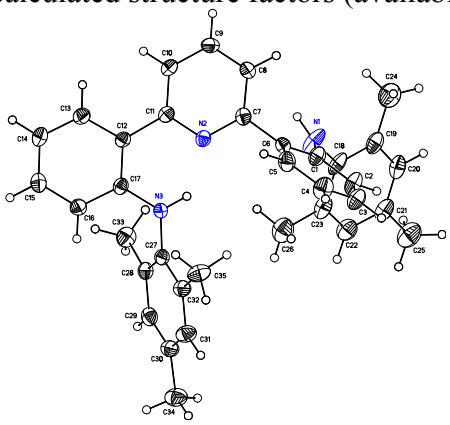
Crystallographic Data

[**2**]H_2

Contents



[**2**]H_2

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 653538. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 653538."

Table 1. Crystal data and structure refinement for [**2**]H_2 (CCDC 653538).

Empirical formula	$C_{35}H_{35}N_3$
Formula weight	497.66
Crystallization Solvent	Not given
Crystal Habit	Blade
Crystal size	0.39 x 0.22 x 0.09 mm^3
Crystal color	Colorless

Data Collection

Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K

θ range for 8568 reflections used in lattice determination	2.54 to 27.95°
Unit cell dimensions	a = 12.1774(12) Å b = 8.3901(8) Å β= 93.803(2)° c = 27.039(3) Å
Volume	2756.5(5) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	$P2_1/n$
Density (calculated)	1.199 Mg/m^3
F(000)	1064
Data collection program	Bruker SMART v5.630
θ range for data collection	1.51 to 28.41°
Completeness to θ = 28.41°	93.2 %
Index ranges	$-15 \le h \le 16$, $-10 \le k \le 11$, $-36 \le l \le 35$
Data collection scan type	ω scans at 5 ϕ settings
Data reduction program	Bruker SAINT v6.45A
Reflections collected	34841
Independent reflections	6474 [R_{int}= 0.0831]
Absorption coefficient	0.070 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.9937 and 0.9732

Table 1 (cont.)

Structure solution and Refinement

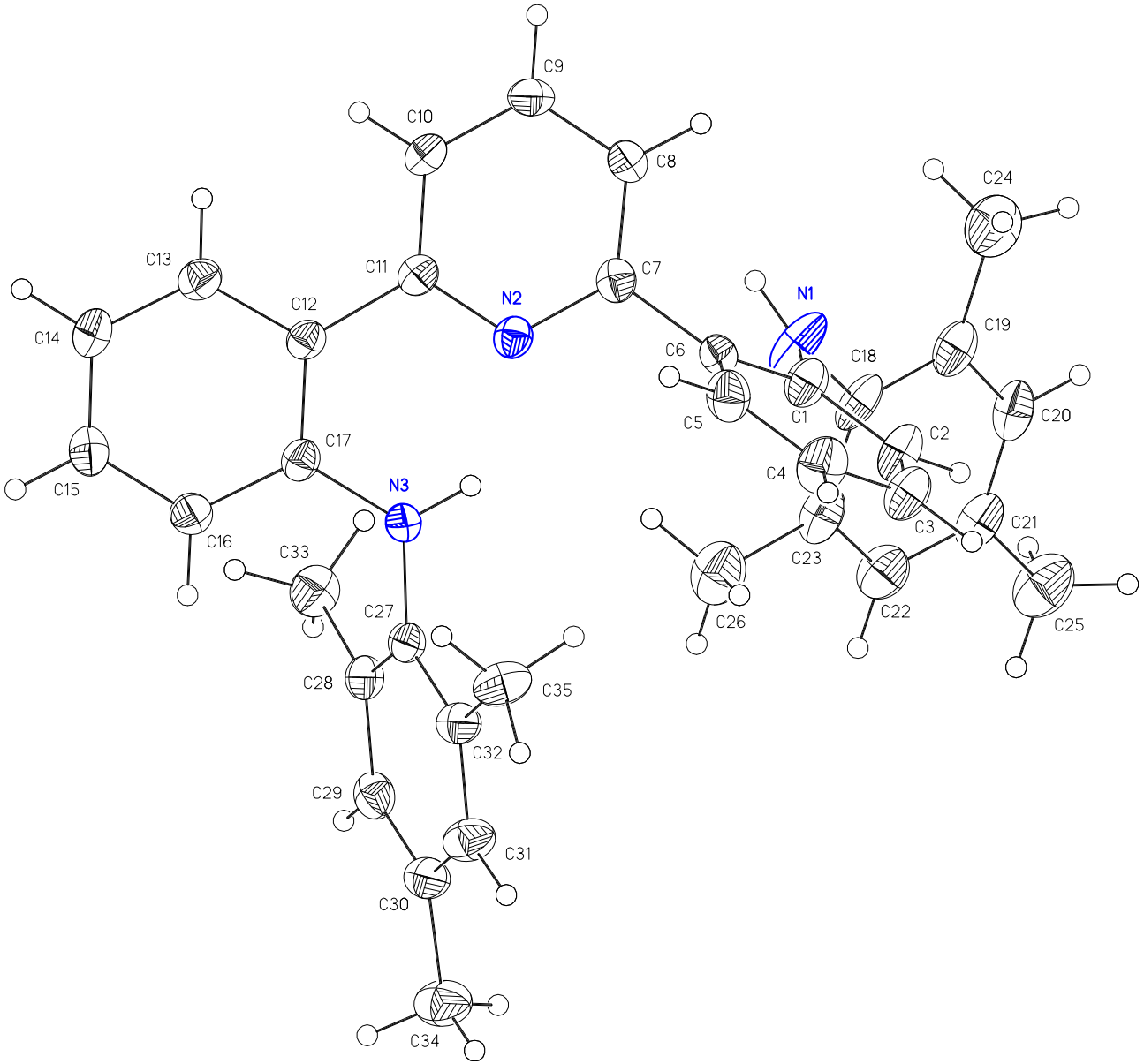
Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	6474 / 0 / 349
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.579
Final R indices [$I>2\sigma(I)$, 4122 reflections]	R1 = 0.0554, *w*R2 = 0.0907
R indices (all data)	R1 = 0.0900, *w*R2 = 0.0939
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$

Max shift/error	0.000
Average shift/error	0.000
Largest diff. peak and hole	0.387 and -0.364 e.Å^{-3}

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.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C32
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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [**2**]H_2 **(CCDC 653538). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.**

	x	y	z	U_{eq}
N(1)	1038(1)	3989(2)	1311(1)	39(1)
N(2)	3731(1)	5158(2)	1856(1)	21(1)
N(3)	4904(1)	2425(2)	1759(1)	24(1)
C(1)	1569(1)	5009(2)	998(1)	27(1)
C(2)	1265(1)	5049(2)	493(1)	33(1)
C(3)	1798(1)	6037(2)	181(1)	34(1)
C(4)	2639(1)	7005(2)	366(1)	36(1)
C(5)	2952(1)	6967(2)	866(1)	31(1)
C(6)	2434(1)	5978(2)	1186(1)	22(1)
C(7)	2781(1)	5934(2)	1727(1)	22(1)
C(8)	2159(1)	6639(2)	2073(1)	27(1)
C(9)	2504(1)	6534(2)	2570(1)	28(1)
C(10)	3462(1)	5726(2)	2705(1)	25(1)
C(11)	4076(1)	5057(2)	2340(1)	21(1)
C(12)	5122(1)	4202(2)	2469(1)	20(1)
C(13)	5747(1)	4626(2)	2903(1)	25(1)
C(14)	6718(1)	3870(2)	3052(1)	30(1)
C(15)	7103(1)	2667(2)	2758(1)	29(1)
C(16)	6516(1)	2220(2)	2327(1)	26(1)
C(17)	5517(1)	2946(2)	2180(1)	22(1)
C(18)	458(2)	2616(2)	1119(1)	31(1)
C(19)	-685(2)	2578(2)	1105(1)	31(1)
C(20)	-1216(2)	1243(2)	903(1)	34(1)
C(21)	-652(2)	-34(2)	722(1)	33(1)
C(22)	485(1)	30(2)	744(1)	36(1)
C(23)	1059(1)	1350(2)	938(1)	34(1)
C(24)	-1328(2)	3938(2)	1312(1)	45(1)
C(25)	-1250(2)	-1478(2)	512(1)	49(1)
C(26)	2300(1)	1393(2)	948(1)	45(1)
C(27)	5218(1)	1155(2)	1452(1)	22(1)
C(28)	5264(1)	-416(2)	1626(1)	25(1)
C(29)	5539(1)	-1613(2)	1302(1)	27(1)
C(30)	5737(1)	-1313(2)	812(1)	28(1)
C(31)	5673(1)	251(2)	649(1)	30(1)
C(32)	5430(1)	1503(2)	963(1)	25(1)
C(33)	4974(1)	-839(2)	2143(1)	34(1)
C(34)	5955(1)	-2667(2)	464(1)	37(1)
C(35)	5391(1)	3205(2)	784(1)	34(1)

Table 3. Bond lengths [Å] and angles [°] for [2]H_2 (CCDC 653538).

N(1)-C(1)	1.3935(19)	C(6)-C(5)-C(4)	121.31(16)
N(1)-C(18)	1.430(2)	C(5)-C(6)-C(1)	118.94(15)
N(2)-C(11)	1.3511(18)	C(5)-C(6)-C(7)	121.10(14)
N(2)-C(7)	1.3525(18)	C(1)-C(6)-C(7)	119.96(14)
N(3)-C(17)	1.3900(17)	N(2)-C(7)-C(8)	122.15(14)
N(3)-C(27)	1.4191(19)	N(2)-C(7)-C(6)	116.41(14)
C(1)-C(2)	1.390(2)	C(8)-C(7)-C(6)	121.44(14)
C(1)-C(6)	1.400(2)	C(7)-C(8)-C(9)	119.20(15)
C(2)-C(3)	1.376(2)	C(10)-C(9)-C(8)	119.07(15)
C(3)-C(4)	1.374(2)	C(9)-C(10)-C(11)	119.67(14)
C(4)-C(5)	1.383(2)	N(2)-C(11)-C(10)	120.90(14)
C(5)-C(6)	1.381(2)	N(2)-C(11)-C(12)	117.71(13)
C(6)-C(7)	1.496(2)	C(10)-C(11)-C(12)	121.39(14)
C(7)-C(8)	1.376(2)	C(13)-C(12)-C(17)	117.77(14)
C(8)-C(9)	1.383(2)	C(13)-C(12)-C(11)	118.97(14)
C(9)-C(10)	1.378(2)	C(17)-C(12)-C(11)	123.25(13)
C(10)-C(11)	1.395(2)	C(14)-C(13)-C(12)	122.38(15)
C(11)-C(12)	1.483(2)	C(13)-C(14)-C(15)	118.92(15)
C(12)-C(13)	1.4016(19)	C(16)-C(15)-C(14)	120.50(15)
C(12)-C(17)	1.416(2)	C(15)-C(16)-C(17)	121.12(15)
C(13)-C(14)	1.378(2)	N(3)-C(17)-C(16)	120.52(14)
C(14)-C(15)	1.386(2)	N(3)-C(17)-C(12)	120.20(13)
C(15)-C(16)	1.376(2)	C(16)-C(17)-C(12)	119.27(14)
C(16)-C(17)	1.395(2)	C(19)-C(18)-C(23)	121.33(16)
C(18)-C(19)	1.390(2)	C(19)-C(18)-N(1)	119.83(17)
C(18)-C(23)	1.396(2)	C(23)-C(18)-N(1)	118.83(16)
C(19)-C(20)	1.387(2)	C(20)-C(19)-C(18)	117.95(17)
C(19)-C(24)	1.512(2)	C(20)-C(19)-C(24)	121.01(16)
C(20)-C(21)	1.380(2)	C(18)-C(19)-C(24)	121.03(16)
C(21)-C(22)	1.384(2)	C(21)-C(20)-C(19)	122.48(17)
C(21)-C(25)	1.505(2)	C(20)-C(21)-C(22)	118.34(17)
C(22)-C(23)	1.393(2)	C(20)-C(21)-C(25)	121.32(17)
C(23)-C(26)	1.511(2)	C(22)-C(21)-C(25)	120.34(18)
C(27)-C(32)	1.394(2)	C(21)-C(22)-C(23)	121.50(18)
C(27)-C(28)	1.400(2)	C(22)-C(23)-C(18)	118.39(16)
C(28)-C(29)	1.390(2)	C(22)-C(23)-C(26)	120.14(18)
C(28)-C(33)	1.505(2)	C(18)-C(23)-C(26)	121.47(16)
C(29)-C(30)	1.385(2)	C(32)-C(27)-C(28)	120.76(15)
C(30)-C(31)	1.385(2)	C(32)-C(27)-N(3)	118.11(14)
C(30)-C(34)	1.509(2)	C(28)-C(27)-N(3)	121.06(14)
C(31)-C(32)	1.395(2)	C(29)-C(28)-C(27)	118.24(15)
C(32)-C(35)	1.507(2)	C(29)-C(28)-C(33)	119.80(15)
		C(27)-C(28)-C(33)	121.89(15)
C(1)-N(1)-C(18)	120.80(13)	C(30)-C(29)-C(28)	122.51(16)
C(11)-N(2)-C(7)	119.00(13)	C(29)-C(30)-C(31)	117.83(15)
C(17)-N(3)-C(27)	124.37(12)	C(29)-C(30)-C(34)	120.51(16)
C(2)-C(1)-N(1)	120.47(15)	C(31)-C(30)-C(34)	121.59(16)
C(2)-C(1)-C(6)	119.30(15)	C(30)-C(31)-C(32)	121.95(16)
N(1)-C(1)-C(6)	120.22(14)	C(27)-C(32)-C(31)	118.67(15)
C(3)-C(2)-C(1)	120.67(16)	C(27)-C(32)-C(35)	119.94(14)
C(4)-C(3)-C(2)	120.27(16)	C(31)-C(32)-C(35)	121.39(15)
C(3)-C(4)-C(5)	119.50(16)		

Table 4. Anisotropic displacement parameters ($Å^2 x 10^4$) for [2]H_2 (CCDC 653538). 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}
N(1)	593(11)	397(10)	180(8)	18(7)	-34(7)	-245(8)
N(2)	217(7)	196(8)	224(7)	-9(6)	-9(6)	-26(6)
N(3)	187(7)	278(8)	235(7)	-60(6)	-24(6)	38(6)
C(1)	323(10)	259(10)	228(9)	37(8)	-17(8)	-39(8)
C(2)	405(11)	328(11)	254(10)	15(9)	-83(8)	-98(9)
C(3)	417(11)	379(11)	219(9)	44(9)	-32(8)	-28(9)
C(4)	364(11)	429(12)	276(10)	94(9)	44(8)	-89(9)
C(5)	239(9)	345(11)	331(10)	26(9)	0(8)	-44(8)
C(6)	207(9)	220(9)	234(9)	-1(8)	-2(7)	31(7)
C(7)	210(9)	188(9)	263(9)	3(7)	-9(7)	-34(7)
C(8)	214(9)	300(11)	291(10)	-40(8)	-10(7)	46(8)
C(9)	262(10)	310(11)	265(10)	-72(8)	51(8)	23(8)
C(10)	274(9)	267(10)	192(9)	-25(7)	1(7)	-27(8)
C(11)	218(9)	184(9)	212(9)	-6(7)	12(7)	-50(7)
C(12)	218(9)	224(10)	171(8)	17(7)	25(7)	-20(7)
C(13)	268(9)	254(10)	234(9)	-32(8)	11(7)	-18(8)
C(14)	276(10)	343(11)	257(10)	-28(8)	-58(8)	-19(8)
C(15)	241(9)	301(11)	306(10)	15(8)	-38(8)	4(8)
C(16)	249(9)	250(10)	275(9)	-43(8)	0(7)	7(8)
C(17)	216(9)	237(10)	192(8)	14(7)	4(7)	-29(7)
C(18)	469(12)	292(11)	163(9)	49(8)	-61(8)	-145(9)
C(19)	415(11)	311(11)	205(9)	87(8)	-51(8)	-48(9)
C(20)	318(10)	412(12)	270(10)	91(9)	-68(8)	-90(9)
C(21)	398(11)	353(12)	232(10)	28(9)	-33(8)	-131(9)
C(22)	400(12)	359(12)	330(11)	1(9)	12(9)	-74(9)
C(23)	367(11)	387(12)	252(10)	58(9)	-45(8)	-125(9)
C(24)	537(13)	407(12)	403(11)	58(10)	-16(10)	-23(11)
C(25)	511(13)	491(14)	459(12)	-65(10)	-1(10)	-207(11)
C(26)	393(12)	494(14)	448(12)	8(10)	-4(9)	-131(10)
C(27)	178(9)	236(10)	253(9)	-55(8)	-15(7)	-19(7)
C(28)	194(9)	280(10)	264(9)	-29(8)	-13(7)	-25(8)
C(29)	227(9)	227(10)	339(10)	-25(8)	-30(8)	-15(8)
C(30)	215(9)	277(11)	337(10)	-92(8)	33(8)	-41(8)
C(31)	310(10)	324(11)	281(10)	-46(8)	88(8)	-66(8)
C(32)	230(9)	248(10)	277(9)	-40(8)	38(7)	-38(8)
C(33)	374(11)	306(11)	327(10)	22(9)	8(8)	-9(9)
C(34)	377(11)	318(11)	418(11)	-116(9)	74(9)	-62(9)
C(35)	462(12)	302(11)	269(10)	-24(8)	101(8)	-42(9)

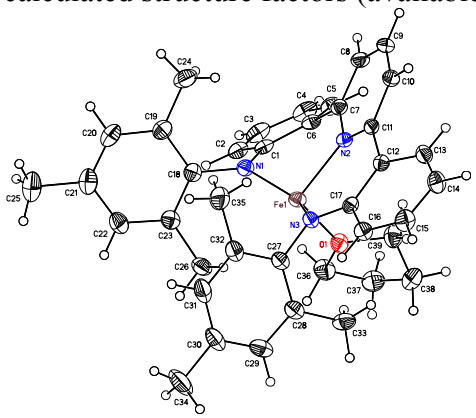
Table 5. Hydrogen bonds for [2]H_2 **(CCDC 653538) [Å and °].**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(3)-H(3)...N(2)	0.88	2.06	2.7235(18)	130.9

Symmetry transformations used to generate equivalent atoms:

[**2**]Fe(THF)

Contents



[**2**]Fe(THF)

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 678268. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 678268."

Table 1. Crystal data and structure refinement for [**2**]Fe(THF) **(CCDC 678268).**

Empirical formula	$C_{39}H_{41}N_3OFe$
Formula weight	623.60
Crystallization Solvent	Toluene/petroleumether
Crystal Habit	Block

Crystal size	0.26 x 0.25 x 0.21 mm^3
Crystal color	Dark red

Data Collection

Type of diffractometer	Bruker KAPPA APEX II
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 9851 reflections used in lattice determination	2.48 to 35.69°
Unit cell dimensions	a = 14.5396(6) Å b = 13.5644(6) Å β= 98.247(2)° c = 16.6014(7) Å
Volume	3240.3(2) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	$P2_1/c$
Density (calculated)	1.278 Mg/m^3
F(000)	1320
Data collection program	Bruker APEX2 v2.1-0
θ range for data collection	1.95 to 36.53°
Completeness to θ = 36.53°	93.3 %
Index ranges	$-24 \leq h \leq 22$, $-22 \leq k \leq 22$, $-26 \leq l \leq 27$
Data collection scan type	ω scans; 17 settings
Data reduction program	Bruker SAINT-Plus v7.34A
Reflections collected	97719
Independent reflections	14879 [R_{int}= 0.0486]
Absorption coefficient	0.501 mm^{-1}
Absorption correction	None

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2

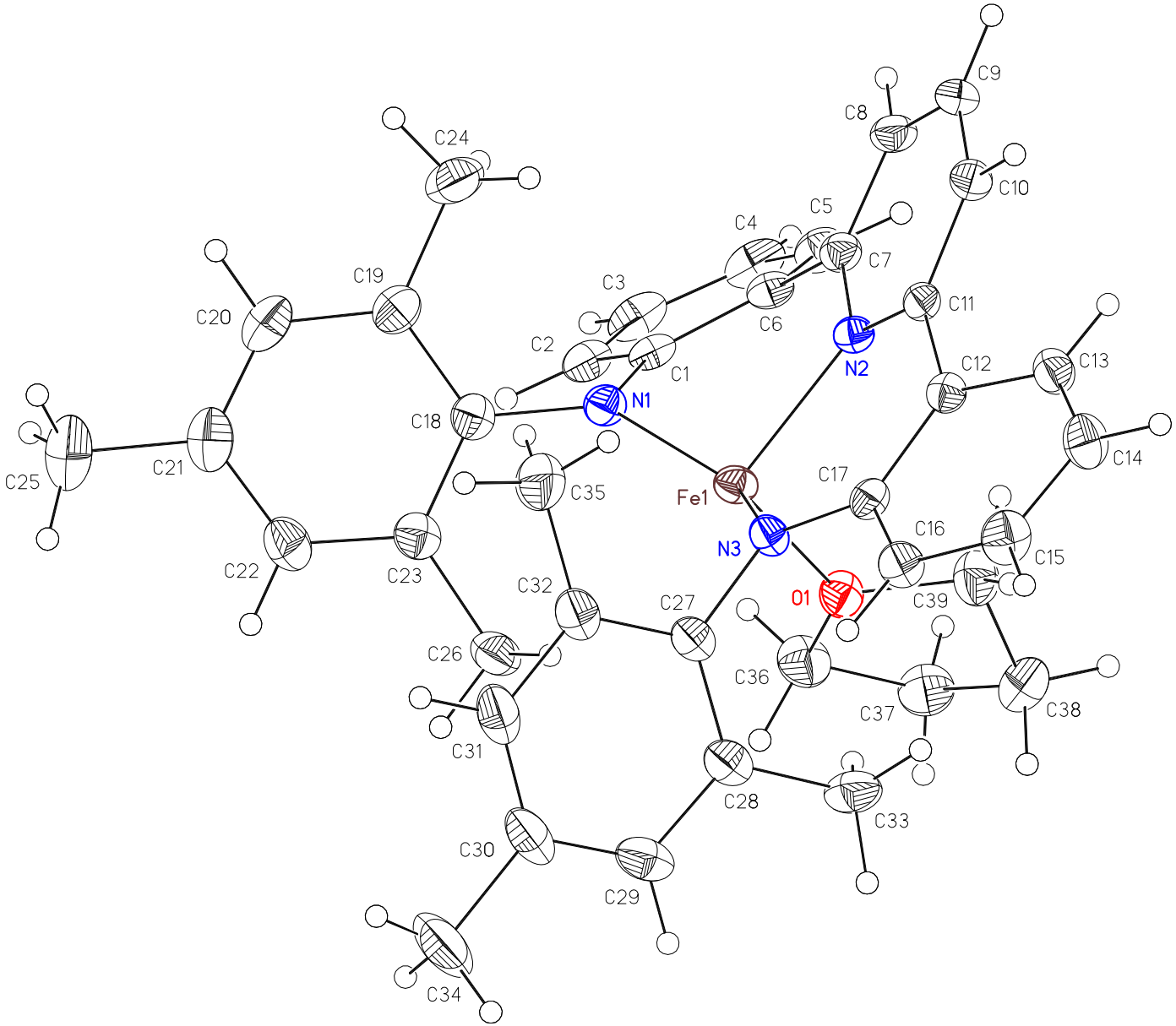
Data / restraints / parameters	14879 / 0 / 403
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	2.823
Final R indices [I>2σ(I), 10317 reflections]	R1 = 0.0501, *w*R2 = 0.0848
R indices (all data)	R1 = 0.0792, *w*R2 = 0.0860
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.003
Average shift/error	0.000
Largest diff. peak and hole	2.279 and -1.067 e.Å^{-3}

Special Refinement Details

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.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C21
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C17
C22
C23
N3
C16
C15
C32
C27
O1
C39
C26
C36
C37
C38
C31
C28
C33
C30
C29
C34

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [**2**]Fe(THF) **(CCDC 678268). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.**

	x	y	z	U_{eq}
Fe(1)	2281(1)	2168(1)	8517(1)	19(1)
O(1)	2086(1)	2910(1)	7387(1)	24(1)
N(1)	1773(1)	860(1)	8316(1)	21(1)
N(2)	1160(1)	2750(1)	8954(1)	17(1)
N(3)	3188(1)	2847(1)	9282(1)	19(1)
C(1)	898(1)	889(1)	7846(1)	21(1)
C(2)	640(1)	204(1)	7222(1)	25(1)
C(3)	-198(1)	270(1)	6716(1)	30(1)
C(4)	-809(1)	1027(1)	6800(1)	30(1)
C(5)	-590(1)	1696(1)	7418(1)	27(1)
C(6)	244(1)	1635(1)	7966(1)	21(1)
C(7)	329(1)	2301(1)	8682(1)	20(1)
C(8)	-444(1)	2470(1)	9065(1)	24(1)
C(9)	-365(1)	3075(1)	9738(1)	26(1)
C(10)	466(1)	3530(1)	10008(1)	23(1)
C(11)	1234(1)	3388(1)	9596(1)	18(1)
C(12)	2101(1)	3946(1)	9852(1)	19(1)
C(13)	2009(1)	4838(1)	10263(1)	24(1)
C(14)	2748(1)	5410(1)	10593(1)	29(1)
C(15)	3637(1)	5083(1)	10530(1)	29(1)
C(16)	3769(1)	4231(1)	10121(1)	24(1)
C(17)	3023(1)	3652(1)	9734(1)	19(1)
C(18)	2226(1)	-67(1)	8422(1)	23(1)
C(19)	1844(1)	-829(1)	8840(1)	28(1)
C(20)	2299(1)	-1734(1)	8933(1)	34(1)
C(21)	3133(1)	-1905(1)	8648(1)	36(1)
C(22)	3521(1)	-1128(1)	8274(1)	31(1)
C(23)	3089(1)	-214(1)	8148(1)	25(1)
C(24)	955(1)	-666(1)	9191(1)	37(1)
C(25)	3616(1)	-2900(1)	8753(1)	49(1)
C(26)	3530(1)	588(1)	7708(1)	30(1)
C(27)	4129(1)	2569(1)	9221(1)	22(1)
C(28)	4607(1)	3015(1)	8642(1)	25(1)
C(29)	5484(1)	2647(1)	8549(1)	31(1)
C(30)	5884(1)	1864(1)	9001(1)	35(1)
C(31)	5406(1)	1449(1)	9574(1)	35(1)
C(32)	4530(1)	1782(1)	9694(1)	28(1)
C(33)	4194(1)	3870(1)	8130(1)	32(1)
C(34)	6839(1)	1497(1)	8872(1)	57(1)
C(35)	4025(1)	1312(1)	10322(1)	38(1)
C(36)	2090(1)	2548(1)	6570(1)	32(1)
C(37)	1640(1)	3365(1)	6009(1)	33(1)
C(38)	1787(1)	4274(1)	6540(1)	34(1)
C(39)	1653(1)	3871(1)	7358(1)	31(1)

Table 3. Selected bond lengths [Å] and angles [°] for [**2**]Fe(THF) **(CCDC 678268).**

Fe(1)-N(3)	1.9278(10)	N(3)-Fe(1)-N(1)	139.52(4)
Fe(1)-N(1)	1.9319(10)	N(3)-Fe(1)-N(2)	94.97(4)
Fe(1)-N(2)	2.0356(10)	N(1)-Fe(1)-N(2)	96.44(4)
Fe(1)-O(1)	2.1126(9)	N(3)-Fe(1)-O(1)	110.45(4)
		N(1)-Fe(1)-O(1)	106.54(4)
		N(2)-Fe(1)-O(1)	96.85(4)

Table 4. Bond lengths [Å] and angles [°] for [**2**]Fe(THF) **(CCDC 678268).**

Fe(1)-N(3)	1.9278(10)	C(27)-C(28)	1.4020(18)
Fe(1)-N(1)	1.9319(10)	C(28)-C(29)	1.3982(18)
Fe(1)-N(2)	2.0356(10)	C(28)-C(33)	1.5114(19)
Fe(1)-O(1)	2.1126(9)	C(29)-C(30)	1.380(2)
O(1)-C(36)	1.4435(15)	C(30)-C(31)	1.376(2)
O(1)-C(39)	1.4453(15)	C(30)-C(34)	1.5190(19)
N(1)-C(1)	1.3950(15)	C(31)-C(32)	1.3919(18)
N(1)-C(18)	1.4184(16)	C(32)-C(35)	1.502(2)
N(2)-C(11)	1.3654(15)	C(36)-C(37)	1.5311(19)
N(2)-C(7)	1.3706(14)	C(37)-C(38)	1.513(2)
N(3)-C(17)	1.3656(15)	C(38)-C(39)	1.5034(19)
N(3)-C(27)	1.4373(15)		
C(1)-C(2)	1.4027(17)	N(3)-Fe(1)-N(1)	139.52(4)
C(1)-C(6)	1.4218(17)	N(3)-Fe(1)-N(2)	94.97(4)
C(2)-C(3)	1.3797(18)	N(1)-Fe(1)-N(2)	96.44(4)
C(3)-C(4)	1.378(2)	N(3)-Fe(1)-O(1)	110.45(4)
C(4)-C(5)	1.3723(19)	N(1)-Fe(1)-O(1)	106.54(4)
C(5)-C(6)	1.4106(17)	N(2)-Fe(1)-O(1)	96.85(4)
C(6)-C(7)	1.4838(17)	C(36)-O(1)-C(39)	109.65(10)
C(7)-C(8)	1.3868(17)	C(36)-O(1)-Fe(1)	130.90(8)
C(8)-C(9)	1.3786(18)	C(39)-O(1)-Fe(1)	117.46(7)
C(9)-C(10)	1.3735(18)	C(1)-N(1)-C(18)	117.65(10)
C(10)-C(11)	1.4028(16)	C(1)-N(1)-Fe(1)	111.48(8)
C(11)-C(12)	1.4788(16)	C(18)-N(1)-Fe(1)	129.32(8)
C(12)-C(13)	1.4036(17)	C(11)-N(2)-C(7)	120.38(10)
C(12)-C(17)	1.4398(16)	C(11)-N(2)-Fe(1)	123.15(8)
C(13)-C(14)	1.3738(18)	C(7)-N(2)-Fe(1)	115.05(8)
C(14)-C(15)	1.3849(18)	C(17)-N(3)-C(27)	119.46(10)
C(15)-C(16)	1.3671(18)	C(17)-N(3)-Fe(1)	125.95(8)
C(16)-C(17)	1.4151(16)	C(27)-N(3)-Fe(1)	113.35(8)
C(18)-C(19)	1.4030(18)	N(1)-C(1)-C(2)	121.35(12)
C(18)-C(23)	1.4103(17)	N(1)-C(1)-C(6)	121.06(11)
C(19)-C(20)	1.3926(19)	C(2)-C(1)-C(6)	117.57(11)
C(19)-C(24)	1.5084(19)	C(3)-C(2)-C(1)	121.66(13)
C(20)-C(21)	1.382(2)	C(4)-C(3)-C(2)	120.85(13)
C(21)-C(22)	1.384(2)	C(5)-C(4)-C(3)	119.03(13)
C(21)-C(25)	1.520(2)	C(4)-C(5)-C(6)	121.93(13)
C(22)-C(23)	1.3905(19)	C(5)-C(6)-C(1)	118.76(12)
C(23)-C(26)	1.5049(18)	C(5)-C(6)-C(7)	116.50(12)
C(27)-C(32)	1.4007(18)	C(1)-C(6)-C(7)	124.43(11)

N(2)-C(7)-C(8)	120.67(11)	C(20)-C(21)-C(22)	117.34(14)
N(2)-C(7)-C(6)	120.17(10)	C(20)-C(21)-C(25)	121.52(15)
C(8)-C(7)-C(6)	119.16(11)	C(22)-C(21)-C(25)	121.13(14)
C(9)-C(8)-C(7)	119.39(12)	C(21)-C(22)-C(23)	122.83(13)
C(10)-C(9)-C(8)	119.92(12)	C(22)-C(23)-C(18)	118.77(13)
C(9)-C(10)-C(11)	120.29(12)	C(22)-C(23)-C(26)	120.19(12)
N(2)-C(11)-C(10)	119.20(11)	C(18)-C(23)-C(26)	121.02(12)
N(2)-C(11)-C(12)	121.14(10)	C(32)-C(27)-C(28)	120.32(11)
C(10)-C(11)-C(12)	119.64(11)	C(32)-C(27)-N(3)	119.01(11)
C(13)-C(12)-C(17)	117.37(11)	C(28)-C(27)-N(3)	120.39(12)
C(13)-C(12)-C(11)	116.38(11)	C(29)-C(28)-C(27)	118.17(13)
C(17)-C(12)-C(11)	126.24(11)	C(29)-C(28)-C(33)	120.43(13)
C(14)-C(13)-C(12)	123.88(12)	C(27)-C(28)-C(33)	121.40(11)
C(13)-C(14)-C(15)	118.24(12)	C(30)-C(29)-C(28)	122.26(14)
C(16)-C(15)-C(14)	120.50(12)	C(31)-C(30)-C(29)	118.40(13)
C(15)-C(16)-C(17)	122.76(12)	C(31)-C(30)-C(34)	121.75(15)
N(3)-C(17)-C(16)	120.67(11)	C(29)-C(30)-C(34)	119.83(15)
N(3)-C(17)-C(12)	122.43(11)	C(30)-C(31)-C(32)	121.93(14)
C(16)-C(17)-C(12)	116.89(11)	C(31)-C(32)-C(27)	118.90(13)
C(19)-C(18)-C(23)	119.24(12)	C(31)-C(32)-C(35)	120.65(13)
C(19)-C(18)-N(1)	120.38(11)	C(27)-C(32)-C(35)	120.45(12)
C(23)-C(18)-N(1)	120.30(12)	O(1)-C(36)-C(37)	105.45(11)
C(20)-C(19)-C(18)	119.27(13)	C(38)-C(37)-C(36)	102.94(11)
C(20)-C(19)-C(24)	120.45(13)	C(39)-C(38)-C(37)	101.77(11)
C(18)-C(19)-C(24)	120.28(12)	O(1)-C(39)-C(38)	104.19(11)
C(21)-C(20)-C(19)	122.43(14)		

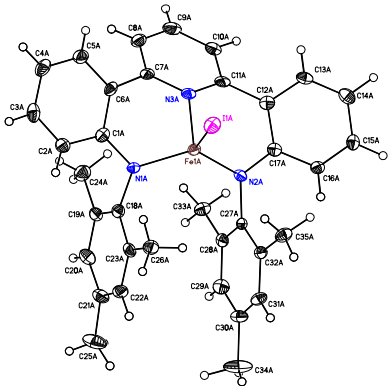
Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for [**2**]Fe(THF) **(CCDC 678268). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	173(1)	212(1)	203(1)	-40(1)	40(1)	-35(1)
O(1)	294(5)	220(5)	199(5)	-29(4)	43(4)	7(4)
N(1)	200(5)	194(6)	223(6)	-27(4)	35(4)	-29(4)
N(2)	170(4)	193(6)	160(5)	9(4)	25(4)	-11(4)
N(3)	150(4)	181(5)	228(5)	-43(5)	15(4)	-3(4)
C(1)	227(6)	218(7)	185(6)	21(5)	51(5)	-74(5)
C(2)	300(7)	238(7)	217(7)	-4(6)	68(6)	-71(6)
C(3)	412(8)	299(8)	181(7)	-6(6)	21(6)	-161(7)
C(4)	294(7)	370(9)	221(7)	63(6)	-48(6)	-129(7)
C(5)	248(6)	295(8)	248(7)	53(6)	2(5)	-45(6)
C(6)	182(6)	238(7)	196(6)	13(5)	20(5)	-61(5)
C(7)	184(5)	212(7)	198(6)	29(5)	20(5)	-5(5)
C(8)	173(6)	263(7)	283(7)	47(6)	52(5)	-23(5)
C(9)	228(6)	258(8)	323(8)	49(6)	137(6)	25(5)
C(10)	285(7)	222(7)	205(7)	2(5)	94(5)	24(6)
C(11)	207(6)	179(6)	166(6)	28(5)	40(5)	21(5)
C(12)	211(6)	190(7)	153(6)	5(5)	19(5)	2(5)
C(13)	257(6)	229(7)	235(7)	-9(6)	49(5)	39(6)

C(14)	353(7)	226(8)	300(8)	-94(6)	36(6)	8(6)
C(15)	290(7)	258(8)	309(8)	-69(6)	-20(6)	-50(6)
C(16)	207(6)	242(7)	259(7)	-32(6)	4(5)	-19(5)
C(17)	222(6)	179(7)	168(6)	16(5)	19(5)	-11(5)
C(18)	247(6)	210(7)	222(7)	-45(5)	17(5)	-25(5)
C(19)	289(7)	249(8)	284(8)	0(6)	29(6)	-46(6)
C(20)	402(8)	242(8)	373(9)	49(7)	21(7)	-75(7)
C(21)	419(8)	257(8)	368(9)	-27(7)	-21(7)	35(7)
C(22)	296(7)	287(8)	336(8)	-75(6)	43(6)	32(6)
C(23)	267(6)	251(7)	226(7)	-56(6)	35(5)	-17(6)
C(24)	356(8)	383(9)	380(9)	114(7)	96(7)	-60(7)
C(25)	574(10)	278(9)	595(12)	4(8)	-6(9)	80(8)
C(26)	275(7)	295(8)	366(8)	-65(7)	134(6)	-3(6)
C(27)	169(6)	222(7)	262(7)	-77(6)	13(5)	-23(5)
C(28)	200(6)	272(8)	284(7)	-85(6)	25(5)	-31(5)
C(29)	236(6)	377(9)	344(8)	-122(7)	99(6)	-66(6)
C(30)	233(7)	329(9)	496(10)	-137(7)	53(7)	59(6)
C(31)	291(7)	269(8)	471(10)	-43(7)	14(7)	79(6)
C(32)	238(6)	251(8)	337(8)	-49(6)	15(6)	17(6)
C(33)	229(6)	384(9)	339(8)	46(7)	59(6)	-66(6)
C(34)	350(9)	522(12)	877(15)	-138(11)	214(9)	147(8)
C(35)	357(8)	337(9)	443(10)	92(7)	46(7)	59(7)
C(36)	393(8)	362(9)	203(7)	-29(6)	73(6)	40(7)
C(37)	370(8)	377(9)	239(8)	15(7)	44(6)	-4(7)
C(38)	381(8)	277(8)	358(9)	56(7)	34(7)	-33(7)
C(39)	370(8)	257(8)	287(8)	-26(6)	39(6)	39(6)

[**2**]FeI

Contents



[**2**]FeI

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 695390. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 695390."

Table 1. Crystal data and structure refinement for [2]FeI (CCDC 695390).

Empirical formula	$2(C_{35}H_{33}N_3FeI)\ 1.5(C_6H_6)$	
Formula weight	1473.98	
Crystallization Solvent	Benzene/petroleumether	
Crystal Habit	Flake	
Crystal size	0.16 x 0.10 x 0.06 mm^3	
Crystal color	Dark brown	

Data Collection

Type of diffractometer	Bruker KAPPA APEX II	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	100(2) K	
θ range for 9935 reflections used in lattice determination	2.54 to 31.80°	
Unit cell dimensions	a = 14.8740(7) Å b = 14.9489(7) Å c = 16.9750(8) Å	α= 69.528(3)° β= 72.061(3)° γ = 76.207(3)°
Volume	3327.7(3) $Å^3$	
Z	4	
Crystal system	Triclinic	
Space group	P-1	
Density (calculated)	1.471 Mg/m^3	
F(000)	1498	
Data collection program	Bruker APEX2 v2.1-0	

θ range for data collection	1.66 to 32.13°
Completeness to θ = 32.13°	94.8 %
Index ranges	$-21 \le h \le 20$, $-22 \le k \le 21$, $-25 \le l \le 24$
Data collection scan type	ω scans; 17 settings
Data reduction program	Bruker SAINT-Plus v7.34A
Reflections collected	85468
Independent reflections	22141 [R_{int}= 0.0607]
Absorption coefficient	1.413 mm^{-1}
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.4344 and 0.3722

Table 1 (cont.)

Structure solution and Refinement

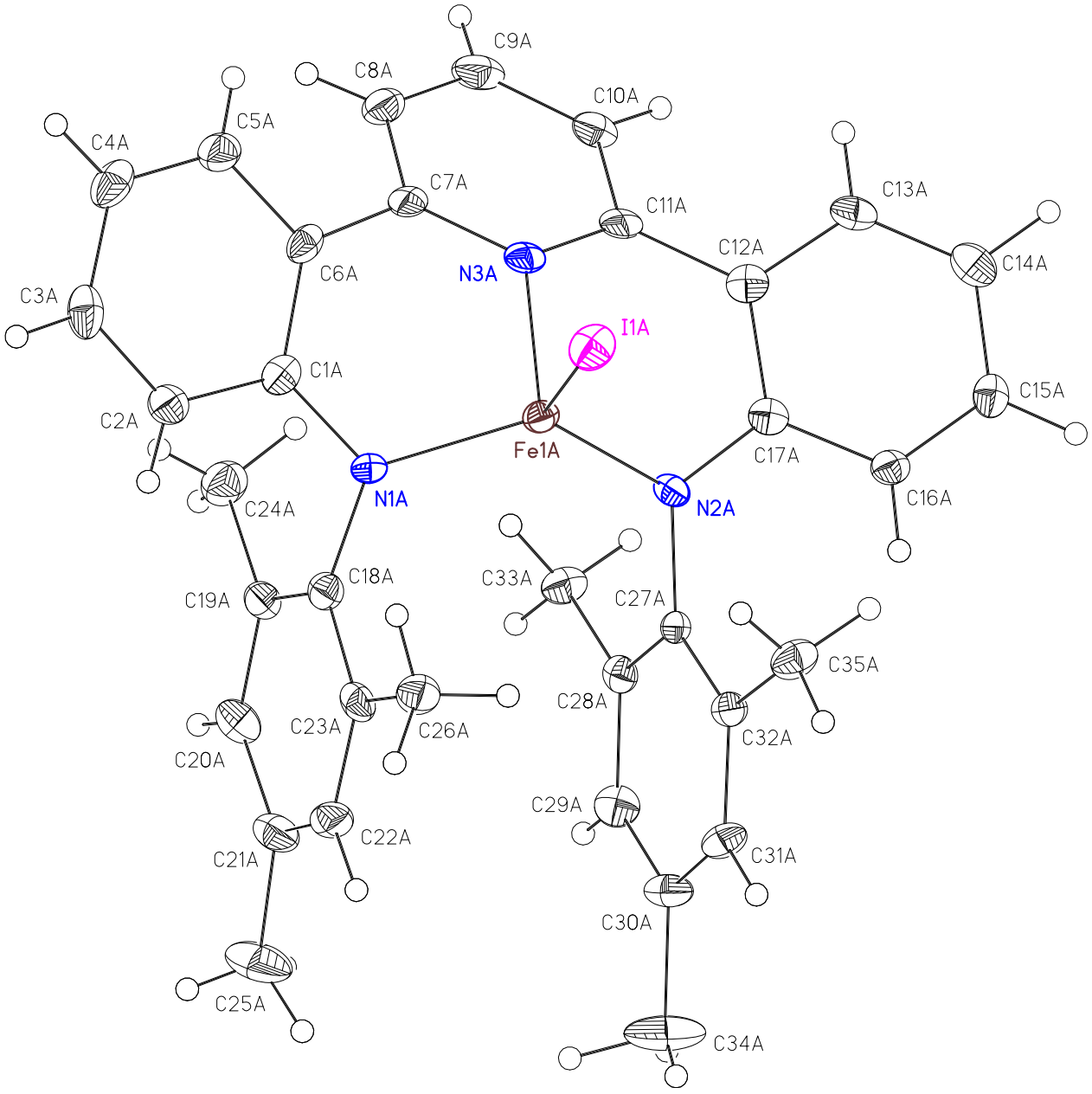
Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	22141 / 0 / 1102
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	1.524
Final R indices [I>2σ(I), 13476 reflections]	R1 = 0.0507, *w*R2 = 0.0602
R indices (all data)	R1 = 0.1132, *w*R2 = 0.0647
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.003
Average shift/error	0.000
Largest diff. peak and hole	1.916 and -1.795 e.$Å^{-3}$

Special Refinement Details

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.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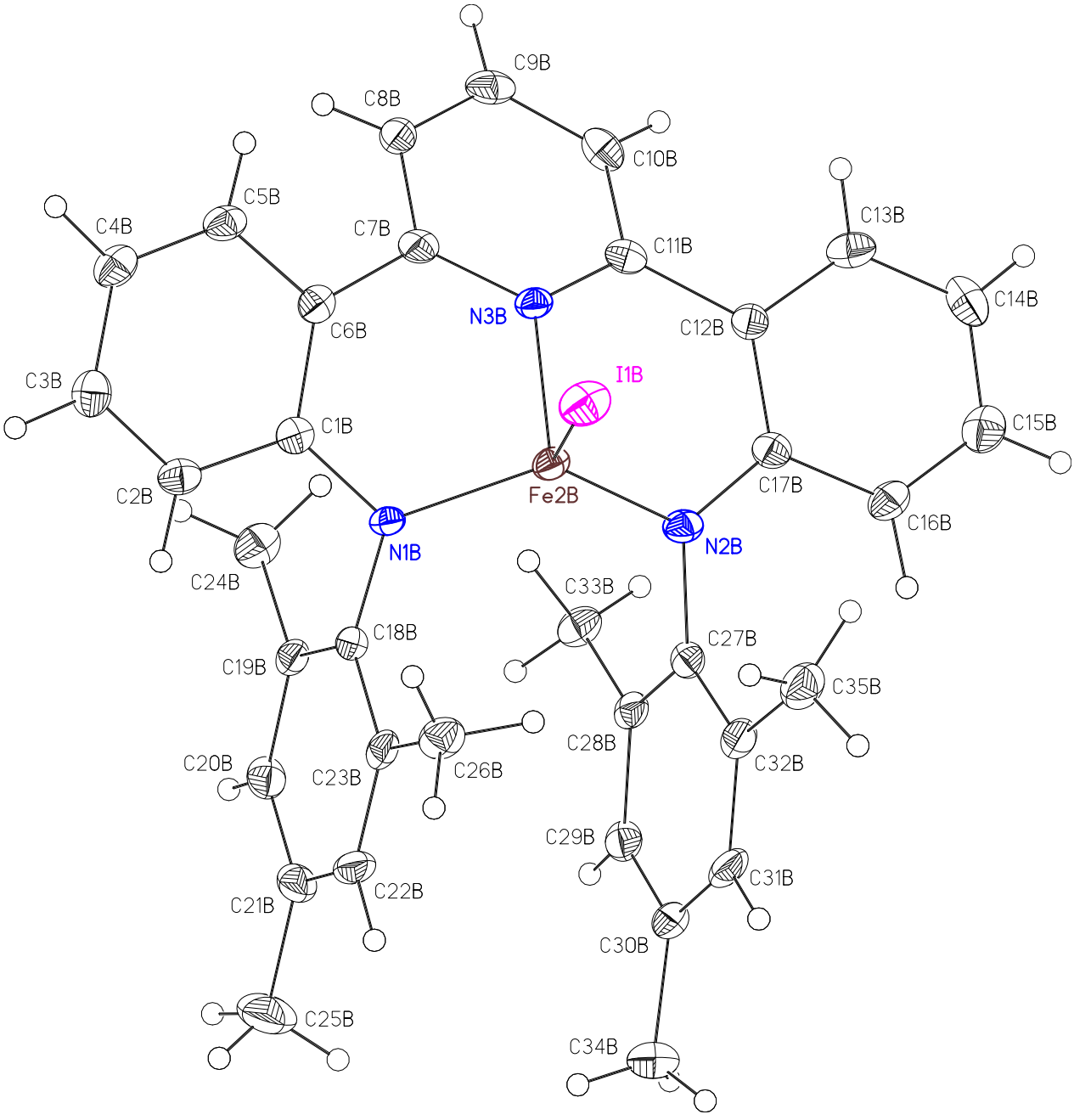
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C34B

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [**2**]FeI **(CCDC 695390). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.**

	x	y	z	U_{eq}
Fe(1A)	7733(1)	6797(1)	9594(1)	14(1)
I(1A)	9034(1)	6803(1)	10304(1)	22(1)
N(1A)	7164(2)	8029(2)	9000(1)	15(1)
N(2A)	6991(2)	5785(2)	10103(1)	14(1)
N(3A)	8373(2)	6424(2)	8490(1)	15(1)
C(1A)	7828(2)	8566(2)	8359(2)	16(1)
C(2A)	7785(2)	9546(2)	8240(2)	18(1)
C(3A)	8485(2)	10070(2)	7659(2)	23(1)
C(4A)	9263(2)	9626(2)	7158(2)	24(1)
C(5A)	9303(2)	8677(2)	7232(2)	22(1)
C(6A)	8601(2)	8124(2)	7809(2)	17(1)
C(7A)	8641(2)	7147(2)	7758(2)	17(1)
C(8A)	8926(2)	6978(2)	6952(2)	21(1)
C(9A)	8919(2)	6077(2)	6911(2)	24(1)
C(10A)	8649(2)	5360(2)	7654(2)	20(1)
C(11A)	8382(2)	5522(2)	8472(2)	16(1)
C(12A)	8097(2)	4739(2)	9261(2)	16(1)
C(13A)	8492(2)	3790(2)	9268(2)	19(1)
C(14A)	8181(2)	2995(2)	9922(2)	21(1)
C(15A)	7410(2)	3130(2)	10613(2)	17(1)
C(16A)	7027(2)	4047(2)	10647(2)	16(1)
C(17A)	7357(2)	4873(2)	10015(2)	14(1)
C(18A)	6176(2)	8444(2)	9186(2)	16(1)
C(19A)	5661(2)	8661(2)	8566(2)	18(1)
C(20A)	4674(2)	8922(2)	8799(2)	21(1)
C(21A)	4192(2)	8966(2)	9634(2)	22(1)
C(22A)	4737(2)	8802(2)	10216(2)	20(1)
C(23A)	5719(2)	8542(2)	10017(2)	17(1)
C(24A)	6135(3)	8585(3)	7663(2)	25(1)
C(25A)	3117(2)	9170(4)	9891(3)	35(1)
C(26A)	6268(2)	8374(3)	10677(2)	22(1)
C(27A)	6023(2)	5936(2)	10621(2)	13(1)
C(28A)	5287(2)	6171(2)	10211(2)	15(1)
C(29A)	4355(2)	6369(2)	10683(2)	19(1)
C(30A)	4150(2)	6325(2)	11550(2)	20(1)
C(31A)	4900(2)	6079(2)	11942(2)	18(1)
C(32A)	5846(2)	5879(2)	11494(2)	14(1)
C(33A)	5483(2)	6220(3)	9275(2)	20(1)
C(34A)	3127(2)	6531(4)	12043(3)	38(1)
C(35A)	6631(2)	5585(3)	11954(2)	21(1)
Fe(2B)	2563(1)	7908(1)	5601(1)	15(1)
I(1B)	1359(1)	9349(1)	5034(1)	25(1)
N(1B)	3345(2)	8156(2)	6179(1)	15(1)
N(2B)	3089(2)	6942(2)	5040(1)	16(1)
N(3B)	1832(2)	7032(2)	6682(1)	15(1)
C(1B)	2814(2)	8512(2)	6866(2)	15(1)

C(2B)	3128(2)	9216(2)	7047(2)	19(1)
C(3B)	2569(2)	9650(2)	7667(2)	21(1)
C(4B)	1679(2)	9394(2)	8131(2)	21(1)
C(5B)	1375(2)	8680(2)	7996(2)	19(1)
C(6B)	1930(2)	8195(2)	7384(2)	16(1)
C(7B)	1617(2)	7311(2)	7417(2)	17(1)
C(8B)	1126(2)	6738(2)	8196(2)	19(1)
C(9B)	895(2)	5884(2)	8233(2)	21(1)
C(10B)	1162(2)	5596(2)	7496(2)	20(1)
C(11B)	1613(2)	6185(2)	6707(2)	16(1)
C(12B)	1870(2)	5893(2)	5899(2)	17(1)
C(13B)	1373(2)	5194(2)	5910(2)	22(1)
C(14B)	1617(2)	4758(2)	5258(2)	25(1)
C(15B)	2389(2)	5023(2)	4563(2)	23(1)
C(16B)	2868(2)	5723(2)	4517(2)	19(1)
C(17B)	2615(2)	6199(2)	5156(2)	17(1)
C(18B)	4357(2)	8138(2)	5915(2)	15(1)
C(19B)	4925(2)	7499(2)	6459(2)	15(1)
C(20B)	5915(2)	7440(2)	6167(2)	20(1)
C(21B)	6348(2)	7993(2)	5361(2)	21(1)
C(22B)	5776(2)	8625(2)	4835(2)	21(1)
C(23B)	4783(2)	8722(2)	5090(2)	17(1)
C(24B)	4486(2)	6884(3)	7340(2)	23(1)
C(25B)	7428(2)	7925(3)	5055(3)	36(1)
C(26B)	4198(2)	9436(2)	4505(2)	23(1)
C(27B)	4033(2)	7003(2)	4476(2)	15(1)
C(28B)	4814(2)	6468(2)	4821(2)	16(1)
C(29B)	5733(2)	6607(2)	4304(2)	20(1)
C(30B)	5894(2)	7239(2)	3474(2)	20(1)
C(31B)	5110(2)	7738(2)	3144(2)	21(1)
C(32B)	4177(2)	7629(2)	3629(2)	19(1)
C(33B)	4662(2)	5779(2)	5719(2)	21(1)
C(34B)	6900(3)	7403(3)	2965(2)	31(1)
C(35B)	3349(2)	8191(3)	3241(2)	26(1)
C(41)	9959(2)	8043(2)	3955(2)	31(1)
C(42)	10483(3)	7138(3)	4013(2)	31(1)
C(43)	10445(2)	6636(3)	3490(2)	37(1)
C(44)	9886(2)	7032(3)	2909(2)	36(1)
C(45)	9370(2)	7937(3)	2841(2)	30(1)
C(46)	9411(2)	8439(2)	3367(2)	29(1)
C(51)	588(2)	421(2)	206(2)	26(1)
C(52)	117(2)	952(2)	-423(2)	25(1)
C(53)	488(2)	-534(3)	629(2)	26(1)

Table 3. Selected bond lengths [Å] and angles [°] for [**2**]FeI **(CCDC 695390).**

Fe(1A)-N(2A)	1.883(2)	N(2A)-Fe(1A)-N(1A)	118.30(10)
Fe(1A)-N(1A)	1.899(2)	N(2A)-Fe(1A)-N(3A)	94.66(9)
Fe(1A)-N(3A)	2.0274(19)	N(1A)-Fe(1A)-N(3A)	93.44(9)
Fe(1A)-I(1A)	2.5784(4)	N(2A)-Fe(1A)-I(1A)	118.77(7)
Fe(2B)-N(2B)	1.888(2)	N(1A)-Fe(1A)-I(1A)	115.77(7)
Fe(2B)-N(1B)	1.902(2)	N(3A)-Fe(1A)-I(1A)	108.74(6)
Fe(2B)-N(3B)	2.008(2)	N(2B)-Fe(2B)-N(1B)	116.72(9)
Fe(2B)-I(1B)	2.5576(5)	N(2B)-Fe(2B)-N(3B)	94.66(9)
		N(1B)-Fe(2B)-N(3B)	94.36(9)
		N(2B)-Fe(2B)-I(1B)	121.38(7)
		N(1B)-Fe(2B)-I(1B)	115.03(7)
		N(3B)-Fe(2B)-I(1B)	107.04(6)

Table 4. Bond lengths [Å] and angles [°] for [**2**]FeI **(CCDC 695390).**

Fe(1A)-N(2A)	1.883(2)	C(14A)-H(14A)	1.00(3)
Fe(1A)-N(1A)	1.899(2)	C(15A)-C(16A)	1.368(4)
Fe(1A)-N(3A)	2.0274(19)	C(15A)-H(15A)	0.97(2)
Fe(1A)-I(1A)	2.5784(4)	C(16A)-C(17A)	1.399(4)
N(1A)-C(1A)	1.381(3)	C(16A)-H(16A)	0.90(2)
N(1A)-C(18A)	1.435(3)	C(18A)-C(19A)	1.393(4)
N(2A)-C(17A)	1.385(3)	C(18A)-C(23A)	1.406(3)
N(2A)-C(27A)	1.449(3)	C(19A)-C(20A)	1.394(4)
N(3A)-C(7A)	1.354(3)	C(19A)-C(24A)	1.508(4)
N(3A)-C(11A)	1.356(3)	C(20A)-C(21A)	1.395(4)
C(1A)-C(2A)	1.396(4)	C(20A)-H(20A)	0.96(2)
C(1A)-C(6A)	1.426(3)	C(21A)-C(22A)	1.386(4)
C(2A)-C(3A)	1.373(4)	C(21A)-C(25A)	1.508(4)
C(2A)-H(2A)	0.85(2)	C(22A)-C(23A)	1.384(4)
C(3A)-C(4A)	1.388(4)	C(22A)-H(22A)	0.92(2)
C(3A)-H(3A)	0.89(2)	C(23A)-C(26A)	1.502(4)
C(4A)-C(5A)	1.369(4)	C(24A)-H(24A)	1.01(3)
C(4A)-H(4A)	0.91(3)	C(24A)-H(24B)	0.94(3)
C(5A)-C(6A)	1.396(4)	C(24A)-H(24C)	0.86(3)
C(5A)-H(5A)	0.82(3)	C(25A)-H(25A)	0.88(3)
C(6A)-C(7A)	1.479(4)	C(25A)-H(25B)	0.80(4)
C(7A)-C(8A)	1.398(3)	C(25A)-H(25C)	0.97(5)
C(8A)-C(9A)	1.374(4)	C(26A)-H(26A)	0.96(2)
C(8A)-H(8A)	0.87(2)	C(26A)-H(26B)	0.95(3)
C(9A)-C(10A)	1.359(4)	C(26A)-H(26C)	0.94(3)
C(9A)-H(9A)	0.90(2)	C(27A)-C(28A)	1.386(4)
C(10A)-C(11A)	1.412(3)	C(27A)-C(32A)	1.398(3)
C(10A)-H(10A)	0.90(2)	C(28A)-C(29A)	1.392(4)
C(11A)-C(12A)	1.462(4)	C(28A)-C(33A)	1.502(4)
C(12A)-C(13A)	1.396(4)	C(29A)-C(30A)	1.388(4)
C(12A)-C(17A)	1.448(3)	C(29A)-H(29A)	0.87(3)
C(13A)-C(14A)	1.372(4)	C(30A)-C(31A)	1.384(4)
C(13A)-H(13A)	0.86(2)	C(30A)-C(34A)	1.511(4)
C(14A)-C(15A)	1.399(4)	C(31A)-C(32A)	1.395(3)

C(31A)-H(31A)	0.91(2)	C(20B)-C(21B)	1.375(4)
C(32A)-C(35A)	1.499(4)	C(20B)-H(20B)	0.96(3)
C(33A)-H(33A)	0.93(3)	C(21B)-C(22B)	1.381(4)
C(33A)-H(33B)	0.92(4)	C(21B)-C(25B)	1.519(4)
C(33A)-H(33C)	0.92(3)	C(22B)-C(23B)	1.393(4)
C(34A)-H(34A)	0.76(3)	C(22B)-H(22B)	0.95(3)
C(34A)-H(34B)	0.79(3)	C(23B)-C(26B)	1.493(4)
C(34A)-H(34C)	1.04(6)	C(24B)-H(24D)	0.94(2)
C(35A)-H(35A)	0.93(3)	C(24B)-H(24E)	0.94(3)
C(35A)-H(35B)	0.86(3)	C(24B)-H(24F)	0.93(3)
C(35A)-H(35C)	0.97(3)	C(25B)-H(25D)	0.89(4)
Fe(2B)-N(2B)	1.888(2)	C(25B)-H(25E)	0.95(3)
Fe(2B)-N(1B)	1.902(2)	C(25B)-H(25F)	0.91(5)
Fe(2B)-N(3B)	2.008(2)	C(26B)-H(26D)	0.93(4)
Fe(2B)-I(1B)	2.5576(5)	C(26B)-H(26E)	0.89(3)
N(1B)-C(1B)	1.391(3)	C(26B)-H(26F)	0.99(3)
N(1B)-C(18B)	1.430(3)	C(27B)-C(32B)	1.398(4)
N(2B)-C(17B)	1.381(3)	C(27B)-C(28B)	1.406(4)
N(2B)-C(27B)	1.438(3)	C(28B)-C(29B)	1.397(4)
N(3B)-C(11B)	1.364(3)	C(28B)-C(33B)	1.495(4)
N(3B)-C(7B)	1.374(3)	C(29B)-C(30B)	1.379(4)
C(1B)-C(2B)	1.403(4)	C(29B)-H(29B)	0.91(3)
C(1B)-C(6B)	1.422(4)	C(30B)-C(31B)	1.388(4)
C(2B)-C(3B)	1.379(3)	C(30B)-C(34B)	1.508(4)
C(2B)-H(2B)	0.93(2)	C(31B)-C(32B)	1.394(4)
C(3B)-C(4B)	1.381(4)	C(31B)-H(31B)	0.91(3)
C(3B)-H(3B)	0.95(2)	C(32B)-C(35B)	1.508(4)
C(4B)-C(5B)	1.364(4)	C(33B)-H(33D)	0.93(2)
C(4B)-H(4B)	0.96(2)	C(33B)-H(33E)	0.96(3)
C(5B)-C(6B)	1.414(3)	C(33B)-H(33F)	1.06(4)
C(5B)-H(5B)	0.88(3)	C(34B)-H(34D)	0.88(4)
C(6B)-C(7B)	1.480(4)	C(34B)-H(34E)	0.92(4)
C(7B)-C(8B)	1.388(4)	C(34B)-H(34F)	0.91(3)
C(8B)-C(9B)	1.375(4)	C(35B)-H(35D)	0.87(3)
C(8B)-H(8B)	0.87(2)	C(35B)-H(35E)	0.98(3)
C(9B)-C(10B)	1.378(4)	C(35B)-H(35F)	0.94(3)
C(9B)-H(9B)	0.98(3)	C(41)-C(46)	1.367(4)
C(10B)-C(11B)	1.386(4)	C(41)-C(42)	1.378(4)
C(10B)-H(10B)	0.88(2)	C(41)-H(41)	0.86(2)
C(11B)-C(12B)	1.495(3)	C(42)-C(43)	1.368(4)
C(12B)-C(13B)	1.410(4)	C(42)-H(42)	0.88(3)
C(12B)-C(17B)	1.417(4)	C(43)-C(44)	1.371(5)
C(13B)-C(14B)	1.387(4)	C(43)-H(43)	1.00(3)
C(13B)-H(13B)	0.89(3)	C(44)-C(45)	1.372(5)
C(14B)-C(15B)	1.386(4)	C(44)-H(44)	0.93(3)
C(14B)-H(14B)	0.84(2)	C(45)-C(46)	1.373(4)
C(15B)-C(16B)	1.368(4)	C(45)-H(45)	0.97(3)
C(15B)-H(15B)	0.92(2)	C(46)-H(46)	0.90(2)
C(16B)-C(17B)	1.408(3)	C(51)-C(52)	1.364(4)
C(16B)-H(16B)	0.97(2)	C(51)-C(53)	1.377(4)
C(18B)-C(19B)	1.399(4)	C(51)-H(51)	0.93(3)
C(18B)-C(23B)	1.409(4)	C(52)-C(53)#1	1.392(4)
C(19B)-C(20B)	1.393(4)	C(52)-H(52)	0.91(2)
C(19B)-C(24B)	1.494(4)	C(53)-C(52)#1	1.392(4)

C(53)-H(53)	0.87(3)	C(14A)-C(13A)-H(13A)	118.4(19)
		C(12A)-C(13A)-H(13A)	118.0(19)
N(2A)-Fe(1A)-N(1A)	118.30(10)	C(13A)-C(14A)-C(15A)	118.9(3)
N(2A)-Fe(1A)-N(3A)	94.66(9)	C(13A)-C(14A)-H(14A)	121.9(17)
N(1A)-Fe(1A)-N(3A)	93.44(9)	C(15A)-C(14A)-H(14A)	119.2(17)
N(2A)-Fe(1A)-I(1A)	118.77(7)	C(16A)-C(15A)-C(14A)	119.3(3)
N(1A)-Fe(1A)-I(1A)	115.77(7)	C(16A)-C(15A)-H(15A)	120.6(13)
N(3A)-Fe(1A)-I(1A)	108.74(6)	C(14A)-C(15A)-H(15A)	119.9(13)
C(1A)-N(1A)-C(18A)	120.0(2)	C(15A)-C(16A)-C(17A)	123.3(3)
C(1A)-N(1A)-Fe(1A)	112.52(18)	C(15A)-C(16A)-H(16A)	121.3(17)
C(18A)-N(1A)-Fe(1A)	127.38(18)	C(17A)-C(16A)-H(16A)	115.3(17)
C(17A)-N(2A)-C(27A)	118.0(2)	N(2A)-C(17A)-C(16A)	121.4(2)
C(17A)-N(2A)-Fe(1A)	121.37(17)	N(2A)-C(17A)-C(12A)	121.2(2)
C(27A)-N(2A)-Fe(1A)	120.59(16)	C(16A)-C(17A)-C(12A)	117.4(2)
C(7A)-N(3A)-C(11A)	122.0(2)	C(19A)-C(18A)-C(23A)	120.7(2)
C(7A)-N(3A)-Fe(1A)	116.75(17)	C(19A)-C(18A)-N(1A)	119.3(2)
C(11A)-N(3A)-Fe(1A)	120.33(18)	C(23A)-C(18A)-N(1A)	119.8(2)
N(1A)-C(1A)-C(2A)	121.6(2)	C(18A)-C(19A)-C(20A)	118.8(2)
N(1A)-C(1A)-C(6A)	120.7(2)	C(18A)-C(19A)-C(24A)	122.0(3)
C(2A)-C(1A)-C(6A)	117.7(3)	C(20A)-C(19A)-C(24A)	119.2(3)
C(3A)-C(2A)-C(1A)	122.4(3)	C(19A)-C(20A)-C(21A)	121.7(3)
C(3A)-C(2A)-H(2A)	117.3(18)	C(19A)-C(20A)-H(20A)	117.1(15)
C(1A)-C(2A)-H(2A)	120.3(18)	C(21A)-C(20A)-H(20A)	121.2(15)
C(2A)-C(3A)-C(4A)	119.8(3)	C(22A)-C(21A)-C(20A)	117.7(3)
C(2A)-C(3A)-H(3A)	118.4(16)	C(22A)-C(21A)-C(25A)	121.7(3)
C(4A)-C(3A)-H(3A)	121.8(16)	C(20A)-C(21A)-C(25A)	120.7(3)
C(5A)-C(4A)-C(3A)	119.1(3)	C(23A)-C(22A)-C(21A)	122.7(3)
C(5A)-C(4A)-H(4A)	123.2(16)	C(23A)-C(22A)-H(22A)	115.3(17)
C(3A)-C(4A)-H(4A)	117.6(16)	C(21A)-C(22A)-H(22A)	121.9(17)
C(4A)-C(5A)-C(6A)	122.6(3)	C(22A)-C(23A)-C(18A)	118.2(3)
C(4A)-C(5A)-H(5A)	121(2)	C(22A)-C(23A)-C(26A)	120.1(2)
C(6A)-C(5A)-H(5A)	117(2)	C(18A)-C(23A)-C(26A)	121.7(3)
C(5A)-C(6A)-C(1A)	118.2(3)	C(19A)-C(24A)-H(24A)	114.5(16)
C(5A)-C(6A)-C(7A)	118.4(2)	C(19A)-C(24A)-H(24B)	108.2(16)
C(1A)-C(6A)-C(7A)	123.1(2)	H(24A)-C(24A)-H(24B)	106(2)
N(3A)-C(7A)-C(8A)	119.9(3)	C(19A)-C(24A)-H(24C)	108.4(18)
N(3A)-C(7A)-C(6A)	120.1(2)	H(24A)-C(24A)-H(24C)	107(3)
C(8A)-C(7A)-C(6A)	120.0(3)	H(24B)-C(24A)-H(24C)	113(3)
C(9A)-C(8A)-C(7A)	119.3(3)	C(21A)-C(25A)-H(25A)	115(2)
C(9A)-C(8A)-H(8A)	122.2(14)	C(21A)-C(25A)-H(25B)	115(3)
C(7A)-C(8A)-H(8A)	118.4(14)	H(25A)-C(25A)-H(25B)	107(4)
C(10A)-C(9A)-C(8A)	119.8(3)	C(21A)-C(25A)-H(25C)	114(3)
C(10A)-C(9A)-H(9A)	120.9(16)	H(25A)-C(25A)-H(25C)	105(4)
C(8A)-C(9A)-H(9A)	119.1(16)	H(25B)-C(25A)-H(25C)	99(4)
C(9A)-C(10A)-C(11A)	121.0(3)	C(23A)-C(26A)-H(26A)	114.4(16)
C(9A)-C(10A)-H(10A)	122.4(15)	C(23A)-C(26A)-H(26B)	110(2)
C(11A)-C(10A)-H(10A)	116.6(15)	H(26A)-C(26A)-H(26B)	109(2)
N(3A)-C(11A)-C(10A)	117.9(3)	C(23A)-C(26A)-H(26C)	113.7(19)
N(3A)-C(11A)-C(12A)	122.2(2)	H(26A)-C(26A)-H(26C)	105(2)
C(10A)-C(11A)-C(12A)	119.9(3)	H(26B)-C(26A)-H(26C)	105(3)
C(13A)-C(12A)-C(17A)	117.1(3)	C(28A)-C(27A)-C(32A)	121.5(2)
C(13A)-C(12A)-C(11A)	118.7(2)	C(28A)-C(27A)-N(2A)	117.6(2)
C(17A)-C(12A)-C(11A)	123.9(2)	C(32A)-C(27A)-N(2A)	120.9(2)
C(14A)-C(13A)-C(12A)	123.6(3)	C(27A)-C(28A)-C(29A)	118.6(2)

C(27A)-C(28A)-C(33A)	121.1(2)	C(2B)-C(3B)-H(3B)	117.4(14)
C(29A)-C(28A)-C(33A)	120.2(3)	C(4B)-C(3B)-H(3B)	122.4(14)
C(30A)-C(29A)-C(28A)	121.6(3)	C(5B)-C(4B)-C(3B)	119.4(3)
C(30A)-C(29A)-H(29A)	121.1(17)	C(5B)-C(4B)-H(4B)	118.7(15)
C(28A)-C(29A)-H(29A)	117.2(17)	C(3B)-C(4B)-H(4B)	121.7(15)
C(31A)-C(30A)-C(29A)	118.3(3)	C(4B)-C(5B)-C(6B)	122.6(3)
C(31A)-C(30A)-C(34A)	121.7(3)	C(4B)-C(5B)-H(5B)	122.4(16)
C(29A)-C(30A)-C(34A)	120.0(3)	C(6B)-C(5B)-H(5B)	115.0(16)
C(30A)-C(31A)-C(32A)	122.1(2)	C(5B)-C(6B)-C(1B)	117.5(2)
C(30A)-C(31A)-H(31A)	119.4(15)	C(5B)-C(6B)-C(7B)	117.4(2)
C(32A)-C(31A)-H(31A)	118.5(15)	C(1B)-C(6B)-C(7B)	124.5(2)
C(31A)-C(32A)-C(27A)	117.8(3)	N(3B)-C(7B)-C(8B)	119.1(3)
C(31A)-C(32A)-C(35A)	120.2(2)	N(3B)-C(7B)-C(6B)	120.4(2)
C(27A)-C(32A)-C(35A)	122.0(2)	C(8B)-C(7B)-C(6B)	120.4(2)
C(28A)-C(33A)-H(33A)	110.7(16)	C(9B)-C(8B)-C(7B)	120.1(3)
C(28A)-C(33A)-H(33B)	116(2)	C(9B)-C(8B)-H(8B)	122.6(17)
H(33A)-C(33A)-H(33B)	106(3)	C(7B)-C(8B)-H(8B)	117.0(17)
C(28A)-C(33A)-H(33C)	108.1(17)	C(8B)-C(9B)-C(10B)	119.6(3)
H(33A)-C(33A)-H(33C)	106(2)	C(8B)-C(9B)-H(9B)	119.3(14)
H(33B)-C(33A)-H(33C)	110(3)	C(10B)-C(9B)-H(9B)	120.5(14)
C(30A)-C(34A)-H(34A)	116(3)	C(9B)-C(10B)-C(11B)	120.6(3)
C(30A)-C(34A)-H(34B)	113(2)	C(9B)-C(10B)-H(10B)	119.2(16)
H(34A)-C(34A)-H(34B)	129(4)	C(11B)-C(10B)-H(10B)	120.2(15)
C(30A)-C(34A)-H(34C)	108(3)	N(3B)-C(11B)-C(10B)	118.9(2)
H(34A)-C(34A)-H(34C)	98(4)	N(3B)-C(11B)-C(12B)	120.4(2)
H(34B)-C(34A)-H(34C)	78(4)	C(10B)-C(11B)-C(12B)	120.8(3)
C(32A)-C(35A)-H(35A)	114.9(19)	C(13B)-C(12B)-C(17B)	117.4(2)
C(32A)-C(35A)-H(35B)	109(2)	C(13B)-C(12B)-C(11B)	116.6(2)
H(35A)-C(35A)-H(35B)	106(2)	C(17B)-C(12B)-C(11B)	125.8(2)
C(32A)-C(35A)-H(35C)	111.9(17)	C(14B)-C(13B)-C(12B)	123.2(3)
H(35A)-C(35A)-H(35C)	105(3)	C(14B)-C(13B)-H(13B)	117.4(17)
H(35B)-C(35A)-H(35C)	109(2)	C(12B)-C(13B)-H(13B)	119.3(16)
N(2B)-Fe(2B)-N(1B)	116.72(9)	C(15B)-C(14B)-C(13B)	118.3(3)
N(2B)-Fe(2B)-N(3B)	94.66(9)	C(15B)-C(14B)-H(14B)	121.7(17)
N(1B)-Fe(2B)-N(3B)	94.36(9)	C(13B)-C(14B)-H(14B)	119.8(18)
N(2B)-Fe(2B)-I(1B)	121.38(7)	C(16B)-C(15B)-C(14B)	120.1(3)
N(1B)-Fe(2B)-I(1B)	115.03(7)	C(16B)-C(15B)-H(15B)	122.5(18)
N(3B)-Fe(2B)-I(1B)	107.04(6)	C(14B)-C(15B)-H(15B)	117.4(18)
C(1B)-N(1B)-C(18B)	119.3(2)	C(15B)-C(16B)-C(17B)	122.8(3)
C(1B)-N(1B)-Fe(2B)	112.61(17)	C(15B)-C(16B)-H(16B)	117.8(13)
C(18B)-N(1B)-Fe(2B)	127.48(15)	C(17B)-C(16B)-H(16B)	119.2(13)
C(17B)-N(2B)-C(27B)	120.1(2)	N(2B)-C(17B)-C(16B)	119.7(2)
C(17B)-N(2B)-Fe(2B)	123.15(17)	N(2B)-C(17B)-C(12B)	122.3(2)
C(27B)-N(2B)-Fe(2B)	116.77(17)	C(16B)-C(17B)-C(12B)	118.0(3)
C(11B)-N(3B)-C(7B)	121.5(2)	C(19B)-C(18B)-C(23B)	120.3(2)
C(11B)-N(3B)-Fe(2B)	122.99(16)	C(19B)-C(18B)-N(1B)	119.6(2)
C(7B)-N(3B)-Fe(2B)	115.34(18)	C(23B)-C(18B)-N(1B)	120.0(3)
N(1B)-C(1B)-C(2B)	120.6(2)	C(20B)-C(19B)-C(18B)	118.9(3)
N(1B)-C(1B)-C(6B)	120.9(2)	C(20B)-C(19B)-C(24B)	120.0(3)
C(2B)-C(1B)-C(6B)	118.5(2)	C(18B)-C(19B)-C(24B)	121.1(3)
C(3B)-C(2B)-C(1B)	121.5(3)	C(21B)-C(20B)-C(19B)	121.9(3)
C(3B)-C(2B)-H(2B)	117.2(13)	C(21B)-C(20B)-H(20B)	118.0(17)
C(1B)-C(2B)-H(2B)	121.2(13)	C(19B)-C(20B)-H(20B)	120.1(17)
C(2B)-C(3B)-C(4B)	120.2(3)	C(20B)-C(21B)-C(22B)	118.4(3)

C(20B)-C(21B)-C(25B)	121.2(3)	C(28B)-C(33B)-H(33E)	111.9(17)
C(22B)-C(21B)-C(25B)	120.4(3)	H(33D)-C(33B)-H(33E)	106(2)
C(21B)-C(22B)-C(23B)	122.5(3)	C(28B)-C(33B)-H(33F)	114(2)
C(21B)-C(22B)-H(22B)	118.3(18)	H(33D)-C(33B)-H(33F)	109(2)
C(23B)-C(22B)-H(22B)	119.2(18)	H(33E)-C(33B)-H(33F)	101(2)
C(22B)-C(23B)-C(18B)	117.9(3)	C(30B)-C(34B)-H(34D)	111(2)
C(22B)-C(23B)-C(26B)	120.3(3)	C(30B)-C(34B)-H(34E)	107(3)
C(18B)-C(23B)-C(26B)	121.7(3)	H(34D)-C(34B)-H(34E)	109(3)
C(19B)-C(24B)-H(24D)	111.5(17)	C(30B)-C(34B)-H(34F)	111.0(19)
C(19B)-C(24B)-H(24E)	114.8(18)	H(34D)-C(34B)-H(34F)	102(3)
H(24D)-C(24B)-H(24E)	109(2)	H(34E)-C(34B)-H(34F)	117(3)
C(19B)-C(24B)-H(24F)	110(2)	C(32B)-C(35B)-H(35D)	112(2)
H(24D)-C(24B)-H(24F)	110(2)	C(32B)-C(35B)-H(35E)	108.9(19)
H(24E)-C(24B)-H(24F)	101(3)	H(35D)-C(35B)-H(35E)	115(3)
C(21B)-C(25B)-H(25D)	113(2)	C(32B)-C(35B)-H(35F)	111(2)
C(21B)-C(25B)-H(25E)	114(2)	H(35D)-C(35B)-H(35F)	102(3)
H(25D)-C(25B)-H(25E)	112(3)	H(35E)-C(35B)-H(35F)	109(3)
C(21B)-C(25B)-H(25F)	113(3)	C(46)-C(41)-C(42)	119.8(3)
H(25D)-C(25B)-H(25F)	97(4)	C(46)-C(41)-H(41)	117(2)
H(25E)-C(25B)-H(25F)	106(3)	C(42)-C(41)-H(41)	123(2)
C(23B)-C(26B)-H(26D)	116(2)	C(43)-C(42)-C(41)	120.0(4)
C(23B)-C(26B)-H(26E)	115.2(19)	C(43)-C(42)-H(42)	118.9(19)
H(26D)-C(26B)-H(26E)	103(3)	C(41)-C(42)-H(42)	121.0(19)
C(23B)-C(26B)-H(26F)	115.6(17)	C(42)-C(43)-C(44)	120.0(3)
H(26D)-C(26B)-H(26F)	103(2)	C(42)-C(43)-H(43)	120.9(18)
H(26E)-C(26B)-H(26F)	103(2)	C(44)-C(43)-H(43)	118.9(18)
C(32B)-C(27B)-C(28B)	120.8(2)	C(43)-C(44)-C(45)	120.3(3)
C(32B)-C(27B)-N(2B)	120.9(2)	C(43)-C(44)-H(44)	118.9(19)
C(28B)-C(27B)-N(2B)	118.2(2)	C(45)-C(44)-H(44)	120.8(19)
C(29B)-C(28B)-C(27B)	118.1(3)	C(44)-C(45)-C(46)	119.5(3)
C(29B)-C(28B)-C(33B)	121.0(3)	C(44)-C(45)-H(45)	118.0(15)
C(27B)-C(28B)-C(33B)	120.8(3)	C(46)-C(45)-H(45)	122.4(15)
C(30B)-C(29B)-C(28B)	122.2(3)	C(41)-C(46)-C(45)	120.5(3)
C(30B)-C(29B)-H(29B)	119.4(18)	C(41)-C(46)-H(46)	120.6(17)
C(28B)-C(29B)-H(29B)	118.3(18)	C(45)-C(46)-H(46)	118.9(17)
C(29B)-C(30B)-C(31B)	118.3(3)	C(52)-C(51)-C(53)	120.7(3)
C(29B)-C(30B)-C(34B)	120.0(3)	C(52)-C(51)-H(51)	121(2)
C(31B)-C(30B)-C(34B)	121.7(3)	C(53)-C(51)-H(51)	118(2)
C(30B)-C(31B)-C(32B)	122.0(3)	C(51)-C(52)-C(53)#1	120.0(3)
C(30B)-C(31B)-H(31B)	119.6(18)	C(51)-C(52)-H(52)	119.3(16)
C(32B)-C(31B)-H(31B)	118.4(18)	C(53)#1-C(52)-H(52)	120.6(16)
C(31B)-C(32B)-C(27B)	118.5(3)	C(51)-C(53)-C(52)#1	119.2(3)
C(31B)-C(32B)-C(35B)	120.0(3)	C(51)-C(53)-H(53)	121.0(19)
C(27B)-C(32B)-C(35B)	121.5(3)	C(52)#1-C(53)-H(53)	119.6(19)
C(28B)-C(33B)-H(33D)	114.1(16)		

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y,-z

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for [2]FeI (CCDC 695390). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1A)	119(2)	156(2)	132(2)	-39(2)	-15(2)	-27(2)
I(1A)	183(1)	268(1)	223(1)	-48(1)	-71(1)	-75(1)
N(1A)	154(13)	146(13)	124(11)	-48(10)	13(10)	-5(10)
N(2A)	116(12)	128(13)	174(12)	-66(10)	-31(10)	0(10)
N(3A)	78(12)	202(14)	161(12)	-62(11)	-35(9)	1(10)
C(1A)	134(15)	211(17)	148(14)	-23(13)	-65(12)	-54(13)
C(2A)	151(16)	210(18)	189(15)	-47(14)	-65(13)	-10(14)
C(3A)	264(19)	154(18)	284(17)	-4(15)	-129(14)	-65(15)
C(4A)	185(18)	290(20)	214(16)	21(15)	-64(14)	-113(15)
C(5A)	151(17)	250(20)	198(16)	-26(15)	-32(13)	-18(14)
C(6A)	135(15)	216(17)	119(13)	13(12)	-51(12)	-45(13)
C(7A)	58(14)	217(17)	178(14)	-19(13)	-24(11)	-6(12)
C(8A)	161(16)	268(19)	140(15)	-17(15)	-19(13)	-13(14)
C(9A)	191(17)	330(20)	180(16)	-128(15)	-30(13)	43(15)
C(10A)	169(16)	218(19)	209(15)	-107(15)	-37(12)	26(14)
C(11A)	49(14)	218(17)	209(15)	-71(13)	-29(11)	-3(12)
C(12A)	134(15)	193(17)	190(15)	-78(13)	-51(12)	-54(13)
C(13A)	122(15)	243(18)	207(15)	-105(14)	-41(13)	10(14)
C(14A)	198(17)	212(18)	265(16)	-113(15)	-96(13)	11(14)
C(15A)	166(16)	162(17)	186(15)	-17(13)	-85(12)	-42(13)
C(16A)	120(15)	202(17)	141(14)	-41(13)	-46(12)	-8(13)
C(17A)	109(14)	183(16)	167(14)	-63(13)	-68(11)	-29(12)
C(18A)	153(15)	141(16)	182(14)	-42(13)	-35(12)	-34(12)
C(19A)	154(16)	150(16)	209(15)	-47(13)	-37(12)	-7(13)
C(20A)	199(17)	210(18)	261(17)	-100(15)	-98(14)	19(14)
C(21A)	154(16)	179(17)	333(18)	-124(15)	-21(14)	-19(13)
C(22A)	217(17)	171(17)	202(15)	-110(14)	19(13)	-43(14)
C(23A)	178(16)	109(15)	219(15)	-65(13)	-53(12)	-8(12)
C(24A)	234(19)	280(20)	199(16)	-45(16)	-52(15)	-38(18)
C(25A)	141(18)	420(30)	520(30)	-270(20)	-40(17)	9(19)
C(26A)	256(19)	203(19)	189(16)	-88(15)	-7(14)	-26(15)
C(27A)	131(15)	95(15)	141(13)	-30(12)	-8(11)	-25(12)
C(28A)	154(15)	113(15)	188(14)	-56(12)	-37(12)	-40(12)
C(29A)	156(17)	230(18)	229(16)	-81(14)	-68(13)	-44(14)
C(30A)	137(16)	241(18)	237(16)	-130(14)	12(12)	-41(13)
C(31A)	196(16)	243(18)	119(14)	-82(13)	3(12)	-61(14)
C(32A)	142(15)	140(15)	151(14)	-54(12)	-24(12)	-29(12)
C(33A)	175(18)	260(20)	161(15)	-74(15)	-18(13)	-39(16)
C(34A)	137(19)	740(30)	360(20)	-360(20)	0(16)	-46(19)
C(35A)	198(18)	290(20)	136(15)	-59(15)	-33(13)	-53(16)
Fe(2B)	128(2)	182(2)	130(2)	-52(2)	-19(2)	-6(2)
I(1B)	190(1)	283(1)	222(1)	-54(1)	-66(1)	52(1)
N(1B)	104(12)	204(14)	124(11)	-59(10)	-2(9)	-32(10)
N(2B)	115(12)	187(14)	167(12)	-55(11)	-20(10)	-3(11)
N(3B)	105(12)	199(14)	136(11)	-52(11)	-14(9)	-16(10)
C(1B)	137(15)	141(15)	143(13)	-19(12)	-59(11)	12(12)

C(2B)	173(17)	184(17)	166(14)	-25(13)	-26(13)	-25(14)
C(3B)	240(18)	167(17)	227(16)	-79(14)	-78(13)	2(14)
C(4B)	188(17)	207(18)	195(15)	-83(14)	-45(13)	49(14)
C(5B)	125(16)	234(18)	168(15)	-50(14)	-33(13)	12(14)
C(6B)	150(15)	167(16)	145(14)	-36(12)	-61(12)	13(13)
C(7B)	80(14)	221(17)	189(14)	-68(13)	-44(12)	22(12)
C(8B)	119(15)	278(19)	176(15)	-96(14)	-45(12)	-8(13)
C(9B)	110(15)	252(19)	200(16)	-9(15)	-38(13)	-8(14)
C(10B)	183(17)	140(17)	271(17)	-42(14)	-91(13)	-23(13)
C(11B)	82(14)	170(16)	209(15)	-51(13)	-53(12)	27(12)
C(12B)	122(15)	208(17)	183(14)	-84(13)	-38(12)	-1(13)
C(13B)	167(17)	229(18)	225(16)	-72(15)	11(13)	-12(14)
C(14B)	223(18)	214(19)	372(19)	-113(16)	-128(15)	-26(15)
C(15B)	201(17)	234(19)	264(17)	-126(15)	-75(14)	57(14)
C(16B)	181(16)	200(18)	179(15)	-79(14)	-26(13)	18(14)
C(17B)	122(15)	187(17)	188(14)	-63(13)	-45(12)	6(13)
C(18B)	146(15)	175(16)	158(14)	-83(13)	-11(12)	-42(13)
C(19B)	173(16)	159(16)	134(13)	-64(12)	-23(12)	-23(13)
C(20B)	156(17)	232(18)	242(16)	-111(15)	-75(13)	16(14)
C(21B)	145(16)	243(18)	281(17)	-141(15)	-31(13)	-26(14)
C(22B)	222(17)	224(18)	176(15)	-79(14)	51(13)	-106(14)
C(23B)	215(16)	154(16)	140(14)	-76(13)	-24(12)	-28(13)
C(24B)	234(19)	230(20)	187(15)	-41(14)	-63(14)	10(16)
C(25B)	162(19)	460(30)	460(20)	-160(20)	-6(17)	-86(19)
C(26B)	266(19)	210(19)	172(16)	-20(15)	-27(14)	-60(16)
C(27B)	136(15)	151(16)	195(14)	-97(13)	-35(12)	3(12)
C(28B)	197(16)	134(16)	162(14)	-79(13)	-5(12)	-36(13)
C(29B)	144(16)	242(18)	231(16)	-139(14)	-49(13)	18(14)
C(30B)	180(16)	250(18)	205(15)	-139(14)	11(13)	-46(14)
C(31B)	285(19)	228(18)	102(14)	-55(14)	19(13)	-81(15)
C(32B)	200(16)	229(17)	162(14)	-89(13)	-37(12)	-22(14)
C(33B)	212(18)	193(19)	193(15)	-77(14)	-12(13)	0(15)
C(34B)	240(20)	410(30)	270(20)	-111(19)	47(16)	-148(19)
C(35B)	270(20)	340(20)	177(17)	-76(16)	-67(15)	-22(17)
C(41)	300(20)	290(20)	400(20)	-127(18)	-116(16)	-86(17)
C(42)	280(20)	330(20)	294(19)	-27(17)	-116(16)	-47(17)
C(43)	320(20)	320(20)	410(20)	-153(19)	-42(17)	58(18)
C(44)	350(20)	440(20)	310(19)	-187(19)	-31(17)	-55(19)
C(45)	200(18)	390(20)	225(17)	-13(16)	-24(14)	-75(16)
C(46)	219(19)	201(19)	370(20)	-17(16)	-48(15)	-34(15)
C(51)	159(17)	330(20)	342(19)	-212(18)	-13(14)	-37(15)
C(52)	208(18)	199(19)	298(18)	-121(16)	25(14)	-8(15)
C(53)	186(18)	310(20)	273(18)	-140(17)	-60(15)	49(16)

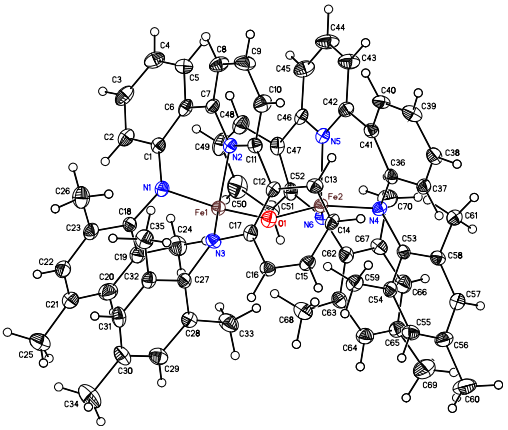
Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for [**2**]FeI **(CCDC 695390).**

	x	y	z	U_{iso}
H(2A)	7314(18)	9842(18)	8526(16)	10(7)
H(3A)	8433(17)	10690(18)	7629(16)	7(7)
H(4A)	9716(19)	9993(19)	6781(17)	20(8)
H(5A)	9730(20)	8420(20)	6909(19)	33(10)
H(8A)	9074(16)	7459(17)	6487(15)	0(6)
H(9A)	9052(16)	5984(16)	6388(15)	3(6)
H(10A)	8655(16)	4756(17)	7655(15)	3(7)
H(13A)	8958(18)	3702(19)	8838(17)	19(8)
H(14A)	8480(20)	2320(20)	9915(18)	34(9)
H(15A)	7192(16)	2574(17)	11090(16)	7(6)
H(16A)	6548(17)	4155(18)	11091(16)	12(7)
H(20A)	4335(17)	9041(17)	8368(16)	11(7)
H(22A)	4464(18)	8842(18)	10773(17)	21(7)
H(24A)	5680(20)	8600(20)	7323(19)	34(9)
H(24B)	6529(19)	7990(20)	7711(17)	21(8)
H(24C)	6440(20)	9060(20)	7377(18)	18(9)
H(25A)	2820(20)	8830(20)	9750(20)	48(12)
H(25B)	2890(30)	9720(30)	9720(30)	72(17)
H(25C)	2850(30)	9070(40)	10510(30)	130(20)
H(26A)	6003(18)	8769(18)	11059(17)	19(7)
H(26B)	6910(20)	8480(20)	10390(20)	51(11)
H(26C)	6320(20)	7740(20)	11050(20)	40(10)
H(29A)	3904(19)	6506(19)	10417(17)	16(8)
H(31A)	4779(16)	6064(17)	12503(16)	7(6)
H(33A)	5980(20)	6580(20)	8934(18)	25(8)
H(33B)	4980(30)	6500(30)	9020(20)	65(13)
H(33C)	5699(19)	5610(20)	9233(17)	22(8)
H(34A)	3050(20)	6640(30)	12470(20)	47(12)
H(34B)	2750(20)	6390(30)	11870(20)	42(12)
H(34C)	2830(40)	7210(40)	11700(40)	170(30)
H(35A)	6440(20)	5600(20)	12520(20)	41(9)
H(35B)	7050(20)	5980(20)	11687(18)	20(8)
H(35C)	6940(20)	4930(20)	11981(18)	35(9)
H(2B)	3708(17)	9429(17)	6736(15)	4(6)
H(3B)	2823(17)	10124(17)	7759(15)	6(7)
H(4B)	1281(17)	9680(17)	8571(16)	12(7)
H(5B)	810(19)	8502(19)	8270(17)	19(8)
H(8B)	1030(16)	6915(17)	8656(15)	7(7)
H(9B)	622(17)	5449(18)	8797(17)	14(7)
H(10B)	1060(16)	5024(17)	7534(15)	1(7)
H(13B)	895(19)	4994(19)	6365(18)	22(8)
H(14B)	1323(18)	4317(18)	5308(17)	10(7)
H(15B)	2554(19)	4717(19)	4144(17)	24(8)
H(16B)	3359(16)	5937(16)	3996(15)	2(6)
H(20B)	6315(19)	6988(19)	6521(17)	20(8)
H(22B)	6080(20)	9010(20)	4283(19)	31(9)
H(24D)	4293(18)	7226(19)	7752(17)	21(8)

H(24E)	4870(20)	6300(20)	7551(19)	35(9)
H(24F)	3970(20)	6650(20)	7320(20)	51(11)
H(25D)	7630(30)	8490(30)	4910(30)	68(14)
H(25E)	7710(30)	7610(30)	4620(30)	80(14)
H(25F)	7730(30)	7610(40)	5490(30)	120(20)
H(26D)	4510(20)	9930(20)	4070(20)	53(11)
H(26E)	3680(20)	9760(20)	4767(19)	29(9)
H(26F)	3940(20)	9170(20)	4178(18)	31(9)
H(29B)	6241(19)	6246(19)	4518(17)	23(8)
H(31B)	5202(19)	8164(19)	2601(18)	23(8)
H(33D)	4449(18)	5220(19)	5776(16)	11(7)
H(33E)	4196(19)	6063(19)	6132(18)	25(8)
H(33F)	5260(30)	5590(30)	5990(20)	75(13)
H(34D)	6930(20)	7670(20)	2410(20)	50(11)
H(34E)	7280(30)	6810(30)	3050(30)	92(17)
H(34F)	7090(20)	7860(20)	3090(20)	40(10)
H(35D)	3160(20)	8750(20)	3338(19)	34(10)
H(35E)	2850(20)	7780(20)	3440(20)	39(10)
H(35F)	3540(20)	8370(20)	2630(20)	52(11)
H(41)	9950(20)	8370(20)	4279(18)	28(9)
H(42)	10870(20)	6890(20)	4360(20)	36(10)
H(43)	10770(20)	5950(20)	3564(19)	42(10)
H(44)	9860(20)	6680(20)	2566(19)	40(10)
H(45)	9020(19)	8216(19)	2391(17)	21(8)
H(46)	9073(18)	9033(19)	3317(16)	15(8)
H(51)	990(20)	690(20)	359(19)	33(9)
H(52)	180(16)	1585(18)	-684(15)	3(7)
H(53)	771(19)	-868(19)	1041(17)	17(8)

([**2**]Fe)$_2$O

Contents



([**2**]Fe)$_2$O

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 697910. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 697910."

Table 1. Crystal data and structure refinement for ([**2**]Fe)$_2$O (CCDC 697910).

Empirical formula	$C_{70}H_{66}N_6OFe_2 \bullet 0.5(C_7H_8)$
Formula weight	1165.05
Crystallization Solvent	Toluene
Crystal Habit	Plate
Crystal size	0.38 x 0.24 x 0.07 mm^3
Crystal color	Green

Data Collection

Type of diffractometer	Bruker KAPPA APEX II
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 9283 reflections used in lattice determination	2.30 to 31.52°
Unit cell dimensions	a = 19.8707(9) Å b = 39.4031(19) Å c = 15.1038(6) Å
Volume	11825.8(9) Å^3
Z	8
Crystal system	Orthorhombic
Space group	I*ba*2
Density (calculated)	1.309 Mg/m^3
F(000)	4904

Data collection program	Bruker APEX2 v2.1-0
θ range for data collection	1.86 to 32.23°
Completeness to θ = 32.23°	93.8 %
Index ranges	$-29 \leq h \leq 29$, $-59 \leq k \leq 42$, $-19 \leq l \leq 22$
Data collection scan type	ω scans; 12 settings
Data reduction program	Bruker SAINT-Plus v7.34A
Reflections collected	121688
Independent reflections	18216 [R_{int}= 0.0571]
Absorption coefficient	0.542 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.9630 and 0.8204

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	18216 / 10 / 757
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.792
Final R indices [$I>2\sigma(I)$, 14462 reflections]	R1 = 0.0416, *w*R2 = 0.0558
R indices (all data)	R1 = 0.0600, *w*R2 = 0.0567
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.003
Average shift/error	0.000
Absolute structure determination	Anomalous differences
Absolute structure parameter	-0.007(6)
Largest diff. peak and hole	1.372 and -0.704 e.$Å^{-3}$

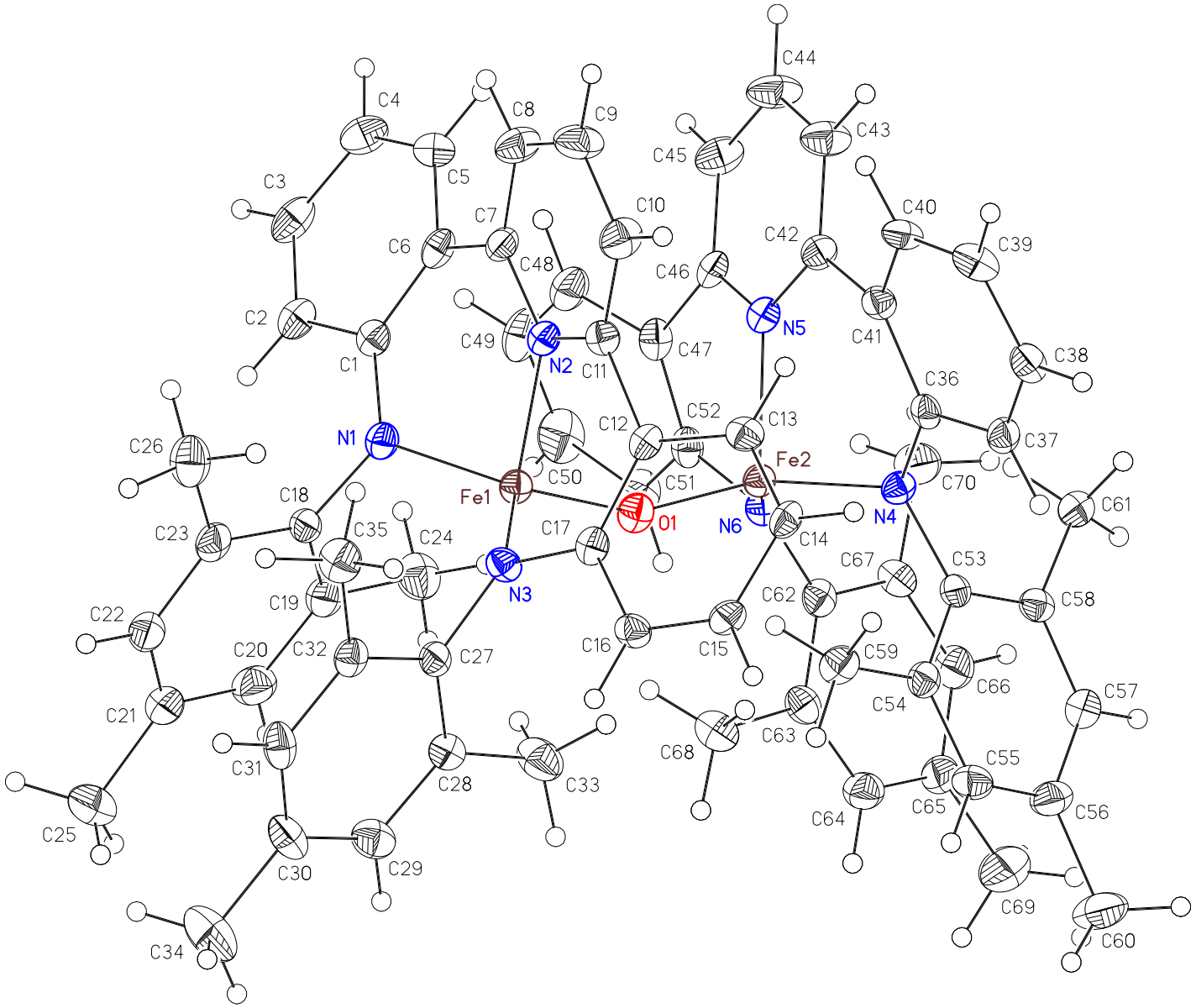
Special Refinement Details

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based

on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.


C44
C4
C8
C9
C43
C45
C5
C3
C10
C40
C7
C42
C39
C6
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C2
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C70
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C24
C17
C14
C67
C53
N3
C62
C58
C22
C19
C16
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C32
C27
C59
C66
C54
C57
C21
C63
C68
C55
C31
C28
C33
C65
C56
C64
C25
C30
C29
C69
C34
C60

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ([**2**]Fe)$_2$O **(CCDC 697910). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.**

	x	y	z	U_{eq}
Fe(1)	7380(1)	8495(1)	10926(1)	16(1)
Fe(2)	7526(1)	8565(1)	8636(1)	16(1)
O(1)	7402(1)	8618(1)	9792(1)	21(1)
N(1)	8180(1)	8518(1)	11632(1)	19(1)
N(2)	7370(1)	7983(1)	10897(1)	16(1)
N(3)	6529(1)	8538(1)	11526(1)	18(1)
N(4)	6787(1)	8425(1)	7895(1)	17(1)
N(5)	8028(1)	8124(1)	8483(1)	17(1)
N(6)	8206(1)	8840(1)	8083(1)	18(1)
C(1)	8708(1)	8299(1)	11484(1)	18(1)
C(2)	9373(1)	8391(1)	11729(1)	23(1)
C(3)	9912(1)	8190(1)	11523(1)	27(1)
C(4)	9823(1)	7887(1)	11070(1)	27(1)
C(5)	9181(1)	7785(1)	10874(1)	22(1)
C(6)	8607(1)	7975(1)	11101(1)	19(1)
C(7)	7949(1)	7801(1)	10999(1)	19(1)
C(8)	7909(1)	7449(1)	11032(1)	26(1)
C(9)	7294(1)	7289(1)	10922(2)	29(1)
C(10)	6722(1)	7481(1)	10808(1)	26(1)
C(11)	6760(1)	7832(1)	10801(1)	18(1)
C(12)	6139(1)	8040(1)	10700(1)	17(1)
C(13)	5624(1)	7897(1)	10185(1)	19(1)
C(14)	4989(1)	8035(1)	10140(1)	20(1)
C(15)	4850(1)	8326(1)	10626(1)	19(1)
C(16)	5349(1)	8483(1)	11104(1)	19(1)
C(17)	6014(1)	8356(1)	11122(1)	18(1)
C(18)	8271(1)	8820(1)	12134(1)	19(1)
C(19)	8463(1)	9122(1)	11722(1)	24(1)
C(20)	8476(1)	9417(1)	12220(1)	30(1)
C(21)	8305(1)	9422(1)	13118(1)	31(1)
C(22)	8132(1)	9116(1)	13510(1)	28(1)
C(23)	8118(1)	8816(1)	13049(1)	22(1)
C(24)	8664(1)	9124(1)	10762(1)	31(1)
C(25)	8297(1)	9749(1)	13633(2)	50(1)
C(26)	7947(1)	8485(1)	13498(1)	31(1)
C(27)	6372(1)	8808(1)	12120(1)	18(1)
C(28)	6424(1)	9147(1)	11842(1)	20(1)
C(29)	6325(1)	9406(1)	12450(1)	25(1)
C(30)	6169(1)	9340(1)	13334(1)	26(1)
C(31)	6107(1)	9004(1)	13585(1)	24(1)
C(32)	6199(1)	8739(1)	13004(1)	20(1)
C(33)	6572(1)	9232(1)	10887(1)	31(1)
C(34)	6062(1)	9631(1)	13968(1)	44(1)
C(35)	6107(1)	8376(1)	13307(1)	27(1)
C(36)	6541(1)	8101(1)	7933(1)	16(1)
C(37)	5878(1)	8026(1)	7672(1)	20(1)
C(38)	5605(1)	7708(1)	7745(1)	22(1)

C(39)	5979(1)	7445(1)	8100(1)	24(1)
C(40)	6632(1)	7506(1)	8338(1)	21(1)
C(41)	6948(1)	7821(1)	8226(1)	18(1)
C(42)	7693(1)	7830(1)	8310(1)	19(1)
C(43)	8061(1)	7535(1)	8154(1)	28(1)
C(44)	8756(1)	7544(1)	8191(1)	32(1)
C(45)	9081(1)	7842(1)	8362(1)	27(1)
C(46)	8716(1)	8137(1)	8517(1)	19(1)
C(47)	9071(1)	8461(1)	8678(1)	20(1)
C(48)	9712(1)	8436(1)	9075(1)	26(1)
C(49)	10152(1)	8702(1)	9122(1)	32(1)
C(50)	9958(1)	9011(1)	8760(1)	35(1)
C(51)	9326(1)	9055(1)	8419(1)	28(1)
C(52)	8853(1)	8785(1)	8390(1)	20(1)
C(53)	6399(1)	8693(1)	7508(1)	17(1)
C(54)	5914(1)	8866(1)	8008(1)	19(1)
C(55)	5601(1)	9149(1)	7644(1)	23(1)
C(56)	5755(1)	9263(1)	6801(1)	25(1)
C(57)	6228(1)	9085(1)	6307(1)	22(1)
C(58)	6548(1)	8800(1)	6647(1)	18(1)
C(59)	5729(1)	8747(1)	8924(1)	23(1)
C(60)	5417(1)	9575(1)	6434(1)	38(1)
C(61)	7040(1)	8606(1)	6082(1)	23(1)
C(62)	8065(1)	9128(1)	7541(1)	19(1)
C(63)	7634(1)	9382(1)	7838(1)	21(1)
C(64)	7468(1)	9649(1)	7285(1)	25(1)
C(65)	7724(1)	9677(1)	6439(1)	26(1)
C(66)	8157(1)	9422(1)	6157(1)	27(1)
C(67)	8334(1)	9149(1)	6676(1)	23(1)
C(68)	7356(1)	9380(1)	8775(1)	28(1)
C(69)	7543(1)	9972(1)	5848(1)	44(1)
C(70)	8796(1)	8877(1)	6331(1)	31(1)
C(81)	10000	10000	7764(3)	288(7)
C(82)	10000	10000	6753(3)	204(4)
C(83)	9909(2)	9699(1)	6290(3)	155(3)
C(84)	9909(2)	9699(1)	5371(3)	381(8)
C(85)	10000	10000	4906(3)	207(6)

Table 3. Selected bond lengths [Å] and angles [°] for ([**2**]Fe)$_2$O **(CCDC 697910).**

Fe(1)-O(1)	1.7802(14)	O(1)-Fe(1)-N(1)	120.08(6)
Fe(1)-N(1)	1.9174(15)	O(1)-Fe(1)-N(3)	116.84(6)
Fe(1)-N(3)	1.9262(14)	N(1)-Fe(1)-N(3)	117.50(6)
Fe(1)-N(2)	2.0161(14)	O(1)-Fe(1)-N(2)	104.57(6)
Fe(2)-O(1)	1.7761(14)	N(1)-Fe(1)-N(2)	93.86(6)
Fe(2)-N(6)	1.9234(15)	N(3)-Fe(1)-N(2)	95.14(6)
Fe(2)-N(4)	1.9262(15)	O(1)-Fe(2)-N(6)	117.27(6)
Fe(2)-N(5)	2.0153(15)	O(1)-Fe(2)-N(4)	119.97(6)
		N(6)-Fe(2)-N(4)	116.39(6)
		O(1)-Fe(2)-N(5)	106.37(6)
		N(6)-Fe(2)-N(5)	95.06(6)
		N(4)-Fe(2)-N(5)	93.67(6)

Table 4. Bond lengths [Å] and angles [°] for ([**2**]Fe)$_2$O **(CCDC 697910).**

Fe(1)-O(1)	1.7802(14)	C(13)-C(14)	1.376(2)
Fe(1)-N(1)	1.9174(15)	C(14)-C(15)	1.387(2)
Fe(1)-N(3)	1.9262(14)	C(15)-C(16)	1.374(2)
Fe(1)-N(2)	2.0161(14)	C(16)-C(17)	1.413(2)
Fe(2)-O(1)	1.7761(14)	C(18)-C(19)	1.397(3)
Fe(2)-N(6)	1.9234(15)	C(18)-C(23)	1.415(2)
Fe(2)-N(4)	1.9262(15)	C(19)-C(20)	1.385(3)
Fe(2)-N(5)	2.0153(15)	C(19)-C(24)	1.503(3)
N(1)-C(1)	1.378(2)	C(20)-C(21)	1.400(3)
N(1)-C(18)	1.421(2)	C(21)-C(22)	1.384(3)
N(2)-C(11)	1.358(2)	C(21)-C(25)	1.506(3)
N(2)-C(7)	1.365(2)	C(22)-C(23)	1.374(3)
N(3)-C(17)	1.391(2)	C(23)-C(26)	1.509(3)
N(3)-C(27)	1.428(2)	C(27)-C(28)	1.402(3)
N(4)-C(36)	1.370(2)	C(27)-C(32)	1.406(2)
N(4)-C(53)	1.431(2)	C(28)-C(29)	1.389(3)
N(5)-C(42)	1.361(2)	C(28)-C(33)	1.509(2)
N(5)-C(46)	1.371(2)	C(29)-C(30)	1.396(3)
N(6)-C(52)	1.384(2)	C(30)-C(31)	1.383(3)
N(6)-C(62)	1.427(2)	C(30)-C(34)	1.508(3)
C(1)-C(2)	1.419(2)	C(31)-C(32)	1.378(3)
C(1)-C(6)	1.414(3)	C(32)-C(35)	1.513(3)
C(2)-C(3)	1.370(3)	C(36)-C(37)	1.406(2)
C(3)-C(4)	1.386(3)	C(36)-C(41)	1.437(3)
C(4)-C(5)	1.370(2)	C(37)-C(38)	1.370(3)
C(5)-C(6)	1.408(2)	C(38)-C(39)	1.382(3)
C(6)-C(7)	1.486(2)	C(39)-C(40)	1.369(2)
C(7)-C(8)	1.389(3)	C(40)-C(41)	1.402(3)
C(8)-C(9)	1.384(2)	C(41)-C(42)	1.487(2)
C(9)-C(10)	1.376(3)	C(42)-C(43)	1.395(3)
C(10)-C(11)	1.385(3)	C(43)-C(44)	1.382(3)
C(11)-C(12)	1.487(2)	C(44)-C(45)	1.362(3)
C(12)-C(13)	1.403(2)	C(45)-C(46)	1.391(3)
C(12)-C(17)	1.421(3)	C(46)-C(47)	1.478(2)

C(47)-C(48)	1.410(2)	C(36)-N(4)-Fe(2)	120.97(12)
C(47)-C(52)	1.416(3)	C(53)-N(4)-Fe(2)	115.93(12)
C(48)-C(49)	1.367(3)	C(42)-N(5)-C(46)	121.72(16)
C(49)-C(50)	1.387(3)	C(42)-N(5)-Fe(2)	120.95(12)
C(50)-C(51)	1.369(3)	C(46)-N(5)-Fe(2)	117.25(12)
C(51)-C(52)	1.422(3)	C(52)-N(6)-C(62)	120.02(15)
C(53)-C(58)	1.398(2)	C(52)-N(6)-Fe(2)	114.75(12)
C(53)-C(54)	1.402(2)	C(62)-N(6)-Fe(2)	123.96(12)
C(54)-C(55)	1.391(3)	N(1)-C(1)-C(2)	120.41(17)
C(54)-C(59)	1.506(2)	N(1)-C(1)-C(6)	121.52(16)
C(55)-C(56)	1.385(2)	C(2)-C(1)-C(6)	118.07(17)
C(56)-C(57)	1.391(3)	C(3)-C(2)-C(1)	121.34(19)
C(56)-C(60)	1.506(3)	C(2)-C(3)-C(4)	120.65(18)
C(57)-C(58)	1.390(3)	C(5)-C(4)-C(3)	118.70(18)
C(58)-C(61)	1.507(2)	C(4)-C(5)-C(6)	122.93(18)
C(62)-C(63)	1.391(3)	C(5)-C(6)-C(1)	117.77(16)
C(62)-C(67)	1.414(2)	C(5)-C(6)-C(7)	116.14(17)
C(63)-C(64)	1.384(3)	C(1)-C(6)-C(7)	125.76(16)
C(63)-C(68)	1.519(2)	N(2)-C(7)-C(8)	118.77(16)
C(64)-C(65)	1.380(3)	N(2)-C(7)-C(6)	120.70(16)
C(65)-C(66)	1.390(3)	C(8)-C(7)-C(6)	120.51(16)
C(65)-C(69)	1.507(3)	C(9)-C(8)-C(7)	120.01(17)
C(66)-C(67)	1.379(3)	C(10)-C(9)-C(8)	119.52(18)
C(67)-C(70)	1.504(3)	C(9)-C(10)-C(11)	120.43(18)
C(81)-C(82)	1.5266(9)	N(2)-C(11)-C(10)	118.91(16)
C(82)-C(83)#1	1.3880(9)	N(2)-C(11)-C(12)	120.75(16)
C(82)-C(83)	1.3881(9)	C(10)-C(11)-C(12)	120.34(16)
C(83)-C(84)	1.3885(9)	C(13)-C(12)-C(17)	118.16(16)
C(84)-C(85)	1.3897(10)	C(13)-C(12)-C(11)	116.22(17)
C(85)-C(84)#1	1.3898(10)	C(17)-C(12)-C(11)	125.50(16)
		C(14)-C(13)-C(12)	122.53(18)
O(1)-Fe(1)-N(1)	120.08(6)	C(13)-C(14)-C(15)	118.88(17)
O(1)-Fe(1)-N(3)	116.84(6)	C(16)-C(15)-C(14)	120.42(17)
N(1)-Fe(1)-N(3)	117.50(6)	C(15)-C(16)-C(17)	121.63(17)
O(1)-Fe(1)-N(2)	104.57(6)	N(3)-C(17)-C(16)	120.89(17)
N(1)-Fe(1)-N(2)	93.86(6)	N(3)-C(17)-C(12)	121.30(16)
N(3)-Fe(1)-N(2)	95.14(6)	C(16)-C(17)-C(12)	117.80(16)
O(1)-Fe(2)-N(6)	117.27(6)	C(19)-C(18)-C(23)	120.15(19)
O(1)-Fe(2)-N(4)	119.97(6)	C(19)-C(18)-N(1)	120.67(16)
N(6)-Fe(2)-N(4)	116.39(6)	C(23)-C(18)-N(1)	119.04(18)
O(1)-Fe(2)-N(5)	106.37(6)	C(20)-C(19)-C(18)	118.61(18)
N(6)-Fe(2)-N(5)	95.06(6)	C(20)-C(19)-C(24)	120.88(19)
N(4)-Fe(2)-N(5)	93.67(6)	C(18)-C(19)-C(24)	120.51(19)
Fe(2)-O(1)-Fe(1)	156.60(7)	C(19)-C(20)-C(21)	122.3(2)
C(1)-N(1)-C(18)	120.93(15)	C(22)-C(21)-C(20)	117.6(2)
C(1)-N(1)-Fe(1)	120.81(12)	C(22)-C(21)-C(25)	121.43(19)
C(18)-N(1)-Fe(1)	116.21(12)	C(20)-C(21)-C(25)	121.0(2)
C(11)-N(2)-C(7)	122.30(15)	C(23)-C(22)-C(21)	122.49(19)
C(11)-N(2)-Fe(1)	116.62(12)	C(22)-C(23)-C(18)	118.85(19)
C(7)-N(2)-Fe(1)	121.04(12)	C(22)-C(23)-C(26)	121.44(18)
C(17)-N(3)-C(27)	120.01(14)	C(18)-C(23)-C(26)	119.71(18)
C(17)-N(3)-Fe(1)	113.20(11)	C(28)-C(27)-C(32)	119.27(18)
C(27)-N(3)-Fe(1)	123.58(12)	C(28)-C(27)-N(3)	120.36(16)
C(36)-N(4)-C(53)	120.80(15)	C(32)-C(27)-N(3)	120.28(18)

C(29)-C(28)-C(27)	119.46(17)	N(6)-C(52)-C(47)	121.93(17)
C(29)-C(28)-C(33)	119.71(18)	N(6)-C(52)-C(51)	120.39(18)
C(27)-C(28)-C(33)	120.81(17)	C(47)-C(52)-C(51)	117.68(17)
C(28)-C(29)-C(30)	121.74(19)	C(58)-C(53)-C(54)	120.03(17)
C(31)-C(30)-C(29)	117.50(18)	C(58)-C(53)-N(4)	119.14(16)
C(31)-C(30)-C(34)	122.66(18)	C(54)-C(53)-N(4)	120.60(16)
C(29)-C(30)-C(34)	119.83(19)	C(55)-C(54)-C(53)	119.01(17)
C(30)-C(31)-C(32)	122.70(18)	C(55)-C(54)-C(59)	120.24(17)
C(31)-C(32)-C(27)	119.28(19)	C(53)-C(54)-C(59)	120.74(17)
C(31)-C(32)-C(35)	120.62(17)	C(56)-C(55)-C(54)	121.66(18)
C(27)-C(32)-C(35)	120.09(18)	C(55)-C(56)-C(57)	118.59(18)
N(4)-C(36)-C(37)	121.31(17)	C(55)-C(56)-C(60)	120.29(18)
N(4)-C(36)-C(41)	121.83(16)	C(57)-C(56)-C(60)	121.12(18)
C(37)-C(36)-C(41)	116.85(18)	C(56)-C(57)-C(58)	121.36(18)
C(38)-C(37)-C(36)	122.77(18)	C(57)-C(58)-C(53)	119.32(17)
C(37)-C(38)-C(39)	120.26(18)	C(57)-C(58)-C(61)	119.89(17)
C(40)-C(39)-C(38)	118.66(19)	C(53)-C(58)-C(61)	120.78(17)
C(39)-C(40)-C(41)	123.27(19)	C(63)-C(62)-C(67)	119.28(18)
C(40)-C(41)-C(36)	117.70(17)	C(63)-C(62)-N(6)	120.59(16)
C(40)-C(41)-C(42)	117.14(17)	C(67)-C(62)-N(6)	120.04(17)
C(36)-C(41)-C(42)	124.69(17)	C(64)-C(63)-C(62)	119.96(18)
N(5)-C(42)-C(43)	119.14(17)	C(64)-C(63)-C(68)	118.63(17)
N(5)-C(42)-C(41)	121.49(17)	C(62)-C(63)-C(68)	121.39(17)
C(43)-C(42)-C(41)	119.24(18)	C(65)-C(64)-C(63)	122.15(19)
C(44)-C(43)-C(42)	119.6(2)	C(64)-C(65)-C(66)	117.03(19)
C(45)-C(44)-C(43)	120.3(2)	C(64)-C(65)-C(69)	121.48(19)
C(44)-C(45)-C(46)	120.32(18)	C(66)-C(65)-C(69)	121.49(19)
N(5)-C(46)-C(45)	118.86(17)	C(67)-C(66)-C(65)	123.23(18)
N(5)-C(46)-C(47)	120.98(16)	C(66)-C(67)-C(62)	118.35(18)
C(45)-C(46)-C(47)	120.10(17)	C(66)-C(67)-C(70)	120.91(17)
C(48)-C(47)-C(52)	117.91(17)	C(62)-C(67)-C(70)	120.73(18)
C(48)-C(47)-C(46)	116.22(17)	C(83)#1-C(82)-C(83)	119.49(17)
C(52)-C(47)-C(46)	125.57(16)	C(83)#1-C(82)-C(81)	120.26(8)
C(49)-C(48)-C(47)	123.2(2)	C(83)-C(82)-C(81)	120.25(8)
C(48)-C(49)-C(50)	118.32(18)	C(82)-C(83)-C(84)	120.28(11)
C(51)-C(50)-C(49)	120.99(19)	C(83)-C(84)-C(85)	120.30(11)
C(50)-C(51)-C(52)	121.45(19)	C(84)-C(85)-C(84)#1	119.36(18)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+2,z

Table 5. Anisotropic displacement parameters (Å^{2}x 10^4) for ([**2**]Fe)$_2$O **(CCDC 697910). The anisotropic displacement factor exponent takes the form: -2π^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)	140(1)	187(1)	163(1)	0(1)	5(1)	2(1)
Fe(2)	140(1)	172(1)	165(1)	-1(1)	-2(1)	0(1)
O(1)	173(7)	257(8)	198(5)	10(7)	8(6)	3(6)
N(1)	160(8)	213(10)	184(8)	2(8)	-18(6)	-5(7)
N(2)	150(7)	188(8)	149(7)	19(8)	10(7)	1(7)
N(3)	146(8)	194(9)	193(8)	-32(7)	23(6)	3(7)

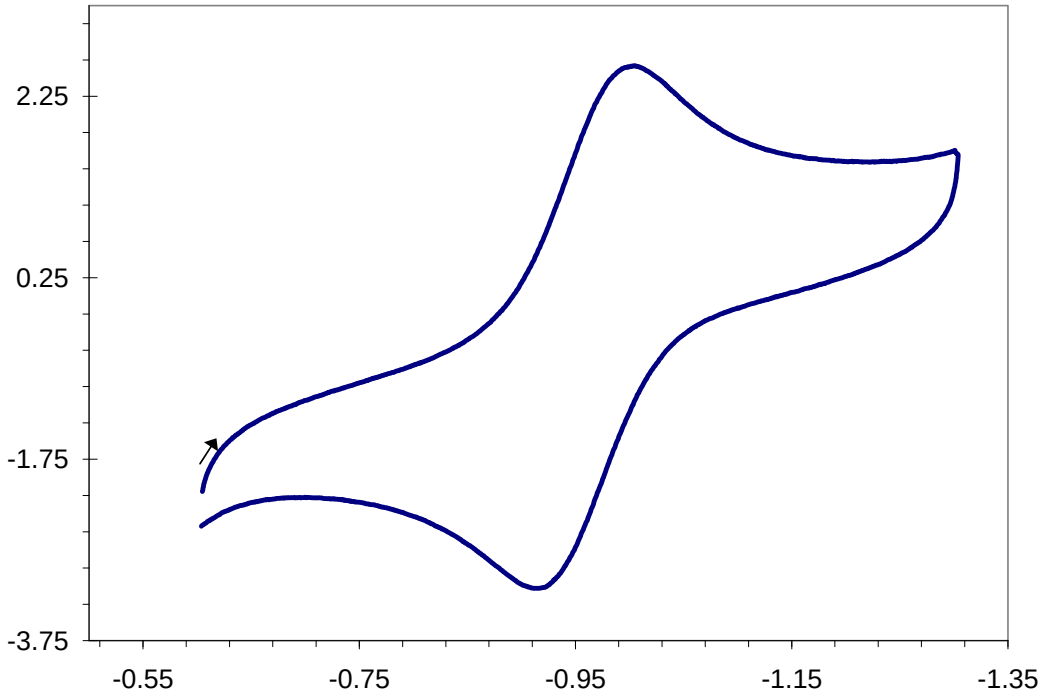
N(4)	135(8)	166(9)	197(8)	11(7)	-13(7)	-5(7)
N(5)	145(8)	195(9)	158(8)	23(7)	5(6)	-7(6)
N(6)	147(8)	207(10)	176(8)	-5(7)	11(6)	-1(7)
C(1)	173(10)	215(12)	141(10)	25(8)	31(8)	2(8)
C(2)	187(10)	254(12)	240(11)	51(9)	-25(8)	-11(9)
C(3)	147(10)	313(13)	337(12)	118(10)	-47(9)	-39(9)
C(4)	172(10)	288(12)	346(12)	45(11)	28(9)	48(8)
C(5)	225(10)	188(11)	259(11)	-4(10)	20(9)	24(8)
C(6)	160(9)	257(12)	163(10)	62(9)	-4(8)	-4(8)
C(7)	179(9)	214(11)	166(10)	18(10)	-17(9)	42(8)
C(8)	172(9)	247(13)	351(12)	27(11)	-15(10)	43(8)
C(9)	257(10)	162(11)	464(12)	-40(12)	-24(10)	-1(9)
C(10)	185(10)	237(12)	364(12)	21(11)	-62(9)	-42(9)
C(11)	174(9)	191(11)	176(11)	-3(9)	9(8)	-5(8)
C(12)	144(9)	189(11)	164(10)	45(8)	7(7)	-20(8)
C(13)	221(10)	151(11)	205(10)	25(9)	24(8)	-26(9)
C(14)	154(10)	222(12)	210(10)	29(9)	-53(7)	-5(9)
C(15)	124(9)	224(12)	215(11)	20(9)	7(8)	22(8)
C(16)	196(9)	203(11)	177(10)	-16(9)	43(7)	22(8)
C(17)	165(9)	222(11)	139(10)	32(8)	28(7)	-21(8)
C(18)	150(10)	209(12)	215(11)	-47(9)	-47(8)	21(8)
C(19)	192(11)	257(13)	260(12)	-8(10)	-37(9)	-5(9)
C(20)	318(13)	220(14)	352(13)	30(10)	-53(10)	9(10)
C(21)	318(12)	287(14)	325(13)	-54(11)	-117(10)	82(10)
C(22)	293(11)	333(13)	209(11)	-32(11)	-35(9)	103(10)
C(23)	136(10)	308(13)	224(11)	-15(10)	-27(8)	46(9)
C(24)	343(12)	282(13)	303(13)	2(10)	-4(10)	-67(10)
C(25)	791(19)	295(14)	414(14)	-104(13)	-133(14)	155(13)
C(26)	305(11)	407(15)	221(11)	11(11)	18(10)	-37(10)
C(27)	124(9)	214(12)	202(10)	-38(9)	-30(8)	7(8)
C(28)	175(10)	199(12)	211(11)	-1(9)	11(8)	-16(8)
C(29)	242(11)	203(12)	317(12)	-17(10)	11(9)	-43(9)
C(30)	233(11)	303(14)	255(11)	-111(10)	34(9)	-37(9)
C(31)	194(10)	355(14)	165(10)	-31(11)	12(9)	-47(8)
C(32)	134(10)	261(12)	190(10)	3(9)	-5(8)	-1(9)
C(33)	418(13)	227(12)	287(12)	-25(11)	50(11)	-42(9)
C(34)	544(16)	412(16)	351(13)	-133(12)	135(11)	-89(12)
C(35)	258(11)	317(13)	240(11)	14(10)	49(9)	-5(10)
C(36)	156(10)	215(12)	120(9)	-29(8)	29(7)	8(8)
C(37)	162(10)	248(12)	179(10)	-24(9)	-13(8)	33(9)
C(38)	147(10)	278(13)	248(11)	-83(10)	-2(8)	-1(9)
C(39)	202(11)	201(12)	321(12)	-56(10)	78(9)	-41(9)
C(40)	212(11)	157(11)	272(11)	-34(9)	19(8)	37(8)
C(41)	146(10)	199(11)	191(10)	-32(8)	11(8)	16(8)
C(42)	164(10)	201(11)	208(10)	8(9)	-3(8)	8(8)
C(43)	192(11)	196(12)	440(13)	-16(10)	23(10)	10(9)
C(44)	197(12)	246(13)	522(15)	-25(11)	30(11)	84(9)
C(45)	158(10)	274(13)	372(13)	48(10)	24(9)	28(9)
C(46)	160(9)	234(11)	165(10)	34(9)	-33(8)	19(8)
C(47)	149(9)	279(12)	171(10)	-5(10)	8(8)	-26(8)
C(48)	195(11)	332(13)	258(11)	26(10)	-32(8)	19(9)
C(49)	175(11)	463(15)	322(12)	27(11)	-82(9)	-38(10)
C(50)	222(11)	387(14)	431(13)	-11(12)	-48(11)	-138(10)
C(51)	264(11)	272(13)	298(12)	22(10)	-26(9)	-60(9)

C(52)	171(10)	272(12)	142(10)	-8(9)	17(8)	-19(9)
C(53)	162(10)	151(11)	207(10)	-33(8)	-52(8)	-18(8)
C(54)	154(10)	211(12)	200(10)	-16(9)	-28(8)	-6(8)
C(55)	210(11)	231(12)	249(11)	-31(10)	28(9)	49(9)
C(56)	261(12)	191(12)	299(12)	29(10)	-20(9)	31(9)
C(57)	220(11)	242(13)	205(11)	9(9)	-19(9)	0(9)
C(58)	148(10)	169(11)	224(11)	-29(9)	-10(8)	-14(8)
C(59)	184(10)	274(12)	220(11)	25(9)	33(8)	30(9)
C(60)	417(14)	314(14)	417(13)	72(11)	40(11)	165(11)
C(61)	243(10)	238(12)	213(11)	-5(9)	-21(9)	47(8)
C(62)	177(10)	182(11)	220(10)	1(9)	-31(8)	-57(9)
C(63)	204(10)	198(11)	225(10)	-29(9)	-9(8)	-44(9)
C(64)	254(12)	203(11)	290(11)	-7(9)	-22(9)	4(9)
C(65)	359(13)	193(12)	240(11)	24(9)	-70(9)	4(10)
C(66)	375(13)	267(13)	175(11)	37(10)	25(9)	-1(10)
C(67)	255(11)	203(12)	224(11)	-34(10)	17(9)	-6(9)
C(68)	311(12)	240(12)	281(12)	-37(10)	35(10)	-9(9)
C(69)	570(15)	342(13)	395(13)	75(13)	-54(14)	91(12)
C(70)	369(13)	310(14)	242(12)	37(10)	83(10)	71(11)
C(81)	2480(110)	4050(170)	2110(80)	0	0	1790(110)
C(82)	1050(60)	1180(70)	3890(150)	0	0	760(60)
C(83)	390(20)	530(20)	3720(80)	140(40)	-280(40)	21(19)
C(84)	1920(80)	5000(200)	4540(140)	1140(110)	-1210(110)	460(110)
C(85)	1180(70)	3590(170)	1430(60)	0	0	940(100)

Electrochemical Data

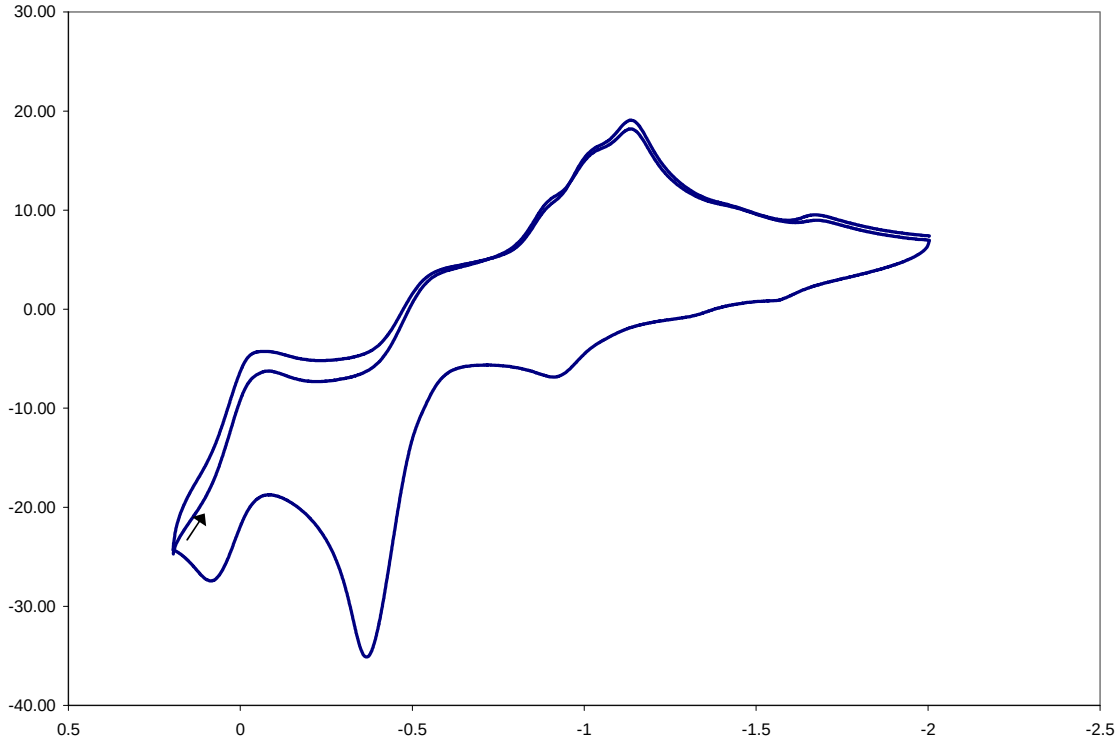
A note on control experiments: Voltammograms of THF, the solution of $^{n}Bu_4BF_4$ in THF, and the protonated ligand [**2**]H_2 were obtained. No peaks were observed, thus supporting that the peaks observed for [**2**]Fe(THF) are attributable to that species exclusively.

Voltammogram showing isolated Fe^{II}/Fe^{I} couple



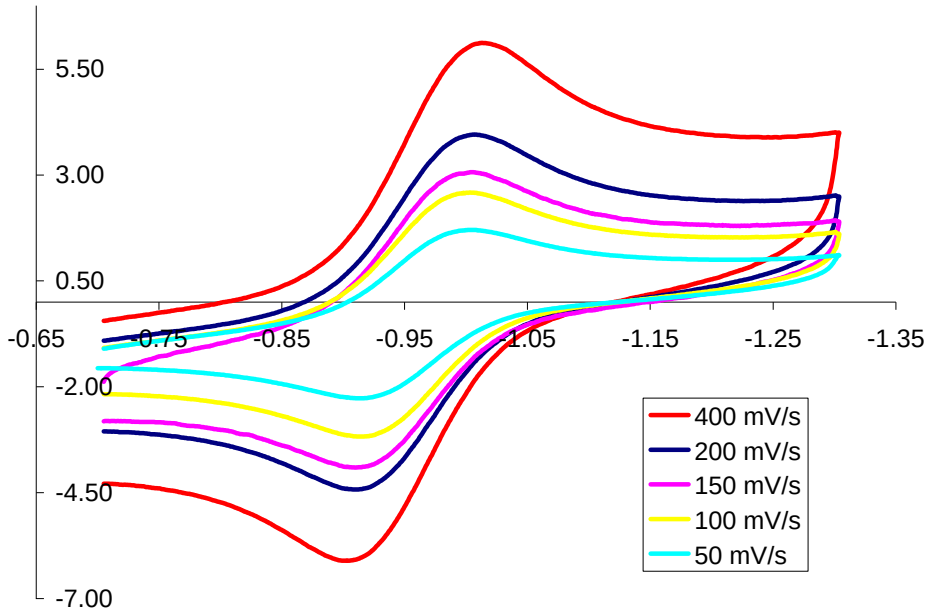
Exp. Conditions:
Init E (mV) = -100
High E (mV) = -100
Low E (mV) = -800
Init P/N = N
V (mV/sec) = 100
Number of Segments = 2
Sample Interval (mV) = 1
Quiet Time (sec) = 2
Sensitivity (A/V) = 1E-6

Voltammogram using expanded window, showing ferrocene/ferrocenium reference. Note the new oxidation wave at more positive potentials, and two new reduction waves which are coupled to the aforementioned wave.



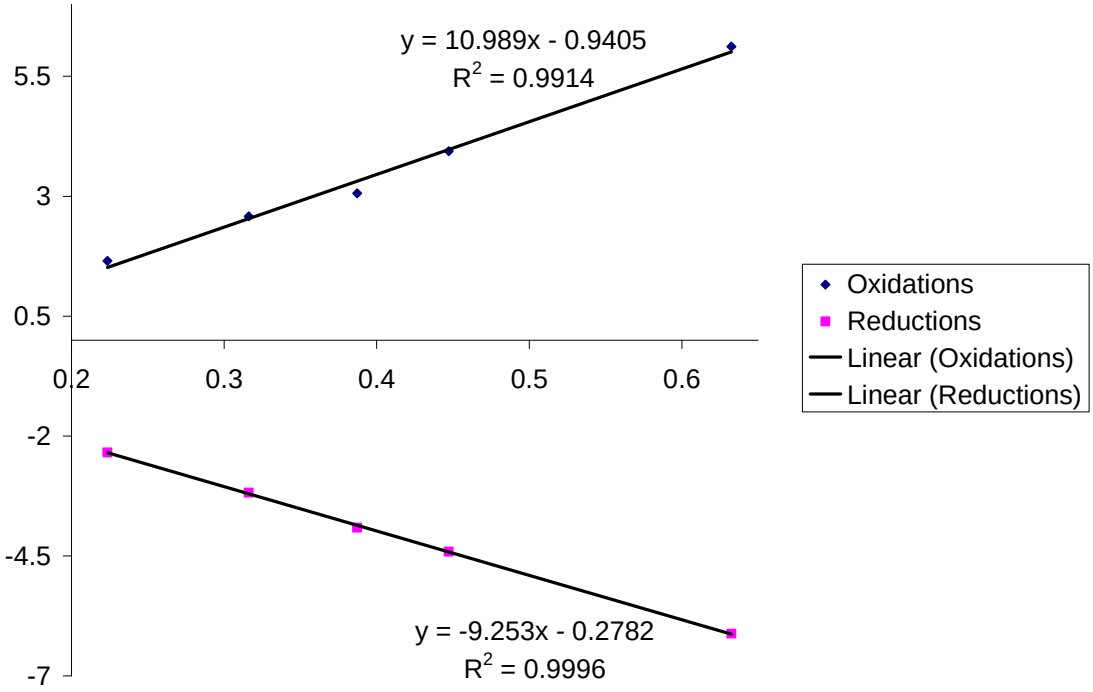
Exp. Conditions:
Init E (mV) = -100
High E (mV) = -100
Low E (mV) = -800
Init P/N = N
V (mV/sec) = 100
Number of Segments = 2
Sample Interval (mV) = 1
Quiet Time (sec) = 2
Sensitivity (A/V) = 1E-6

Scan Rate Dependence Study



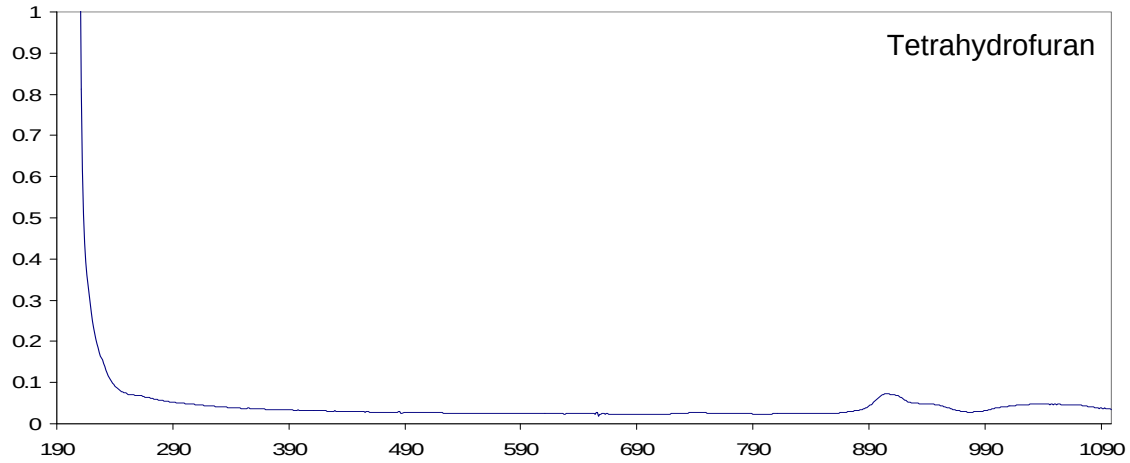
Using the Cottrell equation, it is clear that the root of the scan rate is proportional to current at the peaks (see below), thus indicating a diffusion controlled wave.

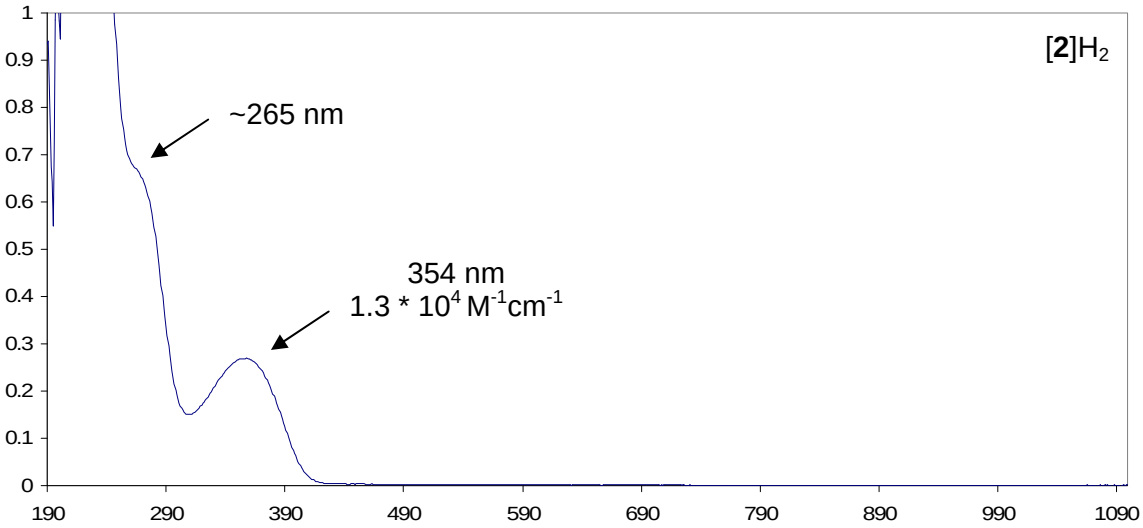
Root of scan rate versus current

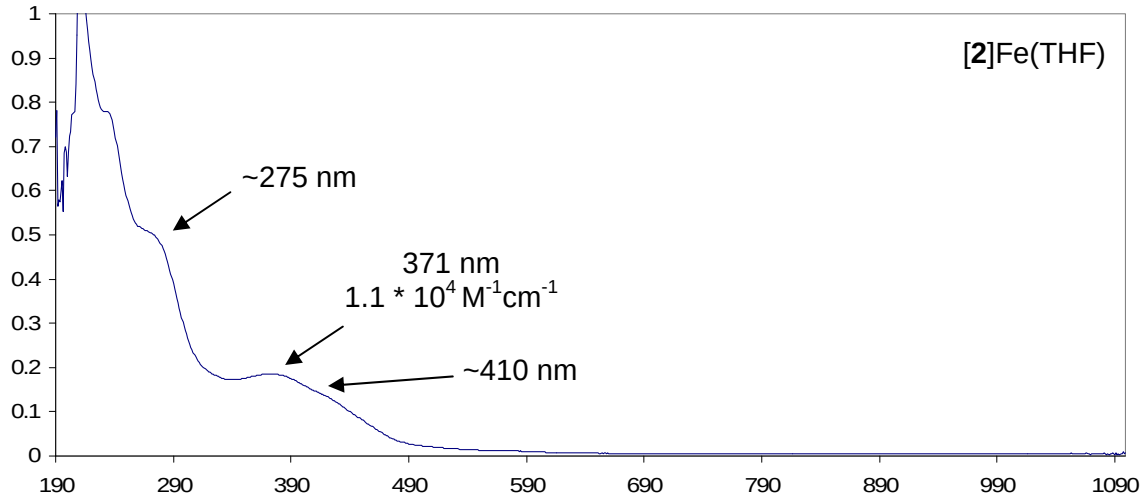


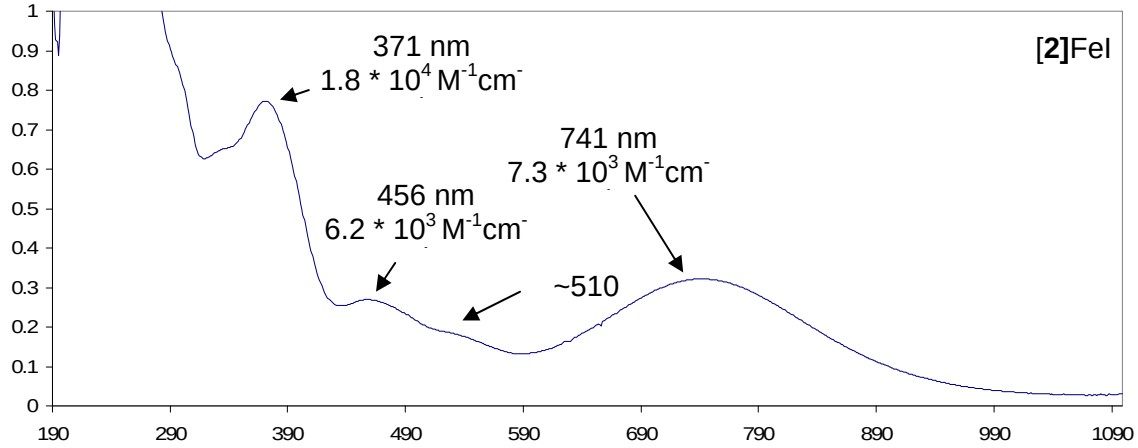
UV-Vis Spectroscopy Data

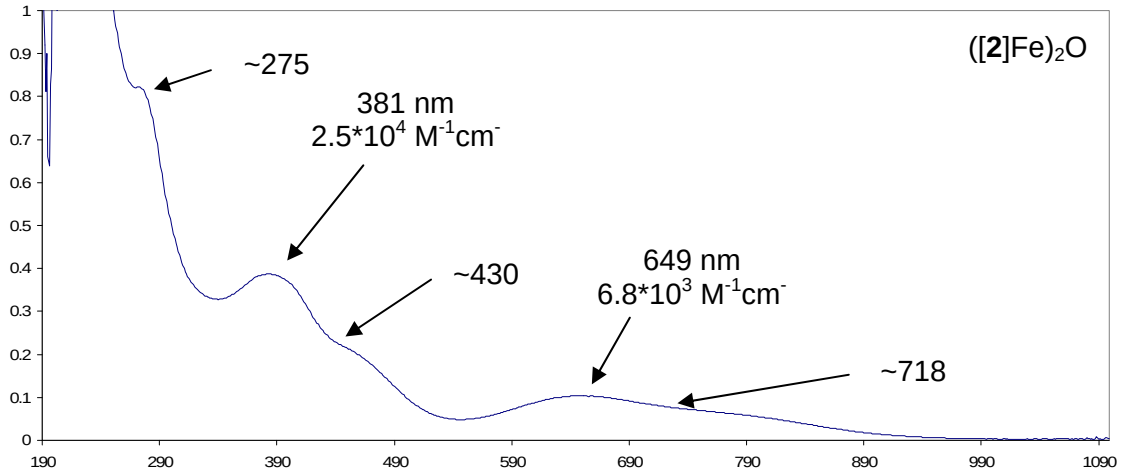
Typical tetrahydrofuran blank used for background subtraction shown below






[2]Fe(THF)
~275 nm
371 nm
1.1 * 10^4 M^-1cm^-1
~410 nm


[2]FeI
371 nm
1.8 * 10^4 M^-1cm^-
741 nm
7.3 * 10^3 M^-1cm^-
456 nm
6.2 * 10^3 M^-1cm^-
~510


([2]Fe)2O
~275
381 nm
2.5*10^4 M^-1cm^-
~430
649 nm
6.8*10^3 M^-1cm^-
~718

Purification of 1 via column chromatography

The column was packed with 1.5 L of silica gel and run initially in methylene chloride. The fractions were collected in 280 18 x 150 mm tubes, then 6 500 mL Erlenmeyer flasks. Thin layer chromatography was performed in methylene chloride, and visualized via a UV lamp. Spot number 5 corresponds to the product. Tubes 171-280, and flasks 1-5 were combined, and concentrated to a yellow solid.

Column chromatography data for **1**.

Tube #	Spot #	Solvent Mixture
1-31	None	CH_2Cl_2
32-41	1	CH_2Cl_2
51-71	1+2	CH_2Cl_2
81-120	2+3	CH_2Cl_2
121-130	3	CH_2Cl_2
131-170	3+4	CH_2Cl_2
171-240	4+5	CH_2Cl_2
241-280	5	4:1 CH_2Cl_2:EtOAc

Spot #	R_f
1	~1
2	0.8
3	0.4
4	0.3
5	0.2
6	~0

Flask #	Spot #	Solvent Mixture
1	5	4:1 CH_2Cl_2:EtOAc
2-3	5	1:1 CH_2Cl_2:EtOAc
4	5	EtOAc
5	5+6	EtOAc
6	6	EtOAc