Supporting information

All reactions were carried out using standard Schlenk techniques under an atmosphere of nitrogen or in a nitrogen filled glove-box. Solvents were dried (Hexane, toluene, Et_2O and THF were passed through activated alumina towers,[1] dichloromethane was distilled from CaH_2), and stored over 4 Å molecular sieves. d_2-dichloromethane and d_5-pyridine were trap-to-trap distilled from activated Al_2O_3, d_8-THF was boiled with K under vacuum and trap-to-trap distilled. The compounds $Me_2C(C_4H_4N)_2$ (H_2[**L**]) and $Fe(THF)[N(SiMe_3)_2]_2$ were synthesised according to literature procedures;[2,3] all other reagents were used as purchased. The ^1H and ^2H NMR spectra were recorded on a Bruker DPX-300 spectrometer operating at 300.13 and 46.07 MHz respectively; residual protio-solvent served as an internal reference. Elemental analyses were carried out by Mr. Stephen Boyer at the London Metropolitan University. Solution magnetic moments were determined by Evan's method in $CD_2Cl_2/SiMe_4$ with a $CD_2Cl_2/SiMe_4$ insert.[4] Variable temperature magnetic susceptibilities were measured using a Quantum Design MPMS-XL 5T SQUID susceptometer operating at 1000 G in the temperature range 5 to 300 K. The sample was loaded in a gel capsule in a nitrogen-filled glovebox and suspended in a plastic straw. Diamagnetic contributions from the ligands were calculated from Pascal's constants.[5] The effective magnetic moments (μ_{eff}) were calculated using the expression $\mu_{eff} = 2.828(\chi T)^{1/2}$. Mössbauer spectra were recorded on an ES-Technology MS-105 spectrometer with a 875 MBq ^{57}Co source in a rhodium matrix at ambient temperature. Spectra were referenced to a 25 μm iron foil at 298 K and were fitted with Lorentzian lines. Errors are $\leq \pm 0.01$ mms^{-1} unless shown otherwise in parenthesis. Cyclic voltametry was carried out under nitrogen using an Autolab PGSTAT potentiostat. A standard three-electrode set-up was used, consisting of a Ag foil psuedo-reference electrode, a platinum wire auxiliary electrode and a platinum disk working electrode. The solute sample was 1.0 mM in freshly distilled CH_2Cl_2 and 0.4 M in $Bu^n{}_4N.BF_4$ supporting electrolyte. The potentials were referenced by the addition of ferrocene ($E_{1/2}$ = 0.438 V).

[1] A. B. Pangborn, M. A. Giardello, R. H. Grubbs, R. K. Rosen, and F. J. Timmers, *Organometallics*, 1998, **15**, 1518.

[2] B. J. Littler, M. A. Miller, C.-H. Hung, R. W. Wagner, D. F. O'Shea, P. D. Boyle, and J. S. Lindsey, *J. Org. Chem.*, 1999, **64**, 1391.

[3] M. M. Olmstead, P. P. Power, and S. C. Shoner, *Inorg. Chem.*, 1991, **30**, 2547.

[4] S. K. Sur, *J. Mag. Reson.*, 1989, **82**, 169; D. F. Evans, *J. Chem. Soc.*, 1959, 2003.

[5] F. E. Mabbs and D. J. Machin, 'Magnetism and Transition Metal Complexes', Chapman and Hall, 1973.

*Synthesis of {Fe[**L**]}$_4$ **1*** - A solution of H_2[**L**] (0.194 g, 0.0011 mol) in THF (20 mL) was added to a stirred solution of Fe(THF)[N(SiMe$_3$)$_2$]$_2$ (0.500 g, 0.0011 mol) in toluene (5 mL) in a teflon-tapped glass pressure vessel at room temperature. The resultant pale green solution was heated at 80 °C for 48 h (during which the colour changed to deep red then to orange), and then transferred into a Schlenk tube. Reduction of the solvent volume under vacuum and cooling to –35 °C for 16 h resulted in the deposition of **1** as bright orange needles. The liquors were decanted and the solids were washed at – 78 °C with cold (– 78 °C) THF (2 x 2 mL), and Et_2O (2 x 5 mL) and dried under vacuum, yielding **1** as an orange powder, 0.120 g, 47 %. Crystals suitable for X-ray diffraction were grown from the washings at –35 °C.

Analysis. Found: C, 58.15; H, 5.34; N, 12.28. $C_{11}H_{12}N_2Fe$ requires: C, 57.93; H, 5.30; N, 12.28 %

μ_{eff} (Evan's method, CD_2Cl_2): 7.15 μ_B

^{1}H NMR (CD_2Cl_2): δ_H 101.5 (vbr.s, 1H, pyrrole H), 65.05 (br.s, 1H, pyrrole H), 58.78 (br.s, 1H, pyrrole H), 43.23 (br.s, 1H, pyrrole H), 37.70 (br.s, 1H, pyrrole H), 11.85 (vbr.s, 1H, pyrrole H), 7.76 (br.s, 3H, *meso*-CH_3), -41.59 (br.s, 3H, *meso*-CH_3).

*Synthesis of {Fe[**L**]}$_n$ **2*** - A solution of H_2[**L**] (0.349 g, 0.0020 mol) in toluene (2 mL) was added to a stirred solution of Fe(THF)[N(SiMe$_3$)$_2$]$_2$ (0.900 g, 0.0020 mol) in toluene (10 mL) in a teflon-tapped glass pressure vessel at room temperature. The resultant pale green solution was heated at 80 °C for 48 h during which **2** was deposited as pale orange solids. The mixture was transferred into a Schlenk tube, the colourless liquors decanted and the solids washed with hexane (3 x 10 mL), yielding **2** as an orange powder, 0.31 g, 68 %.

Analysis. Found: C, 57.74; H, 5.13; N, 12.05. $C_{11}H_{12}N_2Fe$ requires: C, 57.93; H, 5.30; N, 12.28 %

Compound **2** was found to be insoluble in CH_2Cl_2 and THF, but dissolved slowly (15 min) in C_5D_5N to yield an orange solution.

^{1}H NMR (C_5D_5N): δ_H 99.5 (vbr.s, 2H), 46.3 (br.s, 2H), 37.8 (br.s, 2H), 5.25 (br.s, 6H)

*2,2'-$(C_5H_3NH)_2C(CD_3)_2$ H_2[**L**^{d6}]* was synthesised using a modification of a literature procedure[2] - Neat trifluoroacetic acid (0.46 g, 0.004 mol) was added to a stirred mixture of pyrrole (83.9 g, 1.25 mol) and d_6-acetone (3.21 g, 0.05 mol) at room temperature. After 5 min, the reaction mixture was quenched by adding aqueous NaOH (0.1 M, 50 mL) and then extracted with ethyl acetate (2 x 50 mL). The combined extracts were dried ($MgSO_4$) and the solvents removed under vacuum. The remaining beige oil was distilled using a Kugelröhr apparatus at 100 °C / 2.0 mbar, yielding 4.05 g, 45 % of H_2[**L**^{d6}] as a colourless oil that solidified on standing.

Analysis. Found: C, 74.31; H, 9.88; N, 15.54. $C_{11}H_{18}N_2$ requires: C, 74.11; H, 10.18; N, 15.71 %

^{1}H NMR ($CDCl_3$): δ_H 7.58 (br.s, 2H, NH), 6.58 (m, 2H, pyrrole H), 6.16 (m, 2H, pyrrole H), 6.12 (m, 2H, pyrrole H)

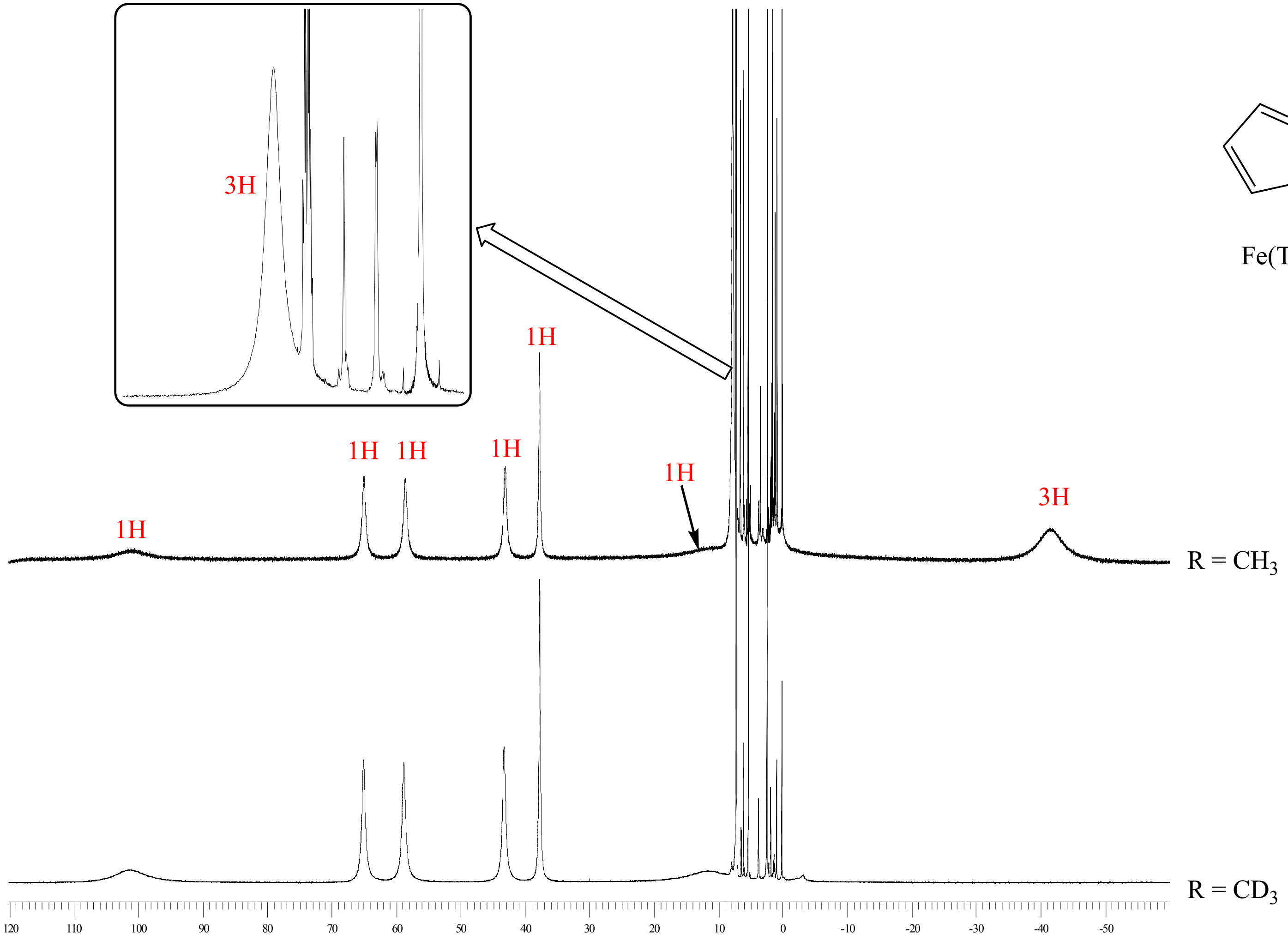
^{2}H NMR ($CDCl_3$): δ 1.63 (s, *meso*-CD_3)

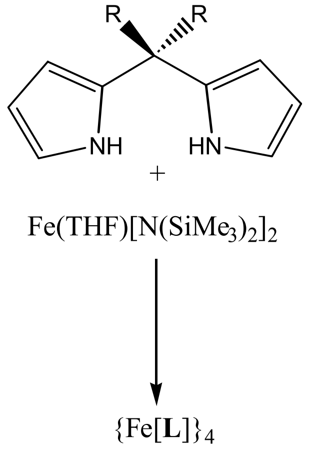
*Synthesis of {Fe[**L**^{d6}]}$_4$* – In a manner similar to **1**, equimolar amounts of Fe(THF)$[N(SiMe_3)_2]_2$ and H_2[**L**^{d6}] were reacted in a toluene/THF mixture (1:4) at 80 °C to yield {Fe[**L**^{d6}]}$_4$ as orange solids.

^{1}H NMR (CD_2Cl_2): δ_H 101.5 (vbr.s, 1H, pyrrole H), 65.05 (br.s, 1H, pyrrole H), 58.78 (br.s, 1H, pyrrole H), 43.23 (br.s, 1H, pyrrole H), 37.70 (br.s, 1H, pyrrole H), 11.85 (vbr.s, 1H, pyrrole H).

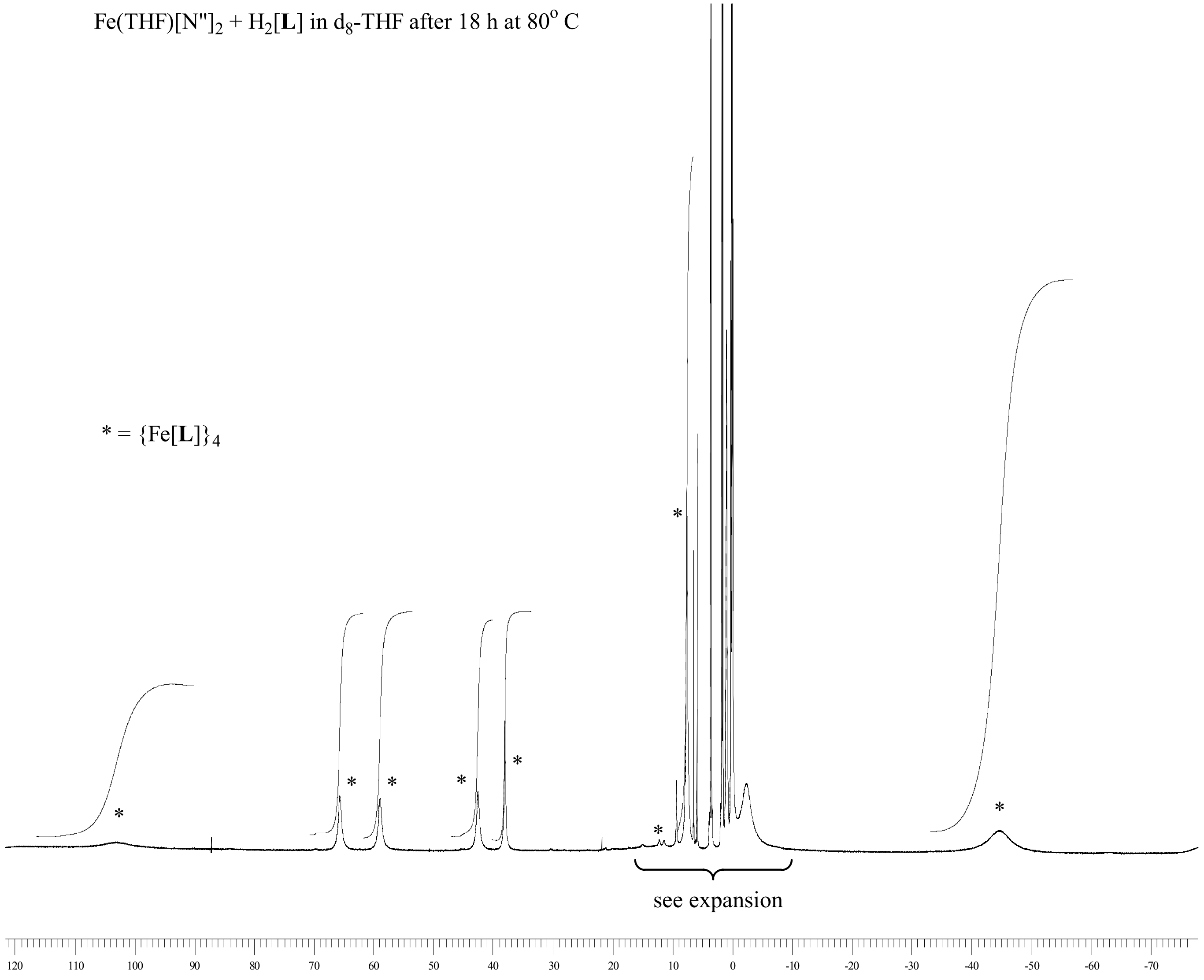
^{2}H NMR (CD_2Cl_2): δ 7.60 (br.s, 3H, *meso* CD_3), -41.1 (br.s, 3H, *meso*-CD_3).

Isolated $\{Fe[\mathbf{L}]\}_4$ in CD_2Cl_2

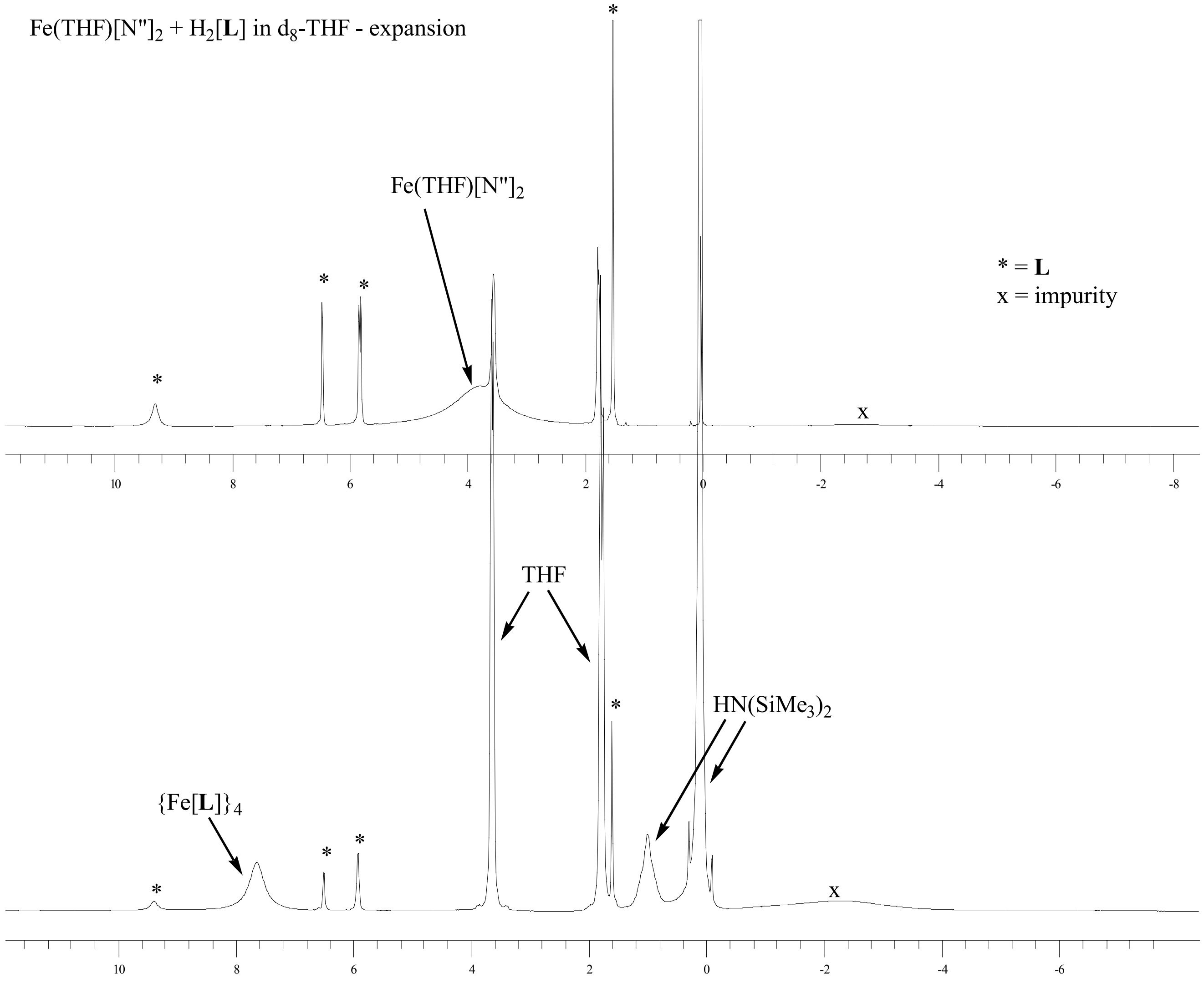




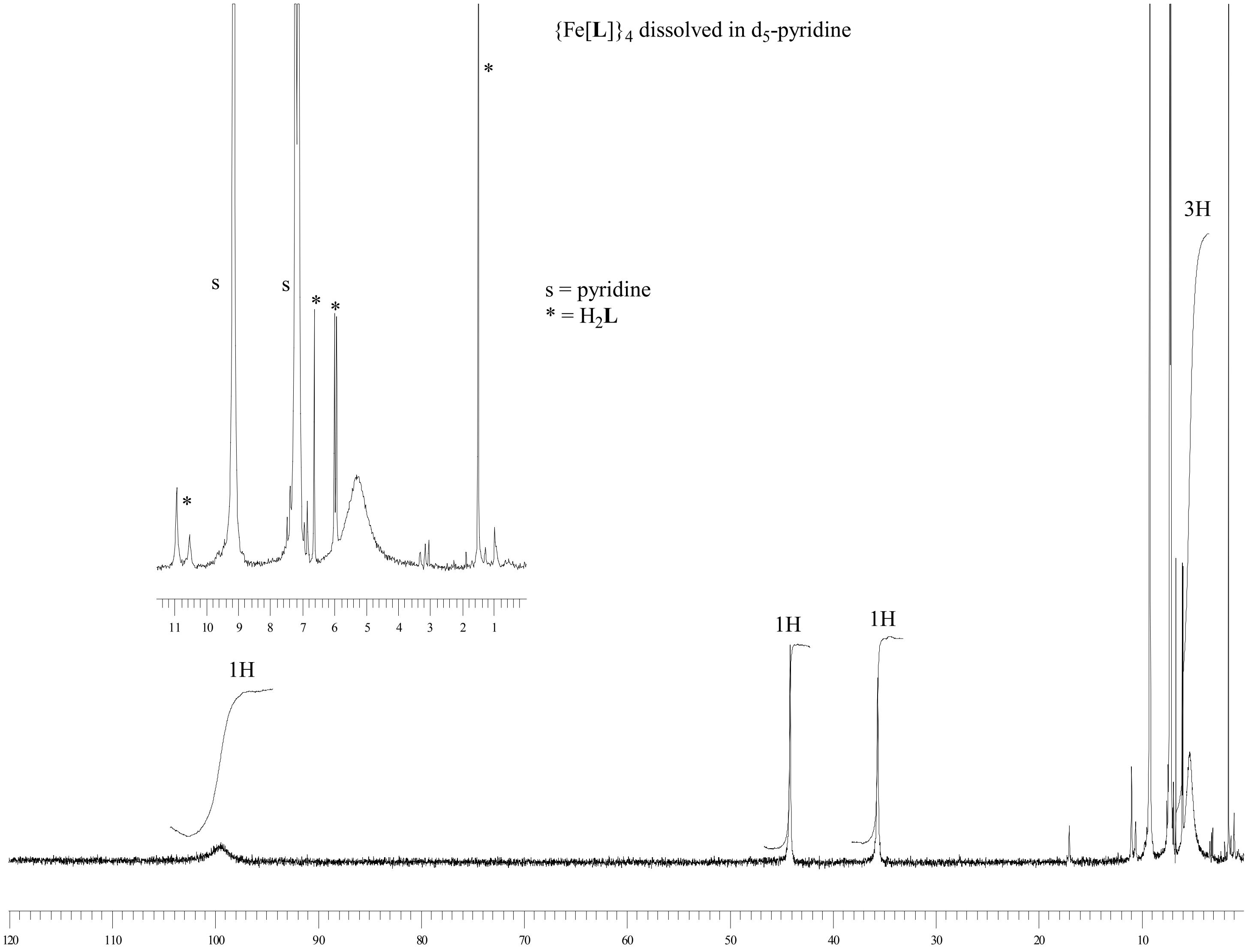
Fe(THF)[N"]$_2$ + H$_2$[**L**] in d$_8$-THF after 18 h at 80^o C



Fe(THF)[N"]$_2$ + H$_2$[**L**] in d$_8$-THF - expansion

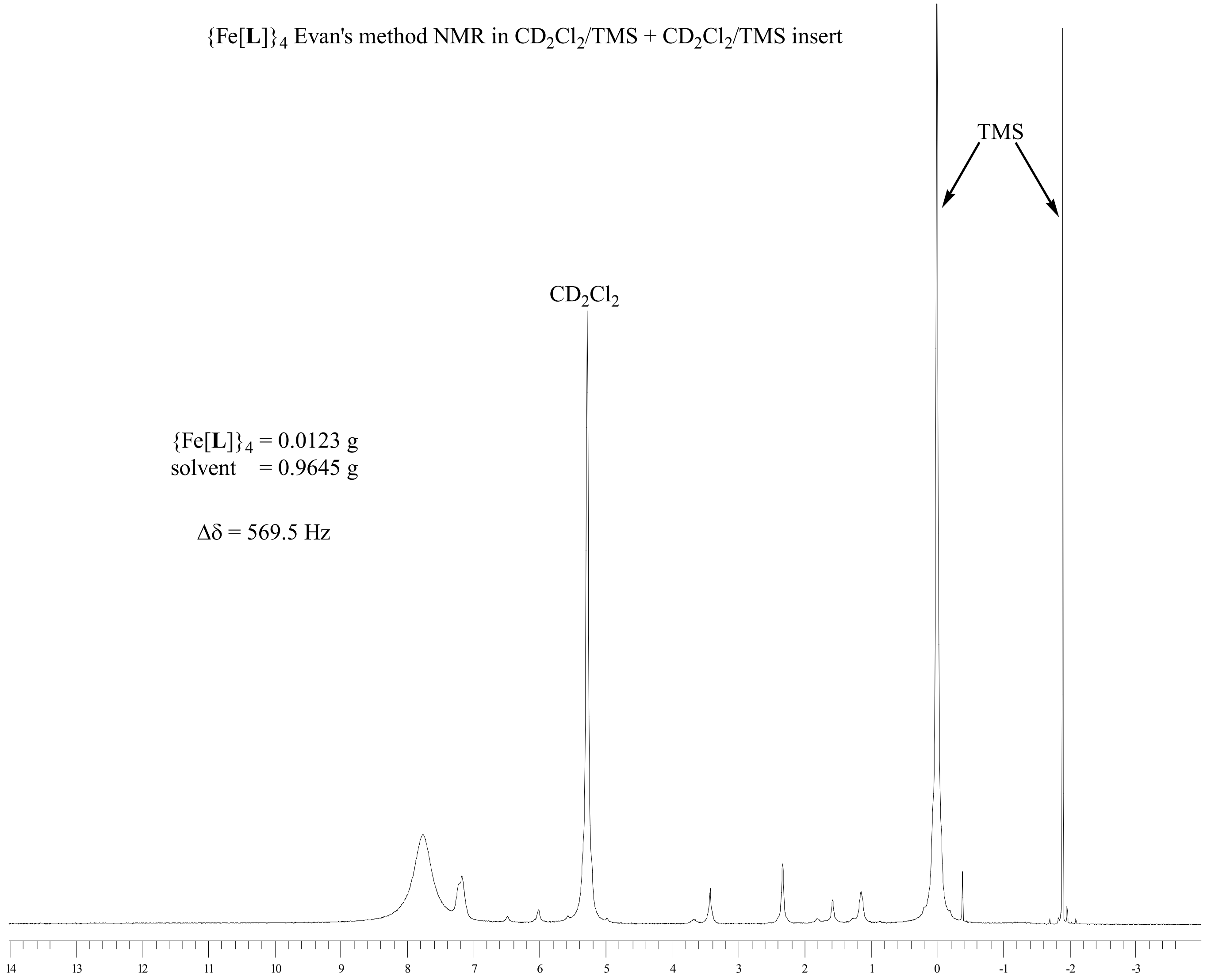


* = **L**
x = impurity



$\{Fe[\mathbf{L}]\}_4$ dissolved in d_5-pyridine

{Fe[**L**]}$_4$ Evan's method NMR in CD_2Cl_2/TMS + CD_2Cl_2/TMS insert



{Fe[**L**]}$_4$ = 0.0123 g
solvent = 0.9645 g

$\Delta\delta$ = 569.5 Hz

Cyclic voltametry

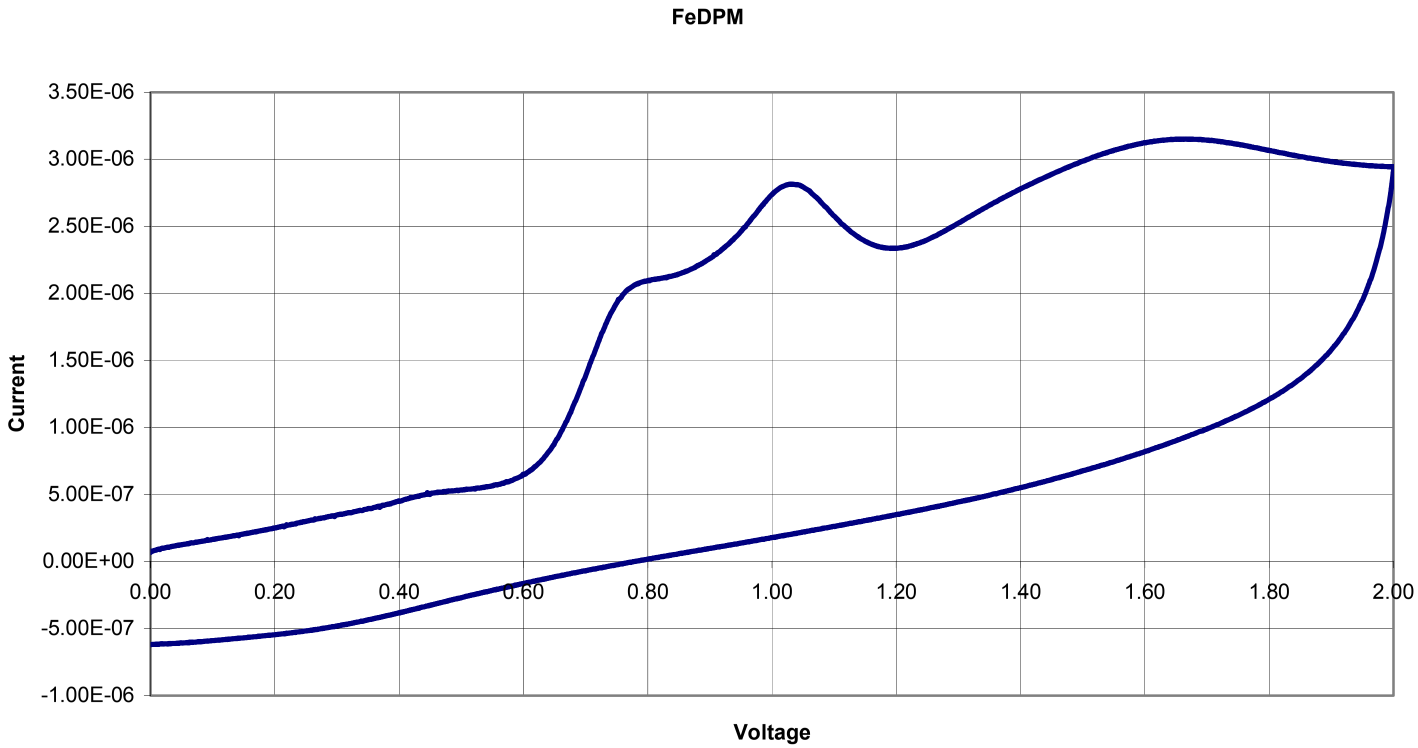


Table 1. Crystal data and structure refinement for fepthf.

Identification code	fepthf	
Empirical formula	C52 H68 Fe4 N8 O2	
Formula weight	1060.54	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	I4(1)/a	
Unit cell dimensions	a = 15.049(3) Å	α= 90°.
	b = 15.049(3) Å	β= 90°.
	c = 42.623(11) Å	γ = 90°.
Volume	9653(4) Å^3	
Z	8	
Density (calculated)	1.460 Mg/m^3	
Absorption coefficient	1.228 mm^{-1}	
F(000)	4448	
Crystal size	0.14 x 0.13 x 0.08 mm^3	
Theta range for data collection	1.97 to 27.35°.	
Index ranges	-19<=h<=11, -19<=k<=13, -53<=l<=52	
Reflections collected	18802	
Independent reflections	5426 [R(int) = 0.09]	
Completeness to theta = 27.35°	97.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.614	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5341 / 0 / 278	
Goodness-of-fit on F^2	0.916	
Final R indices [I>2sigma(I)]	R1 = 0.0574, wR2 = 0.1387	
R indices (all data)	R1 = 0.1147, wR2 = 0.1586	
Extinction coefficient	0.00008(5)	
Largest diff. peak and hole	0.486 and -0.705 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for fepthf. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	3417(1)	3476(1)	1755(1)	36(1)
Fe(2)	4188(1)	1208(1)	1761(1)	37(1)
N(1)	3418(2)	1218(2)	1382(1)	36(1)
N(2)	3489(2)	2285(2)	1966(1)	38(1)
N(3)	4544(2)	3928(2)	1556(1)	37(1)
N(4)	5432(2)	4452(3)	2138(1)	48(1)
C(1)	3695(3)	1143(3)	1073(1)	38(1)
C(2)	3044(3)	1439(3)	877(1)	40(1)
C(3)	2339(3)	1717(3)	1066(1)	36(1)
C(4)	2583(3)	1579(3)	1374(1)	34(1)
C(5)	2099(3)	1790(3)	1677(1)	35(1)
C(6)	1990(3)	938(3)	1878(1)	45(1)
C(7)	1184(3)	2162(3)	1610(1)	48(1)
C(8)	2603(3)	2449(3)	1874(1)	39(1)
C(9)	2309(3)	3230(3)	2025(1)	43(1)
C(10)	3010(3)	3543(3)	2219(1)	46(1)
C(11)	3718(3)	2954(3)	2176(1)	43(1)
C(12)	4073(3)	3417(3)	1342(1)	34(1)
C(13)	3233(3)	3786(3)	1287(1)	41(1)
C(14)	3187(3)	4575(3)	1474(1)	43(1)
C(15)	3997(3)	4651(3)	1640(1)	42(1)
C(16)	4326(3)	5382(3)	1851(1)	53(1)
C(17)	3550(4)	6004(4)	1929(2)	72(2)
C(18)	5024(4)	5918(4)	1661(2)	71(2)
C(19)	4724(3)	5025(3)	2150(1)	52(1)
C(20)	4481(4)	5145(4)	2458(1)	70(2)
C(21)	5055(3)	4628(4)	2646(1)	72(2)
C(22)	5636(3)	4222(4)	2445(1)	56(1)

Table 3. Bond lengths [Å] and angles [°] for fepthf.

Fe(1)-N(2)	2.008(4)
Fe(1)-C(11)	2.011(4)
Fe(1)-N(3)	2.014(4)
Fe(1)-C(12)	2.023(4)
Fe(1)-C(15)	2.032(5)
Fe(1)-C(8)	2.037(5)
Fe(1)-C(9)	2.059(4)
Fe(1)-C(13)	2.067(4)
Fe(1)-C(14)	2.071(5)
Fe(1)-C(10)	2.074(4)
Fe(2)-N(4)#1	1.975(4)
Fe(2)-N(1)	1.987(3)
Fe(2)-N(3)#1	2.109(3)
Fe(2)-N(2)	2.120(4)
N(1)-C(4)	1.369(5)
N(1)-C(1)	1.386(5)
N(2)-C(11)	1.393(5)
N(2)-C(8)	1.411(5)
N(3)-C(12)	1.389(5)
N(3)-C(15)	1.411(5)
N(3)-Fe(2)#1	2.109(3)
N(4)-C(19)	1.372(6)
N(4)-C(22)	1.387(6)
N(4)-Fe(2)#1	1.975(4)
C(1)-C(2)	1.363(6)
C(2)-C(3)	1.398(6)
C(3)-C(4)	1.377(6)
C(4)-C(5)	1.515(6)
C(5)-C(8)	1.506(6)
C(5)-C(7)	1.514(6)
C(5)-C(6)	1.551(6)
C(8)-C(9)	1.410(6)
C(9)-C(10)	1.422(6)
C(10)-C(11)	1.399(6)
C(12)-C(13)	1.400(6)
C(13)-C(14)	1.431(6)
C(14)-C(15)	1.414(6)
C(15)-C(16)	1.506(6)
C(16)-C(19)	1.506(7)
C(16)-C(17)	1.533(7)
C(16)-C(18)	1.552(7)
C(19)-C(20)	1.376(7)
C(20)-C(21)	1.412(8)
C(21)-C(22)	1.367(7)
N(2)-Fe(1)-C(11)	40.55(15)
N(2)-Fe(1)-N(3)	116.35(14)
C(11)-Fe(1)-N(3)	108.53(16)
N(2)-Fe(1)-C(12)	108.88(15)
C(11)-Fe(1)-C(12)	130.57(18)
N(3)-Fe(1)-C(12)	40.24(14)
N(2)-Fe(1)-C(15)	149.54(16)
C(11)-Fe(1)-C(15)	117.33(18)
N(3)-Fe(1)-C(15)	40.81(15)
C(12)-Fe(1)-C(15)	67.54(17)
N(2)-Fe(1)-C(8)	40.84(14)
C(11)-Fe(1)-C(8)	67.46(17)
N(3)-Fe(1)-C(8)	150.17(16)
C(12)-Fe(1)-C(8)	118.53(17)
C(15)-Fe(1)-C(8)	168.22(17)
N(2)-Fe(1)-C(9)	68.51(17)
C(11)-Fe(1)-C(9)	67.30(18)
N(3)-Fe(1)-C(9)	167.88(16)
C(12)-Fe(1)-C(9)	150.94(17)
C(15)-Fe(1)-C(9)	129.74(18)
C(8)-Fe(1)-C(9)	40.27(17)
N(2)-Fe(1)-C(13)	129.78(16)
C(11)-Fe(1)-C(13)	168.38(18)

N(3)-Fe(1)-C(13)	68.29(16)
C(12)-Fe(1)-C(13)	40.02(17)
C(15)-Fe(1)-C(13)	68.14(18)
C(8)-Fe(1)-C(13)	109.35(18)
C(9)-Fe(1)-C(13)	118.10(18)
N(2)-Fe(1)-C(14)	168.63(16)
C(11)-Fe(1)-C(14)	150.01(18)
N(3)-Fe(1)-C(14)	68.16(16)
C(12)-Fe(1)-C(14)	67.21(17)
C(15)-Fe(1)-C(14)	40.30(17)
C(8)-Fe(1)-C(14)	130.49(17)
C(9)-Fe(1)-C(14)	109.33(18)
C(13)-Fe(1)-C(14)	40.46(17)
N(2)-Fe(1)-C(10)	68.47(17)
C(11)-Fe(1)-C(10)	40.01(18)
N(3)-Fe(1)-C(10)	129.37(16)
C(12)-Fe(1)-C(10)	167.96(17)
C(15)-Fe(1)-C(10)	108.39(19)
C(8)-Fe(1)-C(10)	67.73(18)
C(9)-Fe(1)-C(10)	40.24(16)
C(13)-Fe(1)-C(10)	150.49(19)
C(14)-Fe(1)-C(10)	117.65(19)
N(4)#1-Fe(2)-N(1)	146.57(16)
N(4)#1-Fe(2)-N(3)#1	91.52(14)
N(1)-Fe(2)-N(3)#1	101.09(14)
N(4)#1-Fe(2)-N(2)	101.11(15)
N(1)-Fe(2)-N(2)	92.23(14)
N(3)#1-Fe(2)-N(2)	133.88(14)
C(4)-N(1)-C(1)	106.5(3)
C(4)-N(1)-Fe(2)	124.0(3)
C(1)-N(1)-Fe(2)	126.6(3)
C(11)-N(2)-C(8)	106.6(4)
C(11)-N(2)-Fe(1)	69.8(2)
C(8)-N(2)-Fe(1)	70.7(2)
C(11)-N(2)-Fe(2)	134.0(3)
C(8)-N(2)-Fe(2)	119.3(3)
Fe(1)-N(2)-Fe(2)	121.73(16)
C(12)-N(3)-C(15)	107.2(3)
C(12)-N(3)-Fe(1)	70.2(2)
C(15)-N(3)-Fe(1)	70.3(2)
C(12)-N(3)-Fe(2)#1	132.9(3)
C(15)-N(3)-Fe(2)#1	119.9(3)
Fe(1)-N(3)-Fe(2)#1	123.73(17)
C(19)-N(4)-C(22)	107.1(4)
C(19)-N(4)-Fe(2)#1	124.7(3)
C(22)-N(4)-Fe(2)#1	125.4(3)
C(2)-C(1)-N(1)	109.9(4)
C(1)-C(2)-C(3)	106.8(4)
C(4)-C(3)-C(2)	107.6(4)
N(1)-C(4)-C(3)	109.2(4)
N(1)-C(4)-C(5)	120.2(4)
C(3)-C(4)-C(5)	130.6(4)
C(8)-C(5)-C(7)	108.7(4)
C(8)-C(5)-C(4)	111.9(3)
C(7)-C(5)-C(4)	110.8(3)
C(8)-C(5)-C(6)	106.8(3)
C(7)-C(5)-C(6)	108.2(4)
C(4)-C(5)-C(6)	110.3(3)
C(9)-C(8)-N(2)	108.5(4)
C(9)-C(8)-C(5)	130.2(4)
N(2)-C(8)-C(5)	121.0(4)
C(9)-C(8)-Fe(1)	70.7(3)
N(2)-C(8)-Fe(1)	68.5(2)
C(5)-C(8)-Fe(1)	131.5(3)
C(8)-C(9)-C(10)	108.0(4)
C(8)-C(9)-Fe(1)	69.0(2)
C(10)-C(9)-Fe(1)	70.4(2)
C(11)-C(10)-C(9)	106.2(4)
C(11)-C(10)-Fe(1)	67.6(2)
C(9)-C(10)-Fe(1)	69.3(2)
N(2)-C(11)-C(10)	110.7(4)
N(2)-C(11)-Fe(1)	69.6(2)

C(10)-C(11)-Fe(1)	72.4(3)
N(3)-C(12)-C(13)	110.5(4)
N(3)-C(12)-Fe(1)	69.5(2)
C(13)-C(12)-Fe(1)	71.7(2)
C(12)-C(13)-C(14)	106.4(4)
C(12)-C(13)-Fe(1)	68.3(2)
C(14)-C(13)-Fe(1)	69.9(3)
C(15)-C(14)-C(13)	107.6(4)
C(15)-C(14)-Fe(1)	68.3(3)
C(13)-C(14)-Fe(1)	69.6(2)
N(3)-C(15)-C(14)	108.3(4)
N(3)-C(15)-C(16)	121.6(4)
C(14)-C(15)-C(16)	129.9(4)
N(3)-C(15)-Fe(1)	68.9(2)
C(14)-C(15)-Fe(1)	71.4(3)
C(16)-C(15)-Fe(1)	129.2(4)
C(15)-C(16)-C(19)	112.0(4)
C(15)-C(16)-C(17)	109.0(4)
C(19)-C(16)-C(17)	109.8(5)
C(15)-C(16)-C(18)	106.9(4)
C(19)-C(16)-C(18)	110.9(4)
C(17)-C(16)-C(18)	108.1(5)
N(4)-C(19)-C(20)	108.8(5)
N(4)-C(19)-C(16)	120.3(4)
C(20)-C(19)-C(16)	130.9(5)
C(19)-C(20)-C(21)	107.9(5)
C(22)-C(21)-C(20)	106.4(5)
C(21)-C(22)-N(4)	109.8(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1/2,z+0

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for fepthf. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	31(1)	45(1)	33(1)	-6(1)	-1(1)	4(1)
Fe(2)	31(1)	48(1)	33(1)	5(1)	-1(1)	4(1)
N(1)	33(2)	42(2)	32(2)	0(2)	1(2)	2(2)
N(2)	29(2)	57(2)	28(2)	-1(2)	-4(2)	-1(2)
N(3)	35(2)	39(2)	36(2)	-5(2)	-4(2)	2(2)
N(4)	33(2)	63(3)	47(2)	-17(2)	-2(2)	3(2)
C(1)	34(2)	40(2)	40(3)	-4(2)	6(2)	0(2)
C(2)	48(3)	43(3)	29(2)	0(2)	2(2)	-1(2)
C(3)	34(2)	35(2)	39(2)	-1(2)	-6(2)	1(2)
C(4)	30(2)	37(2)	35(2)	-1(2)	-2(2)	-1(2)
C(5)	29(2)	44(2)	31(2)	1(2)	0(2)	-4(2)
C(6)	37(3)	60(3)	36(2)	1(2)	6(2)	-11(2)
C(7)	33(2)	66(3)	44(3)	-10(3)	-4(2)	2(2)
C(8)	34(2)	51(3)	31(2)	1(2)	1(2)	4(2)
C(9)	30(2)	64(3)	34(2)	-8(2)	1(2)	-1(2)
C(10)	41(3)	66(3)	32(2)	-15(2)	-1(2)	-5(2)
C(11)	37(2)	60(3)	32(2)	-6(2)	-2(2)	-5(2)
C(12)	39(2)	35(2)	30(2)	-1(2)	1(2)	0(2)
C(13)	42(3)	50(3)	32(2)	1(2)	-4(2)	3(2)
C(14)	35(2)	41(3)	53(3)	0(2)	-6(2)	6(2)
C(15)	34(2)	44(3)	47(3)	-6(2)	2(2)	7(2)
C(16)	39(3)	46(3)	73(4)	-24(3)	-5(2)	9(2)
C(17)	61(4)	59(3)	96(5)	-35(3)	-10(4)	13(3)
C(18)	66(4)	53(3)	93(5)	-10(3)	-10(4)	-4(3)
C(19)	33(2)	61(3)	61(3)	-27(3)	-7(2)	-1(2)
C(20)	44(3)	96(4)	71(4)	-50(3)	5(3)	1(3)
C(21)	43(3)	121(5)	51(4)	-35(3)	3(3)	-17(3)
C(22)	43(3)	86(4)	40(3)	-16(3)	-6(2)	0(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for fepthf.

	x	y	z	U(eq)
H(1A)	4255	918	1008	44(12)
H(2A)	3066	1454	654	45(12)
H(3A)	1791	1958	996	45(12)
H(6A)	2576	685	1922	51(13)
H(6B)	1693	1087	2075	55(14)
H(6C)	1631	503	1762	44(13)
H(7A)	1240	2699	1481	34(12)
H(7B)	831	1718	1496	43(12)
H(7C)	888	2310	1808	55(14)
H(9A)	1713	3515	1999	52(13)
H(10A)	3002	4083	2356	68(16)
H(11A)	4310	3008	2281	50(13)
H(12A)	4298	2858	1243	49(13)
H(13A)	2762	3548	1145	66(15)
H(14A)	2668	4989	1489	55(13)
H(17A)	3103	5681	2051	72(19)
H(17B)	3768	6511	2051	73(17)
H(17C)	3281	6219	1734	52(15)
H(18A)	5527	5532	1609	120(30)
H(18B)	4751	6140	1468	90(20)
H(18C)	5234	6420	1788	66(16)
H(20A)	4011	5512	2531	72(17)
H(21A)	5040	4572	2868	100(20)
H(22A)	6108	3841	2506	54(15)

$1/\chi$ vs T plot for **1**.