900 | 22.05327700 |
| C | 10.21093900 | 12.49804800 | 20.67608100 |
| H | 9.51125600 | 12.03626300 | 21.36818100 |
| C | 13.94583400 | 13.28864900 | 20.64085400 |
| H | 14.63338100 | 13.20371500 | 19.79205200 |
| H | 14.11913600 | 14.27067700 | 21.10149100 |
| H | 14.22538800 | 12.53048000 | 21.38064100 |
| B | 3.28793900 | 11.82734700 | 20.01945100 |
| B | 8.23260100 | 12.67410700 | 18.92418000 |
| H | 5.42557300 | 12.26481900 | 15.24022700 |
| H | 4.08161300 | 11.42966100 | 15.65033100 |
| Fe | 6.14758400 | 10.06887000 | 12.63056700 |
| N | 7.32658100 | 8.40730100 | 12.55189700 |
| N | 7.20970200 | 7.50995700 | 11.54716700 |
| N | 4.68906000 | 8.82406500 | 12.06349100 |
| N | 4.86457200 | 7.95388700 | 11.04490000 |
| N | 6.69137400 | 10.41337800 | 10.67439100 |
| N | 4.99440100 | 11.63340000 | 12.45342400 |
| N | 5.50096500 | 12.78527600 | 11.96934000 |
| N | 7.62497300 | 11.30058300 | 13.21832200 |
| N | 7.92168600 | 12.42925800 | 12.53780100 |
| N | 5.89159500 | 9.71807200 | 14.33636900 |

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|---|---|---|---|
| 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 | 5.50130500 | 11.24800700 |
| C | 3.53650100 | 8.49954900 | 12.66360000 |
| H | 3.18916200 | 9.04897800 | 13.52693600 |
| C | 2.94917400 | 7.40149000 | 12.03242700 |
| H | 2.01837300 | 6.91167400 | 12.27822600 |
| C | 3.83680700 | 7.07958800 | 11.01988700 |
| H | 3.81441800 | 6.27883100 | 10.29725100 |
| C | 6.29389600 | 6.82351000 | 9.12042200 |
| C | 5.20938000 | 6.73186200 | 8.22782600 |
| H | 4.32075700 | 7.33621400 | 8.39746600 |
| C | 5.23752000 | 5.91857200 | 7.09665600 |
| H | 4.36872800 | 5.88504200 | 6.44100000 |
| C | 6.36656900 | 5.15641600 | 6.78080800 |
| C | 7.47382200 | 5.27543300 | 7.62501100 |
| H | 8.38634600 | 4.72953600 | 7.39034000 |
| C | 7.43783000 | 6.09185600 | 8.75514900 |
| H | 8.34949300 | 6.18537600 | 9.33973600 |
| C | 6.38769800 | 4.24585300 | 5.58144400 |
| H | 7.40241000 | 4.12367100 | 5.18719900 |
| H | 6.01580300 | 3.24434600 | 5.83676700 |
| H | 5.75457500 | 4.62972100 | 4.77396000 |
| C | 6.74502700 | 9.35689300 | 9.82803300 |
| C | 7.27939000 | 9.52668900 | 8.54578200 |
| H | 7.31089700 | 8.68044200 | 7.87007700 |
| C | 7.79859000 | 10.75389900 | 8.16153700 |
| H | 8.26097600 | 10.87915300 | 7.18470000 |
| C | 7.71148700 | 11.82000800 | 9.04620600 |
| H | 8.11598200 | 12.79011000 | 8.78062000 |
| C | 7.10883500 | 11.65107400 | 10.29451400 |
| C | 3.70837100 | 11.85473300 | 12.75229400 |
| H | 3.09018000 | 11.06651800 | 13.14974300 |
| C | 3.37035200 | 13.17772100 | 12.46540100 |
| H | 2.41130700 | 13.65888600 | 12.59014700 |
| C | 4.54036400 | 13.73028600 | 11.96548100 |
| H | 4.75257000 | 14.72335100 | 11.60101500 |
| C | 8.58599900 | 11.12578300 | 14.13184100 |
| H | 8.52887300 | 10.31753200 | 14.84341800 |
| C | 9.54986100 | 12.12991100 | 14.01635000 |
| H | 10.44324300 | 12.25986600 | 14.60888100 |
| C | 9.09123200 | 12.93068200 | 12.98280800 |
| H | 9.51562800 | 13.81813900 | 12.53904300 |
| C | 7.17710300 | 14.37952500 | 10.87986200 |
| C | 7.56874900 | 15.40586900 | 11.75941400 |
| H | 7.79888800 | 15.16990100 | 12.79554900 |
| C | 7.63632500 | 16.74145800 | 11.36541500 |
| H | 7.94915900 | 17.49595400 | 12.08571600 |
| C | 7.29573200 | 17.13189500 | 10.06687000 |
| C | 6.85326500 | 16.13380900 | 9.19342900 |

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|---|---|---|---|
| H | 6.54310800 | 16.40403100 | 8.18517700 |
| C | 6.79139100 | 14.80001300 | 9.59388800 |
| H | 6.40097700 | 14.07307500 | 8.88604300 |
| C | 7.40375500 | 18.56788700 | 9.62625200 |
| H | 6.66980800 | 18.80638400 | 8.84875000 |
| H | 7.24828500 | 19.25797100 | 10.46275600 |
| H | 8.39783500 | 18.78094500 | 9.21057100 |
| B | 6.27448900 | 7.88276300 | 10.34127500 |
| B | 6.96351300 | 12.85449200 | 11.38090300 |
| H | 5.27932300 | 8.90727400 | 14.50083500 |
| H | 5.74349700 | 10.49556300 | 15.18099500 |

**IRCA'** (after **TSA**)

| | | | |
|---|---|---|---|
| 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 | 3.27388500 | 11.23750500 | 19.13248600 |
| N | 6.03675700 | 12.35707400 | 19.87715200 |
| N | 7.03810800 | 10.76939800 | 17.80418800 |
| N | 8.22025700 | 10.89006300 | 18.43985900 |
| N | 7.26857800 | 13.56117600 | 17.67666500 |
| N | 8.41584600 | 13.40187800 | 18.37395300 |
| N | 5.47029100 | 12.19533100 | 15.88336000 |
| C | 3.93270600 | 14.64629200 | 17.12446200 |
| H | 4.53684000 | 14.87410000 | 16.25811000 |
| C | 2.69197600 | 15.18224800 | 17.48107500 |
| H | 2.11873300 | 15.93989500 | 16.96651500 |
| C | 2.36647300 | 14.52035600 | 18.65257700 |
| H | 1.48552600 | 14.58600900 | 19.27175700 |
| C | 3.66629400 | 10.05978100 | 17.36435100 |
| H | 4.20172200 | 9.72556600 | 16.48681100 |
| C | 2.41141600 | 9.65481500 | 17.83212600 |
| H | 1.75680000 | 8.89996400 | 17.42046800 |
| C | 2.19678900 | 10.44268800 | 18.94925300 |
| H | 1.34780600 | 10.50189300 | 19.61253000 |
| C | 2.34058500 | 12.61932700 | 21.19683400 |
| C | 1.91050900 | 11.47943800 | 21.90095300 |
| H | 2.29192800 | 10.50025800 | 21.62002800 |
| C | 1.03399500 | 11.55357700 | 22.98220800 |
| H | 0.73241500 | 10.63816600 | 23.48950700 |
| C | 0.54684800 | 12.78275600 | 23.43663000 |
| C | 1.00490900 | 13.93149400 | 22.78531500 |
| H | 0.68029600 | 14.91038200 | 23.13566500 |
| C | 1.88169800 | 13.84826200 | 21.70414500 |
| H | 2.24266100 | 14.77809600 | 21.27112700 |
| C | -0.43152200 | 12.86607000 | 24.57885900 |
| H | -0.30358600 | 12.03364300 | 25.27971200 |
| 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 |

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|---|---|---|---|
| H | 4.28252500 | 12.94036100 | 22.67930400 |
| C | 6.42823800 | 12.90339700 | 22.56513200 |
| H | 6.58164500 | 13.14657000 | 23.61467800 |
| C | 7.50942500 | 12.68944000 | 21.72121700 |
| H | 8.52305000 | 12.77753000 | 22.09632200 |
| C | 7.30397200 | 12.37449600 | 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 | 18.24294000 |
| 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 | 17.39903600 |
| 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 | 13.33264300 | 12.22374700 | 19.08617500 |
| C | 12.64517600 | 11.25682000 | 20.88191600 |
| C | 11.49585500 | 10.87110700 | 21.57949800 |
| H | 11.59604100 | 10.30270300 | 22.50315400 |
| C | 10.22429000 | 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 | 4.91933900 | 8.40039800 | 11.80118100 |
| N | 5.37338600 | 7.55267400 | 10.85268700 |
| N | 6.42362600 | 10.37001700 | 10.45291400 |
| N | 4.52989300 | 11.20843200 | 12.43839400 |
| N | 4.63946800 | 12.37447900 | 11.77670100 |
| N | 7.18937400 | 11.49140400 | 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 |

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|---|---|---|---|
| C | 3.79398100 | 7.87560800 | 12.30204300 |
| H | 3.25539100 | 8.38166500 | 13.08769800 |
| C | 3.50873300 | 6.66221300 | 11.67713300 |
| H | 2.67327400 | 6.00199800 | 11.85780300 |
| C | 4.54674900 | 6.49108000 | 10.77514800 |
| H | 4.75752400 | 5.67992300 | 10.09605400 |
| C | 7.14654900 | 6.78042000 | 9.02701300 |
| C | 6.17338300 | 6.36628600 | 8.09819800 |
| H | 5.14519500 | 6.70315000 | 8.20843300 |
| C | 6.47978400 | 5.56664100 | 6.99894400 |
| H | 5.68560000 | 5.27406800 | 6.31387100 |
| C | 7.79045900 | 5.14737600 | 6.75086400 |
| C | 8.78096600 | 5.59746700 | 7.62789400 |
| H | 9.82012500 | 5.32900200 | 7.44444000 |
| C | 8.46590200 | 6.39681600 | 8.72646600 |
| H | 9.28828000 | 6.76052600 | 9.33750400 |
| C | 8.11972600 | 4.25043600 | 5.58696600 |
| H | 9.14934800 | 4.39859700 | 5.24390800 |
| H | 8.01754700 | 3.19180300 | 5.86123300 |
| H | 7.45042900 | 4.43053600 | 4.73853500 |
| C | 6.83342900 | 9.35409700 | 9.65589500 |
| C | 7.32066900 | 9.63523100 | 8.37460700 |
| H | 7.64335900 | 8.81875300 | 7.73978200 |
| C | 7.41580300 | 10.94779800 | 7.93557200 |
| H | 7.82996700 | 11.17543600 | 6.95562900 |
| C | 6.97264800 | 11.96410800 | 8.77042200 |
| H | 7.04698200 | 13.00127200 | 8.46403400 |
| C | 6.44354600 | 11.65874100 | 10.02651400 |
| C | 3.33525700 | 11.19332800 | 13.03739300 |
| H | 3.05150100 | 10.37056400 | 13.67487200 |
| C | 2.63726700 | 12.36621400 | 12.74063400 |
| H | 1.64721600 | 12.64895200 | 13.06700900 |
| C | 3.50649300 | 13.08974000 | 11.94006900 |
| H | 3.40336000 | 14.06195200 | 11.48385100 |
| C | 8.24326900 | 11.59700300 | 13.71856400 |
| H | 8.49547100 | 10.80264000 | 14.40254300 |
| C | 8.86362200 | 12.83458600 | 13.54636600 |
| H | 9.72957700 | 13.21852700 | 14.06465600 |
| C | 8.10409700 | 13.46620400 | 12.57302900 |
| H | 8.22543800 | 14.43115600 | 12.10601900 |
| C | 5.77921900 | 14.30358100 | 10.55241900 |
| C | 5.94540800 | 15.44008300 | 11.36487100 |
| H | 6.29253800 | 15.32648000 | 12.38902000 |
| C | 5.64203800 | 16.72656400 | 10.92246400 |
| H | 5.79368100 | 17.57183300 | 11.59199600 |
| C | 5.13197400 | 16.94916100 | 9.63960300 |
| C | 4.90913400 | 15.82746700 | 8.83559100 |
| H | 4.47799600 | 15.95732100 | 7.84423500 |
| C | 5.21995700 | 14.54463000 | 9.28415800 |
| H | 4.99168100 | 13.70626600 | 8.63036100 |
| C | 4.83830600 | 18.34058300 | 9.14433700 |
| H | 4.05440100 | 18.33757700 | 8.37936800 |
| H | 4.51514600 | 18.99801200 | 9.95894200 |

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|---|---|---|---|
| H | 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)**

| | | | |
|---|---|---|---|
| Fe | 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 | 2.84133600 | 8.29733100 | 17.21188000 |
| H | 2.40620400 | 7.43333300 | 16.73152100 |
| C | 2.21682700 | 9.20860800 | 18.04889800 |
| H | 1.19155400 | 9.26840800 | 18.37908300 |
| C | 1.53842400 | 11.50952600 | 20.08763700 |
| C | 0.93733700 | 10.37430200 | 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 | 22.09979500 |
| 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 |

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|---|---|---|---|
| C | 7.54770900 | 8.75185200 | 17.42290000 |
| H | 7.06131300 | 8.56822900 | 16.47688000 |
| C | 8.61524200 | 8.07222200 | 18.01338600 |
| H | 9.13049200 | 7.19725700 | 17.64524300 |
| C | 8.87517200 | 8.78402200 | 19.17214200 |
| H | 9.62312500 | 8.64016000 | 19.93626100 |
| C | 7.53490500 | 13.68322800 | 17.79086800 |
| H | 6.97878900 | 14.02047500 | 16.93132500 |
| C | 8.55765600 | 14.31968300 | 18.49572300 |
| H | 8.98460000 | 15.29459500 | 18.31147200 |
| C | 8.90386900 | 13.41626700 | 19.48901500 |
| H | 9.62854300 | 13.49232300 | 20.28485300 |
| C | 9.21261200 | 10.78046000 | 21.28261200 |
| C | 10.53910100 | 11.14659800 | 20.99053300 |
| H | 10.76309300 | 11.66953500 | 20.06404600 |
| C | 11.60506000 | 10.82270200 | 21.82864400 |
| H | 12.61265800 | 11.13320900 | 21.55630200 |
| C | 11.40590900 | 10.09133900 | 23.00345100 |
| C | 10.10189700 | 9.67244800 | 23.28432900 |
| H | 9.91313400 | 9.06859500 | 24.17064400 |
| C | 9.04074800 | 10.00513000 | 22.44379900 |
| H | 8.05348500 | 9.62244800 | 22.69161900 |
| C | 12.54892100 | 9.77025000 | 23.92997500 |
| H | 12.67619600 | 10.55389400 | 24.68908200 |
| H | 12.38201600 | 8.82770500 | 24.46281600 |
| H | 13.49663000 | 9.68936600 | 23.38640500 |
| B | 2.96710600 | 11.42153000 | 19.33442900 |
| B | 7.98840800 | 11.02207400 | 20.25246800 |
| H | 5.60063500 | 10.45162800 | 15.64525100 |

**4**$_{\mathbf{Tol}}$ (LS)

| | | | |
|---|---|---|---|
| Fe | 6.21009400 | 3.52411400 | 12.15761000 |
| Fe | 2.81725200 | 5.91211200 | 14.55051900 |
| N | 1.24194600 | 5.06656200 | 13.59935900 |
| N | 6.43786400 | 4.13784900 | 9.34426800 |
| N | 2.57533400 | 4.50422500 | 15.98198500 |
| N | 7.61647800 | 2.27433700 | 11.33732200 |
| N | 3.08564600 | 7.28244900 | 13.09037200 |
| N | 0.17353900 | 4.63750300 | 14.30592400 |
| N | 4.01828100 | 4.67187000 | 13.71265600 |
| N | 4.94987400 | 2.00710200 | 12.39890300 |
| N | 4.41012400 | 8.17684300 | 15.54586100 |
| N | 7.45699200 | 5.11055900 | 11.88280200 |
| N | 4.31696700 | 6.82779100 | 15.53901400 |
| N | 5.00244100 | 4.76820700 | 12.92727400 |
| N | 7.00361700 | 3.01897800 | 13.96476100 |
| 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 | 10.76256400 |
| N | 7.23215200 | 1.72030800 | 14.27534000 |

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|---|---|---|---|
| N | 3.29405100 | 8.58015700 | 13.40695000 |
| C | 1.83537600 | 8.42553200 | 15.56501700 |
| C | 7.90875200 | 1.10546700 | 11.96709700 |
| C | -1.28859200 | 4.58902200 | 16.53921800 |
| C | 8.41223100 | 2.75013700 | 10.34320100 |
| C | 0.42264100 | 6.57249900 | 16.01007800 |
| C | 3.41691300 | 3.57756300 | 16.46259400 |
| H | 4.47603400 | 3.62364800 | 16.25452100 |
| C | 3.34021000 | 7.16237100 | 11.77877100 |
| H | 3.25225000 | 6.21168800 | 11.27597400 |
| C | 4.32920600 | 3.96048300 | 9.76674200 |
| H | 3.44453400 | 3.78541000 | 10.35698800 |
| C | 9.62145400 | 2.10953700 | 10.05555600 |
| H | 10.28267900 | 2.53984500 | 9.31169100 |
| C | 7.93043600 | 1.64245400 | 15.42573900 |
| H | 8.24703200 | 0.68688300 | 15.81425700 |
| C | 7.09181700 | -0.89039800 | 13.71469600 |
| C | 9.10728100 | 0.44394600 | 11.68187100 |
| H | 9.35944800 | -0.45484600 | 12.23356200 |
| C | 0.94549700 | 9.27435900 | 16.23054000 |
| H | 1.17536200 | 10.33105000 | 16.30006700 |
| C | 4.42935100 | 4.24557400 | 8.40271200 |
| H | 3.62921300 | 4.35428900 | 7.68514400 |
| C | 7.53767200 | 3.74787800 | 14.95225900 |
| H | 7.48654600 | 4.82297400 | 14.92783800 |
| C | -0.47232500 | 7.40831800 | 16.68522300 |
| H | -1.37034600 | 6.98171200 | 17.11623500 |
| C | 9.07921700 | 3.53145500 | 7.30292800 |
| H | 8.95457800 | 2.48306900 | 7.56244700 |
| C | 8.70231700 | 4.52413800 | 8.22579700 |
| C | 3.62704800 | 1.85892700 | 12.23600000 |
| H | 2.99979100 | 2.69101700 | 11.95611000 |
| C | 1.07810600 | 4.62695600 | 12.34647700 |
| H | 1.79808900 | 4.87375100 | 11.58267300 |
| C | 5.44495000 | 6.35825000 | 16.08248500 |
| H | 5.59384200 | 5.29790800 | 16.20373300 |
| C | 1.39960400 | 3.02102800 | 17.11989900 |
| H | 0.50293200 | 2.56698000 | 17.51175600 |
| C | 2.72050300 | 2.61422500 | 17.19589800 |
| H | 3.11971700 | 1.74825800 | 17.70321400 |
| C | -0.63180600 | 3.90220800 | 13.51274900 |
| H | -1.52254300 | 3.43971600 | 13.90816900 |
| C | 7.80315000 | 6.13638400 | 12.67401600 |
| H | 7.30442200 | 6.30661400 | 13.61788000 |
| C | 9.05475600 | 6.25462800 | 10.87567300 |
| H | 9.76769500 | 6.47025400 | 10.09517700 |
| C | 5.79076100 | 4.34940300 | 8.17787200 |
| H | 6.34268900 | 4.55809400 | 7.27489800 |
| C | -3.74389000 | 4.54347600 | 16.50747700 |
| H | -4.66550200 | 4.68705500 | 15.94530200 |
| C | 6.74725100 | -1.26990000 | 15.02488300 |
| H | 6.41854100 | -0.51426300 | 15.73497400 |
| C | 3.24416800 | 0.54340400 | 12.50604900 |

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|---|---|---|---|
| H | 2.25158000 | 0.12028500 | 12.46121700 |
| C | 3.33553000 | 10.59488800 | 15.14346100 |
| C | -2.51909800 | 4.75698000 | 15.87730500 |
| H | -2.53363300 | 5.10191700 | 14.84623800 |
| 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 | -0.08985000 | 12.85040300 |
| H | 4.61914700 | -1.10918300 | 13.14518900 |
| C | 8.80811000 | 5.84878900 | 7.76242400 |
| H | 8.45402200 | 6.66762200 | 8.38414100 |
| C | 6.30135500 | 7.40968300 | 16.42337500 |
| H | 7.27646400 | 7.35352500 | 16.88543200 |
| C | 2.70513800 | 12.87917000 | 14.49586100 |
| H | 2.21923300 | 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 | -1.38093600 | 4.26291300 | 17.90459500 |
| H | -0.47800200 | 4.20828600 | 18.50778300 |
| C | -0.09644100 | 3.87881100 | 12.23530900 |
| H | -0.49988800 | 3.39669300 | 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 | 3.83674600 | 6.03968000 |
| H | 9.85991500 | 3.02789600 | 5.36497700 |
| C | 3.73691700 | 8.38762300 | 11.23824400 |
| H | 4.00853400 | 8.60483300 | 10.21572000 |
| C | -2.60188500 | 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 | -2.59768900 | 15.44882200 |
| H | 6.49618900 | -2.83645100 | 16.47570100 |
| C | 9.73052600 | 5.16206900 | 5.61948500 |
| C | 7.39746200 | -1.94751600 | 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 |

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|---|---|---|---|
| H | 2.40638000 | 15.39589100 | 15.47555700 |
| C | -5.13048600 | 3.89332200 | 18.52517000 |
| H | -5.42824000 | 2.84243900 | 18.40848700 |
| H | -5.08233600 | 4.09877300 | 19.60015100 |
| H | -5.93269500 | 4.50581900 | 18.09894300 |
| B | 7.98317100 | 4.14736700 | 9.62981100 |
| C | 7.41657600 | -3.27857100 | 13.25324000 |
| H | 7.65957000 | -4.05909500 | 12.53380800 |
| B | 6.93401300 | 0.63035100 | 13.17927200 |
| B | 3.22251600 | 8.99613500 | 14.91973800 |
| C | 7.18153700 | -5.06236300 | 15.03553200 |
| H | 6.46869500 | -5.25518100 | 15.84477400 |
| H | 6.96266800 | -5.75796400 | 14.21802600 |
| H | 8.18063800 | -5.31359900 | 15.41656700 |
| B | 0.11960400 | 4.97540300 | 15.84212800 |
| C | 10.31584400 | 5.49672600 | 4.27289900 |
| H | 10.09395800 | 4.71928600 | 3.53355500 |
| H | 9.92932600 | 6.44798900 | 3.89091700 |
| H | 11.40897000 | 5.58925700 | 4.32784600 |
| H | 5.14315000 | 5.75427500 | 12.67320900 |
| H | 3.87041100 | 3.68072400 | 13.94194700 |

**4$_{Tol}$** (HS)

| | | | |
|---|---|---|---|
| Fe | 6.24087600 | 3.60611000 | 12.12147900 |
| Fe | 2.67432600 | 6.02954500 | 14.60844200 |
| N | 1.12437800 | 5.15650200 | 13.65273500 |
| N | 6.53819900 | 4.09520900 | 9.16117800 |
| N | 2.44877800 | 4.60117800 | 16.01601800 |
| N | 7.68768400 | 2.19556500 | 11.23986700 |
| N | 2.91059500 | 7.43103800 | 13.17997300 |
| N | 0.04737900 | 4.72795400 | 14.34589600 |
| N | 3.86406000 | 4.86096400 | 13.74747100 |
| N | 4.91508700 | 1.95319400 | 12.44572000 |
| N | 4.25646200 | 8.28727800 | 15.63180300 |
| N | 7.62043700 | 5.24561400 | 11.71025900 |
| N | 4.18298000 | 6.93801600 | 15.58098300 |
| N | 4.89790900 | 5.01414900 | 13.03899400 |
| N | 7.06592600 | 2.97860800 | 14.08459600 |
| N | 1.39749600 | 7.19192400 | 15.56164400 |
| N | 5.47460900 | 0.77517300 | 12.80501400 |
| N | 1.21613900 | 4.24302000 | 16.43904600 |
| N | 5.58495900 | 3.99317600 | 10.11204600 |
| N | 8.35581200 | 5.20109700 | 10.57452600 |
| N | 7.34056900 | 1.67178800 | 14.30120900 |
| N | 3.10724200 | 8.72529000 | 13.51875600 |
| C | 1.67530100 | 8.51369100 | 15.68478800 |
| C | 7.99385200 | 1.07681500 | 11.94518000 |
| C | -1.41881700 | 4.63211400 | 16.57141300 |
| C | 8.50436300 | 2.68313900 | 10.27025400 |
| C | 0.27235900 | 6.64275800 | 16.08356400 |
| C | 3.30204600 | 3.67680800 | 16.47882700 |
| H | 4.35903200 | 3.73698700 | 16.26464900 |

| | | | |
|---|---|---|---|
| C | 3.15679800 | 7.33488900 | 11.86518400 |
| H | 3.07751900 | 6.38983200 | 11.35089600 |
| C | 4.40299000 | 4.03972400 | 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 | 15.39672100 |
| H | 8.47314900 | 0.57964900 | 15.71593200 |
| C | 7.17798000 | -0.90994200 | 13.69415200 |
| C | 9.22651200 | 0.44828700 | 11.73069900 |
| H | 9.49621300 | -0.41822700 | 12.32499400 |
| C | 0.78161600 | 9.34082300 | 16.37189600 |
| H | 1.00665700 | 10.39641600 | 16.46878500 |
| C | 4.57669200 | 4.17009100 | 8.11217600 |
| H | 3.81930000 | 4.23105300 | 7.34413800 |
| C | 7.65334200 | 3.66715100 | 15.06979400 |
| H | 7.56995000 | 4.74423300 | 15.09959000 |
| 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 | 12.19893400 |
| H | 2.96408200 | 2.52250300 | 11.89486800 |
| C | 1.00147800 | 4.67781700 | 12.40894800 |
| H | 1.74420000 | 4.90272300 | 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 | 17.52574400 |
| C | 2.61845700 | 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 | 10.65900700 |
| 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 | -0.37686900 | 8.81342100 | 16.92388200 |
| H | -1.07483900 | 9.45140800 | 17.46193200 |

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|---|---|---|---|
| C | 10.11833500 | 0.96290200 | 10.79866200 |
| H | 11.09354200 | 0.50182100 | 10.65425800 |
| C | 3.50081800 | 9.42467700 | 12.43471300 |
| H | 3.74304600 | 10.47299200 | 12.51308200 |
| C | 4.53146700 | -0.19082700 | 12.77769000 |
| H | 4.77881100 | -1.20877800 | 13.03463900 |
| C | 8.96406200 | 5.67632200 | 7.58225800 |
| H | 8.60510200 | 6.51948400 | 8.16847800 |
| C | 6.19767300 | 7.51893800 | 16.39274300 |
| H | 7.19332100 | 7.46229000 | 16.80851700 |
| C | 2.51058600 | 12.99753600 | 14.71136300 |
| H | 2.01331000 | 13.66937800 | 14.01330300 |
| C | 5.46631800 | 8.65815500 | 16.09567100 |
| H | 5.73207100 | 9.70082300 | 16.17207900 |
| C | -3.94233600 | 4.15290100 | 17.86106300 |
| C | -1.51402700 | 4.28354700 | 17.93078100 |
| H | -0.61373700 | 4.23144000 | 18.53820700 |
| C | -0.16039400 | 3.91197000 | 12.28938000 |
| H | -0.53511600 | 3.40058500 | 11.41469200 |
| C | 7.23255100 | -3.65033000 | 14.54657300 |
| C | 3.10256200 | 13.52037100 | 15.86514700 |
| C | 9.26502600 | 6.76939700 | 11.86686900 |
| H | 9.90493900 | 7.55811800 | 12.23495000 |
| C | 8.33609500 | 2.80730800 | 15.93467500 |
| H | 8.90674200 | 3.05846900 | 16.81710700 |
| C | 9.77156200 | 3.59210600 | 5.96207100 |
| H | 10.06295700 | 2.75571500 | 5.32838200 |
| C | 3.53430800 | 8.57370600 | 11.34296800 |
| H | 3.79557200 | 8.81192100 | 10.32241600 |
| C | -2.73576100 | 4.04167600 | 18.55778800 |
| H | -2.75011200 | 3.77244500 | 19.61285000 |
| C | 3.69440000 | 11.24250300 | 16.48199200 |
| H | 4.10735600 | 10.58069300 | 17.23927900 |
| C | 9.50047800 | 5.93736100 | 6.32252800 |
| H | 9.57541600 | 6.96685200 | 5.97511900 |
| C | 6.85985700 | -2.62462000 | 15.42132600 |
| H | 6.58032000 | -2.86979200 | 16.44498900 |
| C | 9.92915200 | 4.89864600 | 5.49011200 |
| C | 7.51184800 | -1.95940400 | 12.82027200 |
| H | 7.73553400 | -1.73810100 | 11.77923600 |
| C | 3.67806000 | 12.60985200 | 16.75554600 |
| H | 4.11123500 | 12.97290500 | 17.68630300 |
| C | 3.11780500 | 15.00172500 | 16.13597300 |
| H | 3.17697100 | 15.21369800 | 17.20901200 |
| H | 3.98341100 | 15.48317500 | 15.66115800 |
| H | 2.22006900 | 15.49172700 | 15.74294100 |
| C | -5.26193500 | 3.85424300 | 18.52250700 |
| H | -5.55130700 | 2.80481400 | 18.37580500 |
| H | -5.21896500 | 4.03055600 | 19.60280400 |
| H | -6.06728100 | 4.47215100 | 18.11020600 |
| B | 8.08109400 | 4.06782400 | 9.49771000 |
| C | 7.54247900 | -3.29141300 | 13.23136100 |
| H | 7.80663900 | -4.06684200 | 12.51381400 |

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|---|---|---|---|
| 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 |
| B | -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**

| | | | |
|---|---|---|---|
| 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 | -3.77404100 | 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 |

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|---|---|---|---|
| C | -5.58414400 | 3.85198300 | 0.95053500 |
| C | -7.01977000 | 1.04402500 | 0.73704700 |
| H | -7.51360600 | 1.90474500 | 1.17361000 |
| C | 6.43766700 | -0.79207200 | 1.84131800 |
| H | 6.67718200 | -1.18402600 | 2.82251200 |
| C | -2.48967800 | -1.78427800 | -3.76602900 |
| H | -2.04934900 | -1.94904000 | -4.73842400 |
| C | -2.44409100 | 0.77807600 | 2.94288800 |
| H | -1.66058000 | 0.04472100 | 3.04506800 |
| C | 7.12795200 | 0.01571000 | -0.30872200 |
| H | 7.91022900 | 0.25830500 | -1.01780400 |
| C | -6.82153900 | -3.40546800 | -2.27332900 |
| H | -7.21826900 | -2.39747800 | -2.36999500 |
| C | -5.65333600 | -3.62177700 | -1.51976800 |
| C | -2.12165300 | 2.31649500 | -1.78987100 |
| H | -1.32587200 | 1.74600100 | -2.23833200 |
| C | 2.64773700 | -1.38187600 | -3.14275500 |
| H | 1.75138200 | -1.90451700 | -2.83337300 |
| C | 1.62120900 | 1.88023100 | 2.20053500 |
| H | 1.14795000 | 2.58627100 | 1.53035700 |
| C | 4.48978600 | 3.25781500 | -2.71780500 |
| H | 5.21873000 | 3.43593100 | -3.49368800 |
| C | 3.43677600 | 4.04423400 | -2.27681000 |
| H | 3.15477100 | 5.02654800 | -2.62776500 |
| C | 4.37105000 | -0.53976100 | -4.20859100 |
| H | 5.12786300 | -0.21388400 | -4.90549200 |
| C | -2.47608000 | -2.38372400 | 1.90069400 |
| H | -1.68013600 | -1.86429900 | 2.40906100 |
| C | -3.96867400 | -3.82712800 | 1.18822800 |
| H | -4.65090700 | -4.64482100 | 1.01482600 |
| C | -3.57979600 | -2.43042500 | -3.20733300 |
| H | -4.20707200 | -3.21865500 | -3.59318300 |
| C | 8.62309100 | 0.27988300 | -4.35565400 |
| H | 9.07631600 | -0.54052400 | -4.91042400 |
| C | -5.05448900 | 4.91029800 | 1.71139100 |
| H | -4.10129100 | 4.78557700 | 2.21965200 |
| C | -2.51207000 | 3.63276600 | -2.03970900 |
| H | -2.08958400 | 4.32575600 | -2.75238000 |
| C | 4.52348800 | -1.52327500 | 3.92376300 |
| C | 7.39377600 | 0.08426900 | -3.72800900 |
| H | 6.94262400 | -0.90349400 | -3.78860700 |
| C | 4.88528200 | -2.87254400 | 4.09036800 |
| H | 4.67689700 | -3.58585600 | 3.29620100 |
| C | 7.45248900 | -0.48646700 | 0.94443000 |
| H | 8.49398200 | -0.63855700 | 1.22152800 |
| C | -7.70954800 | -0.14577400 | 0.55203800 |
| H | -8.75356900 | -0.23412700 | 0.84500400 |
| C | 2.24333000 | -3.06924600 | 2.42929600 |
| H | 2.44403100 | -3.38465500 | 3.44196000 |
| C | -3.56619200 | 3.84877200 | -1.16758300 |
| H | -4.17715400 | 4.72208500 | -1.00067100 |
| C | -5.16269400 | -4.94020000 | -1.52843200 |
| H | -4.21724000 | -5.16831300 | -1.04213700 |

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|---|---|---|---|
| C | 1.44959200 | 1.72085300 | 3.58026500 |
| H | 0.80890100 | 2.28275500 | 4.24456400 |
| C | 5.54399800 | -3.33582500 | 5.22856100 |
| H | 5.79973600 | -4.39173200 | 5.30551300 |
| C | 2.30971500 | 0.68285800 | 3.90575800 |
| H | 2.50389100 | 0.20666200 | 4.85489900 |
| C | 9.29091500 | 1.50552700 | -4.27366400 |
| C | 7.46134900 | 2.30627000 | -2.88432100 |
| H | 7.06516600 | 3.10859700 | -2.26630000 |
| C | 3.24816800 | -1.32764600 | -4.40528200 |
| H | 2.92441000 | -1.79747900 | -5.32296300 |
| C | -6.88102300 | 6.40757300 | 1.13052200 |
| C | 5.89504800 | -2.46697200 | 6.26594400 |
| C | -3.02126400 | -3.63660100 | 2.18180900 |
| H | -2.76345700 | -4.30664500 | 2.98870000 |
| C | -2.97598700 | 1.62407500 | 3.91626300 |
| H | -2.71669900 | 1.67672400 | 4.96341200 |
| C | -7.48503900 | -4.43701600 | -2.93531800 |
| H | -8.38552500 | -4.21433700 | -3.50559800 |
| C | 1.35913200 | -3.57540700 | 1.48885800 |
| H | 0.69850800 | -4.42435200 | 1.59092900 |
| C | 8.69100200 | 2.51031500 | -3.50931600 |
| H | 9.19852000 | 3.46659700 | -3.39039600 |
| C | 4.92922400 | -0.65837000 | 4.95650900 |
| H | 4.75539500 | 0.41106700 | 4.86056800 |
| C | -5.82397900 | -5.97873500 | -2.18252400 |
| H | -5.40244000 | -6.98231300 | -2.15488700 |
| C | -5.68629800 | 6.14900700 | 1.80924000 |
| H | -5.23457200 | 6.93336400 | 2.41457000 |
| C | -7.00966600 | -5.75121200 | -2.88742600 |
| C | -6.76129500 | 4.14763200 | 0.23955500 |
| H | -7.18756500 | 3.40084200 | -0.42616400 |
| C | 5.58831100 | -1.11336300 | 6.09770000 |
| H | 5.87980100 | -0.39944000 | 6.86690600 |
| C | 6.57314700 | -2.96806100 | 7.51417500 |
| H | 7.23038600 | -2.20618800 | 7.94782900 |
| H | 5.83904000 | -3.23940900 | 8.28513000 |
| H | 7.17624600 | -3.86041000 | 7.31340400 |
| C | 10.60034100 | 1.73396000 | -4.98221100 |
| H | 10.44089200 | 2.09708500 | -6.00669100 |
| H | 11.21187800 | 2.48172100 | -4.46533300 |
| H | 11.18494400 | 0.81004700 | -5.05444400 |
| B | -4.82757800 | -2.38283200 | -0.88555600 |
| C | -7.39638500 | 5.38532200 | 0.32777500 |
| H | -8.30550700 | 5.56160900 | -0.24498800 |
| B | -4.78558400 | 2.46388100 | 0.71564700 |
| B | 3.88440400 | -0.97005000 | 2.53912600 |
| C | -7.58592000 | 7.73186100 | 1.26132700 |
| H | -6.88033200 | 8.54452500 | 1.46542500 |
| H | -8.13982700 | 7.98413500 | 0.35053600 |
| H | -8.30976900 | 7.71528400 | 2.08723500 |
| B | 5.39357500 | 0.81621700 | -2.15152800 |
| C | -7.74710500 | -6.87603600 | -3.56468600 |

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|---|---|---|---|
| H | -8.26893500 | -6.53095000 | -4.46399200 |
| H | -7.06765800 | -7.68442000 | -3.85570300 |
| H | -8.50352800 | -7.31134100 | -2.89785800 |
| H | -0.66012000 | -1.00269500 | 0.24420000 |
| H | 0.62894700 | 1.44226200 | -0.96998800 |
| H | 0.70095600 | 0.05646100 | -1.80503300 |
| H | -0.66552700 | 0.51414300 | 0.88982500 |

[**Fe(II)NH(·)-$NH_2$-Fe(II)]** (LS)

| | | | |
|---|---|---|---|
| Fe | -0.10584700 | 0.24000900 | 0.22300600 |
| Fe | -0.03729700 | -0.29181800 | 5.08400200 |
| N | 1.87506400 | -0.82607600 | 5.44764000 |
| N | 0.75546000 | -2.17472500 | -1.09487300 |
| N | 0.60237700 | 1.58372900 | 5.43456500 |
| N | 0.12624800 | 0.68318600 | -1.75144400 |
| N | -0.65240200 | -2.16870900 | 4.72485400 |
| N | 2.57431300 | -0.27114800 | 6.46251900 |
| N | 0.32609100 | -0.05308800 | 3.29073600 |
| N | 1.53972200 | 1.30524600 | 0.63198800 |
| N | -2.95307500 | -0.50122100 | 5.38655600 |
| N | -1.74729200 | -0.90130900 | -0.25903000 |
| N | -1.95153800 | 0.27526300 | 4.91671300 |
| N | -0.54450800 | -0.29112500 | 2.19175800 |
| N | -1.18230900 | 1.97193200 | 0.41949100 |
| N | -0.40846100 | -0.55768000 | 7.04720500 |
| N | 1.70112100 | 2.49403700 | 0.01412600 |
| N | 1.40116100 | 1.86862800 | 6.48834000 |
| N | 0.93160600 | -1.42562800 | 0.01087600 |
| N | -1.69751900 | -1.71982800 | -1.33636000 |
| N | -0.73307500 | 3.11499200 | -0.14963500 |
| N | -1.79917800 | -2.65261700 | 5.24772500 |
| C | -1.52933000 | -1.22937300 | 7.41100100 |
| C | 0.28924700 | 1.98075100 | -2.12499100 |
| C | 2.70580100 | 1.17679800 | 8.70530900 |
| C | -0.15180500 | -0.27715400 | -2.67256300 |
| C | 0.47401900 | -0.07888200 | 7.95616500 |
| C | 0.58287200 | 2.66967000 | 4.65029700 |
| H | 0.04102300 | 2.66807000 | 3.71686100 |
| C | -0.24295700 | -3.04178200 | 3.79540500 |
| H | 0.64791000 | -2.85274000 | 3.21745000 |
| C | 1.84560000 | -2.04847800 | 0.76161600 |
| H | 2.13311900 | -1.63111100 | 1.71346600 |
| C | -0.41095000 | 0.08534100 | -3.99862100 |
| H | -0.69763900 | -0.68142500 | -4.70990400 |
| C | -1.67942500 | 4.07243800 | -0.07280600 |
| H | -1.51867800 | 5.04398100 | -0.51382300 |
| C | 1.13589100 | 4.53260500 | -1.41528200 |
| C | 0.03169300 | 2.36128500 | -3.44580300 |
| H | 0.09572700 | 3.40945100 | -3.71647700 |
| C | -1.78382500 | -1.44538000 | 8.76809100 |
| H | -2.67663800 | -1.98588700 | 9.05883600 |

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|---|---|---|---|
| C | 2.28628600 | -3.21666900 | 0.13116500 |
| H | 3.02521300 | -3.92456400 | 0.47802600 |
| C | -2.40712000 | 2.24246000 | 0.88867700 |
| H | -2.97910600 | 1.48986100 | 1.40615100 |
| C | 0.22699700 | -0.27798000 | 9.31810600 |
| H | 0.93166400 | 0.10898100 | 10.04440700 |
| C | 0.50486400 | -2.89437700 | -4.39640600 |
| H | 1.08206200 | -1.98914100 | -4.56853800 |
| C | -0.32338600 | -2.98065000 | -3.26306300 |
| C | 2.64839900 | 1.09966800 | 1.35742400 |
| H | 2.76805300 | 0.20843200 | 1.95167200 |
| C | 2.74532100 | -1.50362700 | 4.69261800 |
| H | 2.40827600 | -2.03040200 | 3.81614500 |
| C | -2.51634300 | 1.27068600 | 4.22049100 |
| H | -1.91224000 | 2.03715900 | 3.76201500 |
| C | 1.89194300 | 3.11765400 | 6.35315900 |
| H | 2.58834800 | 3.51588500 | 7.07425700 |
| C | 1.37919100 | 3.67727100 | 5.19551900 |
| H | 1.56441500 | 4.66346300 | 4.79633500 |
| C | 3.88010800 | -0.57532700 | 6.32535900 |
| H | 4.61126200 | -0.18844600 | 7.01779200 |
| C | -2.99729700 | -0.98039100 | 0.21749000 |
| H | -3.28986900 | -0.44590900 | 1.10886700 |
| C | -2.91274500 | -2.25753800 | -1.56188300 |
| H | -3.08138400 | -2.90240600 | -2.41017200 |
| C | 1.56415900 | -3.25649000 | -1.04884400 |
| H | 1.56480300 | -3.97654900 | -1.85205700 |
| C | 4.31315800 | 0.69511500 | 10.49765700 |
| H | 5.01973300 | -0.00230800 | 10.94499900 |
| C | 0.97364000 | 5.67211400 | -0.60565300 |
| H | 0.42865000 | 5.59118700 | 0.33227400 |
| C | 3.54083100 | 2.16471800 | 1.21027300 |
| H | 4.51261100 | 2.28363200 | 1.66672900 |
| C | -3.84394100 | -2.48306500 | 6.94797600 |
| C | 3.62956800 | 0.32640900 | 9.34000100 |
| H | 3.80162200 | -0.67272100 | 8.94727400 |
| C | -3.81180100 | -3.84986900 | 7.28307100 |
| H | -2.93922400 | -4.44669200 | 7.02960400 |
| C | -0.90426300 | -0.96719900 | 9.72927400 |
| H | -1.09950700 | -1.12956200 | 10.78716000 |
| C | -0.34777200 | 1.41553800 | -4.38769200 |
| H | -0.58701700 | 1.70952800 | -5.40773000 |
| C | -2.12393100 | -3.80713200 | 4.63097900 |
| H | -3.03464200 | -4.32851900 | 4.88086700 |
| C | 2.89701400 | 3.02900500 | 0.34433700 |
| H | 3.20133100 | 3.98169100 | -0.05961800 |
| C | -0.95841200 | -4.22224000 | -3.07393200 |
| H | -1.54600700 | -4.39544500 | -2.17540000 |
| C | -3.90534600 | 1.12562500 | 4.21013100 |
| H | -4.63725800 | 1.76974700 | 3.74507200 |
| C | -4.84464200 | -4.47477400 | 7.97982700 |
| H | -4.76722800 | -5.53613200 | 8.21030600 |
| C | -4.13444200 | -0.02112400 | 4.95521400 |

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|---|---|---|---|
| H | -5.05567100 | -0.52751700 | 5.19658000 |
| C | 4.09784100 | 1.93705700 | 11.10201100 |
| C | 2.46097600 | 2.39682500 | 9.36216500 |
| H | 1.69266600 | 3.06774100 | 8.98497200 |
| C | 4.03583200 | -1.38127100 | 5.20888200 |
| H | 4.94952300 | -1.81055500 | 4.82458800 |
| C | 2.28479400 | 7.07581900 | -2.09660500 |
| C | -5.97032700 | -3.76098700 | 8.40128800 |
| C | -3.78150600 | -1.82065200 | -0.57582600 |
| H | -4.82489900 | -2.07178500 | -0.45210700 |
| C | -2.77303800 | 3.56066900 | 0.60464900 |
| H | -3.69820200 | 4.06375900 | 0.84599100 |
| C | 0.64246400 | -3.94283300 | -5.30498100 |
| H | 1.29820500 | -3.82148100 | -6.16598000 |
| C | -1.14329700 | -4.10416200 | 3.69865400 |
| H | -1.09211400 | -4.95749300 | 3.03863700 |
| C | 3.14033000 | 2.77292100 | 10.51988700 |
| H | 2.91249000 | 3.73097900 | 10.98461800 |
| C | -4.95622900 | -1.77212000 | 7.43446700 |
| H | -5.00783700 | -0.69354200 | 7.30755700 |
| C | -0.83099700 | -5.27412200 | -3.98000100 |
| H | -1.34730200 | -6.21334000 | -3.78606000 |
| C | 1.52102600 | 6.91052600 | -0.93712100 |
| H | 1.36179700 | 7.76132800 | -0.27597300 |
| C | -0.03880300 | -5.15028800 | -5.12540600 |
| C | 1.94608800 | 4.71015200 | -2.55104700 |
| H | 2.17518600 | 3.85612000 | -3.18367900 |
| C | -5.99374400 | -2.38985300 | 8.13128100 |
| H | -6.83150200 | -1.78935200 | 8.48244800 |
| C | -7.10785900 | -4.43942200 | 9.11770500 |
| H | -7.59643400 | -3.76317300 | 9.82777100 |
| H | -7.87690500 | -4.77674100 | 8.40977100 |
| H | -6.76620600 | -5.32161100 | 9.66982500 |
| C | 4.86464100 | 2.35696100 | 12.32811700 |
| H | 5.77874800 | 2.90202000 | 12.05648500 |
| H | 4.27058100 | 3.01981100 | 12.96682900 |
| H | 5.16934000 | 1.49214500 | 12.92744800 |
| B | -0.34788600 | -1.80286200 | -2.14667300 |
| C | 2.50180600 | 5.94384300 | -2.88777200 |
| H | 3.12271800 | 6.02544300 | -3.77876800 |
| B | 0.61484700 | 3.06582300 | -0.95647900 |
| B | -2.57386200 | -1.75076100 | 6.26713500 |
| C | 2.84627000 | 8.41987400 | -2.47995600 |
| H | 3.04927600 | 9.03739300 | -1.59795000 |
| H | 3.77911300 | 8.31948800 | -3.04561700 |
| H | 2.14238500 | 8.97846700 | -3.11176800 |
| B | 1.81594600 | 0.69457500 | 7.44512000 |
| C | 0.07260200 | -6.26994300 | -6.12671400 |
| H | 1.04657400 | -6.26512600 | -6.62840200 |
| H | -0.05920300 | -7.24872400 | -5.65234100 |
| H | -0.69483000 | -6.18198600 | -6.90771300 |
| H | -0.70518500 | -1.29818900 | 2.13373400 |
| H | 0.94530500 | 0.70828700 | 3.03171700 |

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|---|---|---|---|
| H | -1.46040700 | 0.10777400 | 2.41695600 |

**[Fe(II)NH(·)-$NH_2$-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 | -0.91027200 | -0.39343000 |
| N | -2.10257400 | 0.39772700 | 4.99656800 |
| N | -0.58009800 | -0.18383200 | 2.06056000 |
| N | -1.25095900 | 1.97913300 | 0.24865000 |
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| 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 | 3.78168600 |
| 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 |
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| 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 |
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| C | 2.25504000 | -3.17895700 | 0.19107100 |
| H | 2.97102800 | -3.88261500 | 0.59065900 |
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| 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 |

| | | | |
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| H | 1.23710200 | -2.02795800 | -4.58776200 |
| C | -0.20075300 | -3.02244500 | -3.32020100 |
| C | 2.60836600 | 1.17852200 | 1.20302200 |
| H | 2.75775000 | 0.27870100 | 1.77739700 |
| C | 2.93596600 | -1.46854700 | 4.76821900 |
| H | 2.62373800 | -2.00238300 | 3.88245500 |
| C | -2.70759400 | 1.31941000 | 4.23719900 |
| H | -2.12803400 | 2.09569300 | 3.75639300 |
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| H | 2.86874400 | 3.42222300 | 7.33271700 |
| C | 1.62116000 | 3.79716800 | 5.50801800 |
| H | 1.86051800 | 4.79837100 | 5.18086600 |
| C | 4.01166600 | -0.53102700 | 6.43506300 |
| H | 4.72002300 | -0.13349400 | 7.14555800 |
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| C | -2.84998300 | -2.31410700 | -1.69823600 |
| H | -2.98591700 | -2.97547300 | -2.53964000 |
| C | 1.59827500 | -3.23919600 | -1.02588100 |
| H | 1.63811100 | -3.97594200 | -1.81268900 |
| C | 4.34085200 | 0.43407500 | 10.66105500 |
| H | 5.02266500 | -0.30149200 | 11.08523700 |
| C | 0.83695300 | 5.70990100 | -0.80259200 |
| H | 0.28527500 | 5.63115800 | 0.13148400 |
| C | 3.47362300 | 2.26650600 | 1.06041400 |
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| C | -3.89310800 | -2.39271100 | 7.05297800 |
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| H | -3.03986000 | -4.38023900 | 7.07586500 |
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| H | -1.07106700 | -1.19828700 | 10.84954200 |
| C | -0.30477600 | 1.34771300 | -4.53843700 |
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| C | 2.80366700 | 3.12232200 | 0.20567200 |
| H | 3.08430900 | 4.08424700 | -0.19348400 |
| C | -0.82125800 | -4.27158800 | -3.13392500 |
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| C | -3.75079900 | -1.87949800 | -0.74043700 |
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| C | 3.21674100 | 2.53666800 | 10.76645400 |
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| C | 1.84830100 | 4.74158900 | -2.72462400 |
| H | 2.10209400 | 3.88418700 | -3.34295600 |
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| H | 4.31318300 | 2.65701700 | 13.23014200 |
| H | 5.13169300 | 1.08601100 | 13.16285100 |
| B | -0.28006300 | -1.82296500 | -2.23027400 |
| C | 2.38244700 | 5.98147400 | -3.07275700 |
| H | 3.01052300 | 6.06327500 | -3.95869400 |
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| H | 1.97537000 | 8.99740600 | -3.35723100 |
| B | 1.90065100 | 0.64351800 | 7.56763700 |
| C | 0.36350300 | -6.35260000 | -6.10732500 |
| H | 1.34564600 | -6.32270200 | -6.59171100 |
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