Supporting information for

B-C Bond Cleavage by a Low-Coordinate Iron Hydride Complex and N-N Bond Cleavage by the Hydridoborate Product

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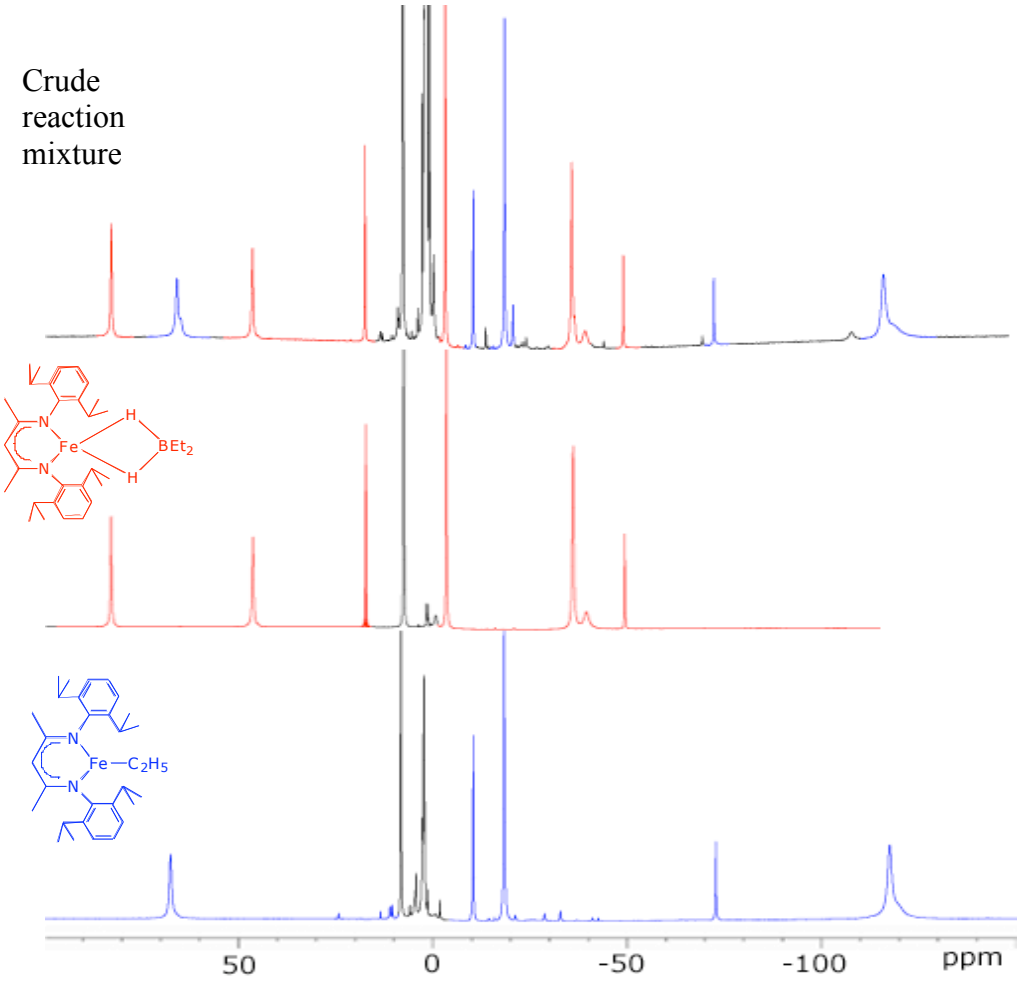
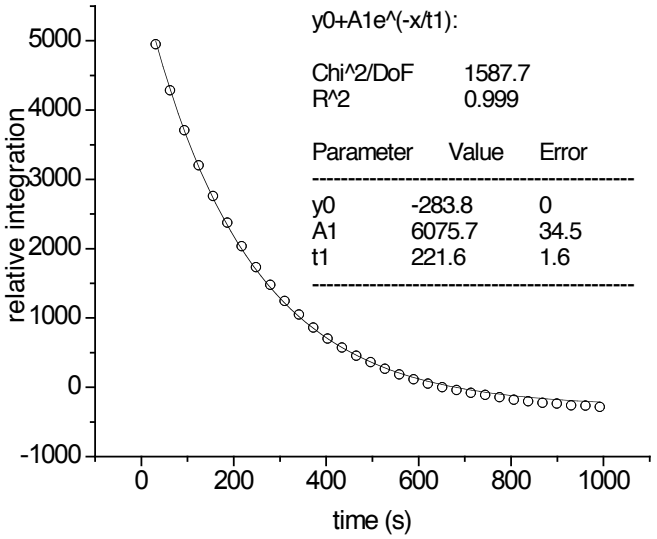
NMR for the reaction of $[L^{Me}FeH]_2 + BEt_3 \rightarrow L^{Me}Fe(\mu\text{-}H)_2BEt_2 + L^{Me}FeEt$



The ratio between $L^{Me}Fe(\mu\text{-}H)_2BEt_2$ and $L^{Me}FeEt$ is 1 : 1 based on NMR integration of the reaction mixture.

Kinetic Experiments

1. BEt_3 effect. Figure SI-1 shows a typical time course for the disappearance of $L^{Me}Fe(\mu\text{-}H)_2FeL^{Me}$ in the presence of excess BEt_3. The plot of ln[**1a**] vs. time confirms the first-order dependence on [Fe]. Attempted fits to 1/[**1a**] (2nd order) or [**1a**]$^{1/2}$ (half-order) were markedly curved.



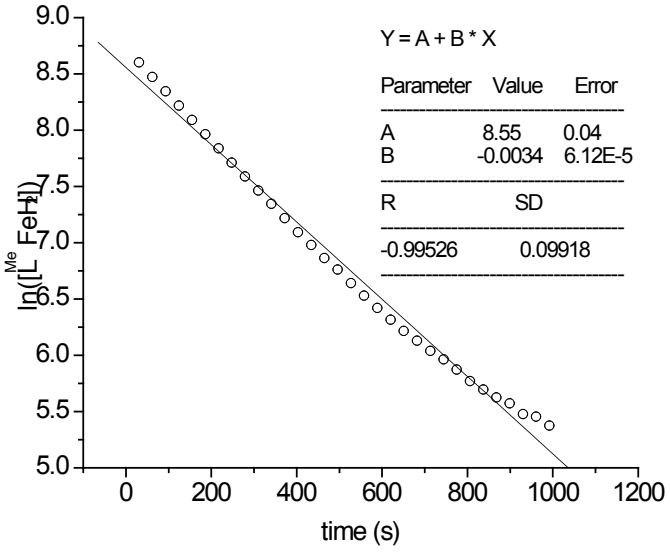


Figure SI-1. (a) Top: The disappearance of **1a** at 313.8 K. (b) Bottom: plot of ln[**1a**] vs. time using the same data.

2. [$\mathbf{L^{Me}Fe(\mu\text{-}H)_2FeL^{Me}}$] **effect.** Without Hg^0, we observed a slightly decreased k_{obs} with increasing [**1a**].

Table SI.1. Observed rate constant vs. [**1a**] without Hg^0

1a / mg	[**1a**]	k_{obs} / s^{-1}
4.8 mg	11.1 mM	$k_{obs} = 3.97(7)\times10^{-3}$
8.0 mg	21.1 mM	$k_{obs} = 3.33(1)\times10^{-3}$
12.6 mg	31.5 mM	$k_{obs} = 2.79(4)\times10^{-3}$
16.9 mg	42.3 mM	$k_{obs} = 2.51(2)\times10^{-3}$

However, when a drop of Hg^0 is used, k_{obs} remains constant within 20 mM < [**1**] < 40 mM (see table in paper).

3. Rate constants from following the concentration of different compounds

Table SI.2. Observed rate constants from integration of different compounds

[**1a**]	[BEt_3]	k_{obs} / s^{-1} calculated by		
		1a	$L^{Me}FeH_2BEt_2$	$L^{Me}FeEt$
4.0×10^{-3}	0.12	$5.3(2)\times10^{-3}$	$5.8(2)\times10^{-3}$	$5.5(4)\times10^{-3}$
8.0×10^{-3}	0.24	$5.2(1)\times10^{-3}$	$4.8(4)\times10^{-3}$	$4.8(3)\times10^{-3}$
15.9×10^{-3}	0.48	$4.8(4)\times10^{-3}$	$4.4(3)\times10^{-3}$	$4.5(3)\times10^{-3}$

4. Solvent effect on rate constant

Table SI.3. Solvent effect on rate constant (without Hg^0)

Solvent	[BEt_3]	[1**a**]	Observed rate constant k_{obs} (s^{-1})
C_6D_6	419 mM	21.1 mM	$3.33(1)\times10^{-3}$
THF-d_8	419 mM	23.2 mM	$5.77(5)\times10^{-3}$
75% o-$C_6H_4F_2$ + 25% C_6D_6	419 mM	24.5 mM	$2.57(3)\times10^{-3}$ [a]

a. THF may coordinate to iron during the reaction. An instant color change of the reaction mixture from brown to red in liquid nitrogen supports this possibility. Thus, the rate constant obtained from THF may not be representative of the same reaction.

3. Activation parameters

1a + BEt_3 → $L^{Me}Fe(\mu\text{-}H)_2BEt_2$ + $L^{Me}FeEt$

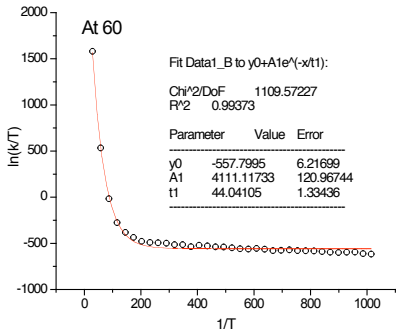
Table SI.3. Reaction rate constants at different temperature.

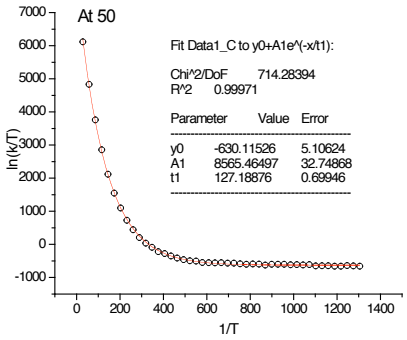
Entry	Δδ(std)	T / K	1/ T (x value)	k	ln(k/T) (y value)
1	1.3194	332.86	0.00300	$5.42(2)\times10^{-2}$	-8.72
2	1.4074	324.03	0.00309	$1.88(2)\times10^{-2}$	-9.76
3	1.5095	313.79	0.00319	$5.24(1)\times10^{-3}$	-11.00
4	1.5991	304.80	0.00328	$1.45(1)\times10^{-3}$	-12.26
5	1.6014	294.71	0.00339	$4.99(1)\times10^{-4}$	-13.29
6	1.6726	287.16	0.00348	$2.10(9)\times10^{-4}$	-14.13
7	1.7391	279.69	0.00358	$8.79(2)\times10^{-5}$	-14.97

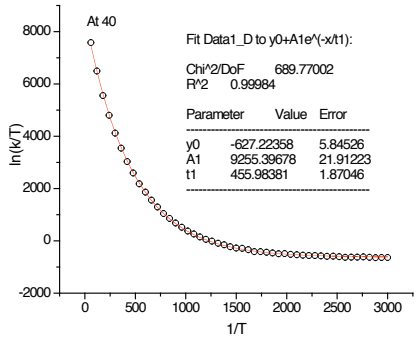
$\ln(k/T) = -(\Delta H^{\neq}/R)(1/T)+(\Delta S^{\neq}/R)+\ln(k_B/T)$,
where $\ln(k_B/h) = 23.76$ and $R=1.987$ cal.K^{-1}.mol^{-1}
$\Delta H^{\neq} = 21.8 \pm 0.8$ kcal.mol^{-1}
$\Delta S^{\neq} = 1 \pm 2$ eu

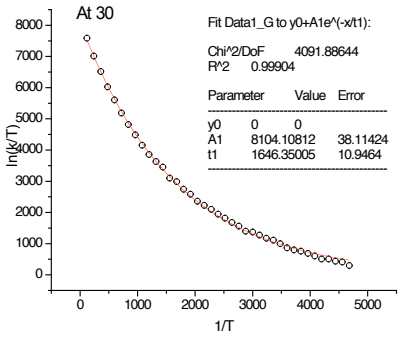
The Eyring plot is shown in the paper.

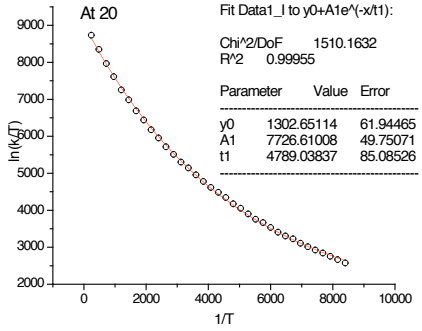
Table SI.4. Observed rate constant at various temperature.

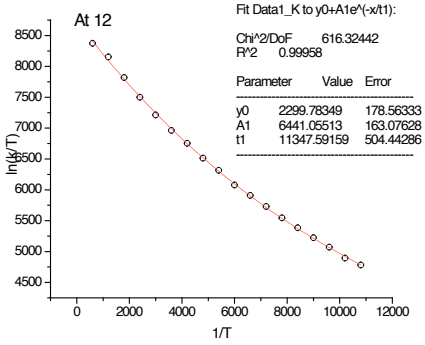


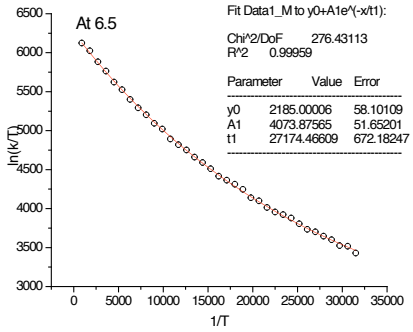












$k_{obs} = 1/t_1$, $k = k_{obs}/[BEt_3] = k_{obs}/0.419$

t	k_{obs}	k
60°C	2.27×10^{-2}	5.42×10^{-2}
50°C	7.86×10^{-3}	1.88×10^{-2}
40°C	2.19×10^{-3}	5.24×10^{-3}
30°C	6.07×10^{-4}	1.45×10^{-3}
20°C	2.09×10^{-4}	4.99×10^{-4}
12°C	8.81×10^{-5}	2.10×10^{-4}
6.6°C	3.68×10^{-5}	8.79×10^{-5}

NMR titration of H_2NNH_2 binding. To a solution of **1a** (21 mg) in benzene-d_6 (1.0 mL) was added hydrazine in small aliquots (0.4 μL each time) using a syringe. The ^{1}H NMR spectrum was recorded after each addition. The titration curve and Job plot show that the stoichiometry is 1:1.

Table SI.5a. NMR titration data at 260 ppm.

H_2NNH_2 : $L^{Me}Fe(H)_2BEt_2$	Chemical shift / ppm
0	208.072
0.17	215.762
0.33	224.498
0.49	232.503
0.66	242.134
0.82	258.893
0.99	261.421
1.15	262.758
1.32	262.911
1.48	263.487
1.65	264.034
1.81	264.607
1.98	264.882
2.14	265.095

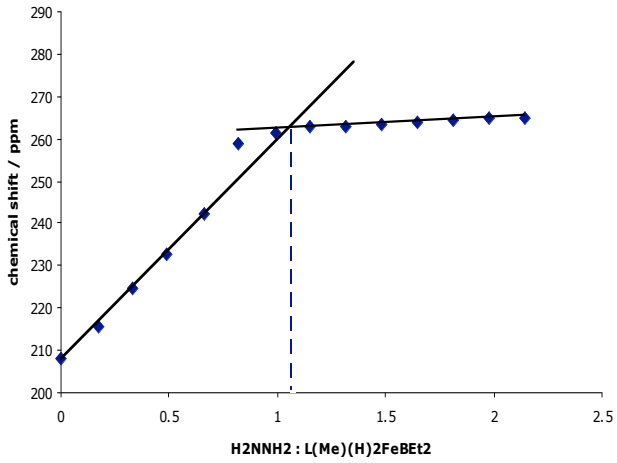


Figure SI.2a. Job plot using peak near 260 ppm

Table SI.5b. NMR titration data at 19 ppm.

H_2NNH_2 : $L^{Me}Fe(H)_2BEt_2$	Chemical shift / ppm
0	46.008
0.17	41.573
0.33	36.581
0.49	31.935
0.66	26.828
0.82	20.197
0.99	18.8
1.15	17.962
1.32	17.522
1.48	17.256
1.65	17.108
1.81	17.047
1.98	16.925
2.14	16.85

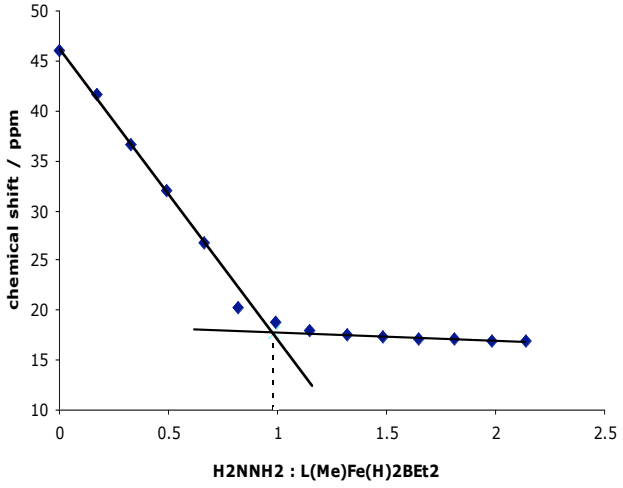


Figure SI.2b. Job plot using peak near 19 ppm

Gas Chromatography Method for Detecting Free Hydrogen. Calibration plot: toluene (3 mL) and a magnetic stir bar were placed in a 25 mL round bottom flask. The flask was capped by an adaptor with a Teflon pin. The open end of the adaptor was closed with a rubber septum. Using a syringe, 8 mL of the gas inside was removed and 8 mL CH_4 (1043 mbar) was injected into the closed system as an internal standard. A sample of H_2 was added to the flask (2 mL each time, 1051 mbar). Finally, 20 μL of the gas was withdrawn and injected into the GC. The amount of hydrogen was detected by GC-17A (Shimadzu) with a molecular 5Å column (30 m × 0.25 mm, oven temperature 26 °C, carrier gas N_2, 600 kPa). A calibration plot was obtained by plotting GC peak integration ratio of H_2:CH_4 versus the amount of hydrogen added to the flask.

Table SI.6. GC calibration plot data.

V_{H_2} / mL	Amount of H_2 / μmol	H_2 peak integration	CH_4 peak integration	Integration Ratio H_2:CH_4
0.2	8.60	6.085	67.29	0.090
0.2	8.60	7.598	78.033	0.097
0.3	12.89	10.899	70.002	0.156
0.6	25.79	19.571	70.701	0.277
0.6	25.79	18.441	70.165	0.263
0.8	34.39	24.54	66.257	0.370
0.8	34.39	22.226	62.222	0.357
1.0	42.98	28.784	62.661	0.459
1.0	42.98	29.119	63.838	0.456
1.2	51.58	27.994	52.773	0.530
1.2	51.58	30.233	55.601	0.544
1.4	60.17	32.736	55.16	0.593
1.4	60.17	34.504	57.272	0.602
1.6	68.77	38.649	54.45	0.710
1.6	68.77	38.348	53.232	0.720
1.8	77.37	41.791	51.406	0.813
2.0	85.96	45.382	49.326	0.920
2.0	85.96	43.223	47.342	0.913

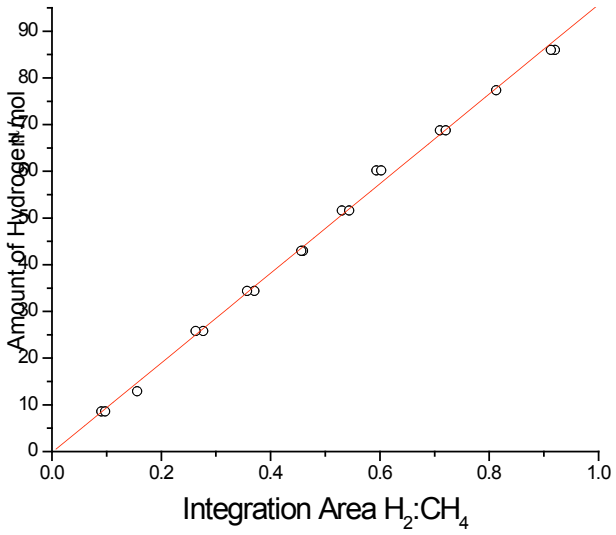


Figure SI.3. GC calibration plot

Detection of H_2 in reactions: To a solution of $L^{Me}Fe(H_2NNH_2)(\mu\text{-}H)_2BEt_2$ in toluene (3 mL) was added 1 eq. of H_2NNH_2 and a stir bar in the same round bottom flask used for the calibration plot. The system was closed. Using a syringe, 8 mL gas was taken out. The mixture was shaken at room temperature for 22 h to make $L^{Me}Fe(H_2NNH_2)(\mu\text{-}H)_2BEt_2$ (**4**). After heating complex **4** at 60 °C for 22 h, 8 mL CH_4 was added and the headspace was subjected to GC analysis as described above. The integration ratio was compared to the calibration plot to quantify the amount of free hydrogen released from the reaction (Table SI.7). The average amount of hydrogen detected from the reaction is 1.67 ± 0.03 per iron.

Table SI.7. Hydrogen detection data.

$L^{Me}Fe(H_2NNH_2)(\mu\text{-}H)_2BEt_2$ (**3**)/ μmol	H_2 detected / μmol	H_2 : Fe ratio
18.8	32.3	1.72 : 1
35.2	58.1	1.65 : 1
40.6	67.0	1.65 : 1

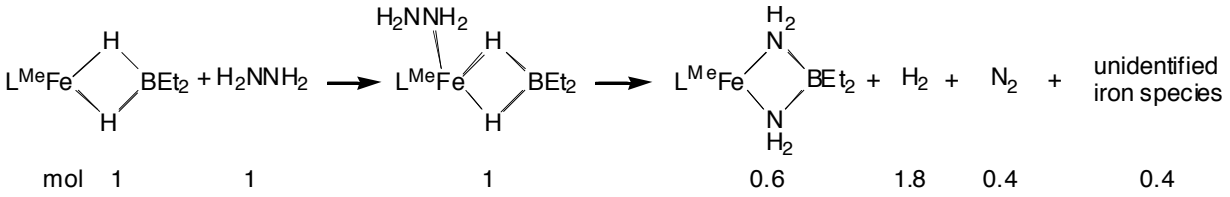
Control experiments were carried out to determine whether there are alternative paths to form gaseous H_2. The results are listed in table SI.8.

1. Heating $L^{Me}Fe(\mu\text{-}H)_2BEt_2$ without any hydrazine.
2. Stirring hydrazine with iron powder (unactivated) in toluene.
3. Heating hydrazine with iron powder (unactivated) in toluene.

Table SI.8. Control experiments

Entry	Reactions	Reaction Condition	Iron Starting Material/ μmol	H_2 detected / μmol	H_2 : Fe ratio
1	$L^{Me}Fe(\mu\text{-}H)_2BEt_2$	80 °C, 22 hr, tol.	45.0	3.8	0.08
2	$Fe + H_2NNH_2$	RT, 22 hr, tol.	71.6	0	0
3	$Fe + H_2NNH_2$	80 °C, 22 hr, tol.	71.6	1.26	0.02

These data show that $L^{Me}Fe(\mu\text{-}H)_2BEt_2$ itself does not lead to the H_2, and that trace iron metal (possibly formed during heating) are not competent to produce the excess H_2. It is possible that other iron species are capable of catalyzing hydrazine decomposition and releasing free hydrogen. An unidentified black precipitate was always observed along with the formation of $L^{Me}Fe(\mu\text{-}NH_2)_2BEt_2$ (**4**). Given that the yield of complex **4** is only 60% , the remaining H_2NNH_2 may in principle release hydrogen up to 1.8 times of starting material $L^{Me}Fe(\mu\text{-}H)_2BEt_2$ (Scheme SI.1) if it disproportionates to N_2 and H_2. Given the good agreement between the calculated and observed stoichiometries, we tentatively propose that the excess H_2 is generated through catalytic decomposition of hydrazine by some unidentified iron species.



Scheme SI.1. Balanced reaction between iron starting material and free hydrogen.

IR Spectra of Complex 4 and 5.

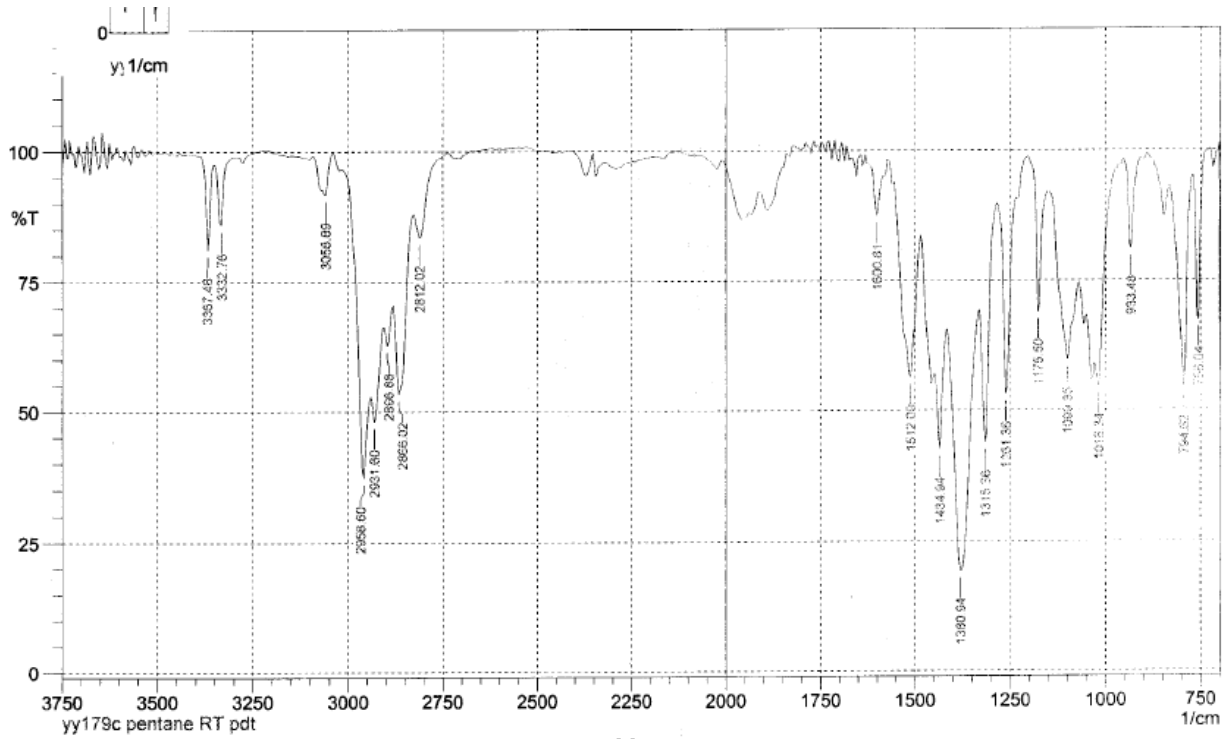


Figure SI.4a. IR spectrum of $L^{Me}Fe(H_2NNH_2)(\mu\text{-}H)_2BEt_2$ (**4**).

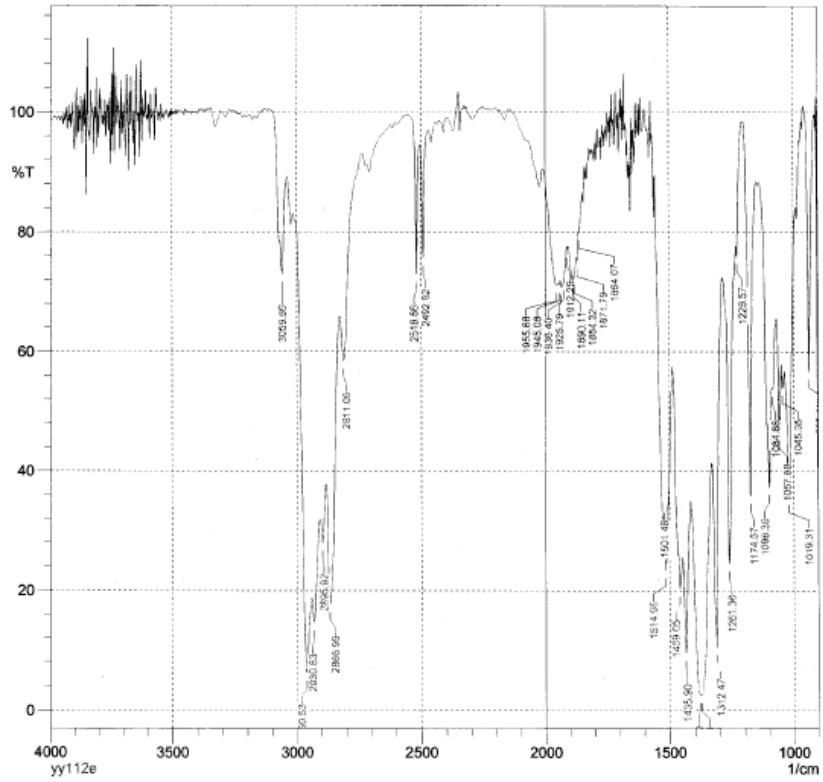


Figure SI.4b. IR spectrum of $L^{Me}Fe(D_2NND_2)(\mu\text{-}H)_2BEt_2$ (**4-*d*$_4$**).

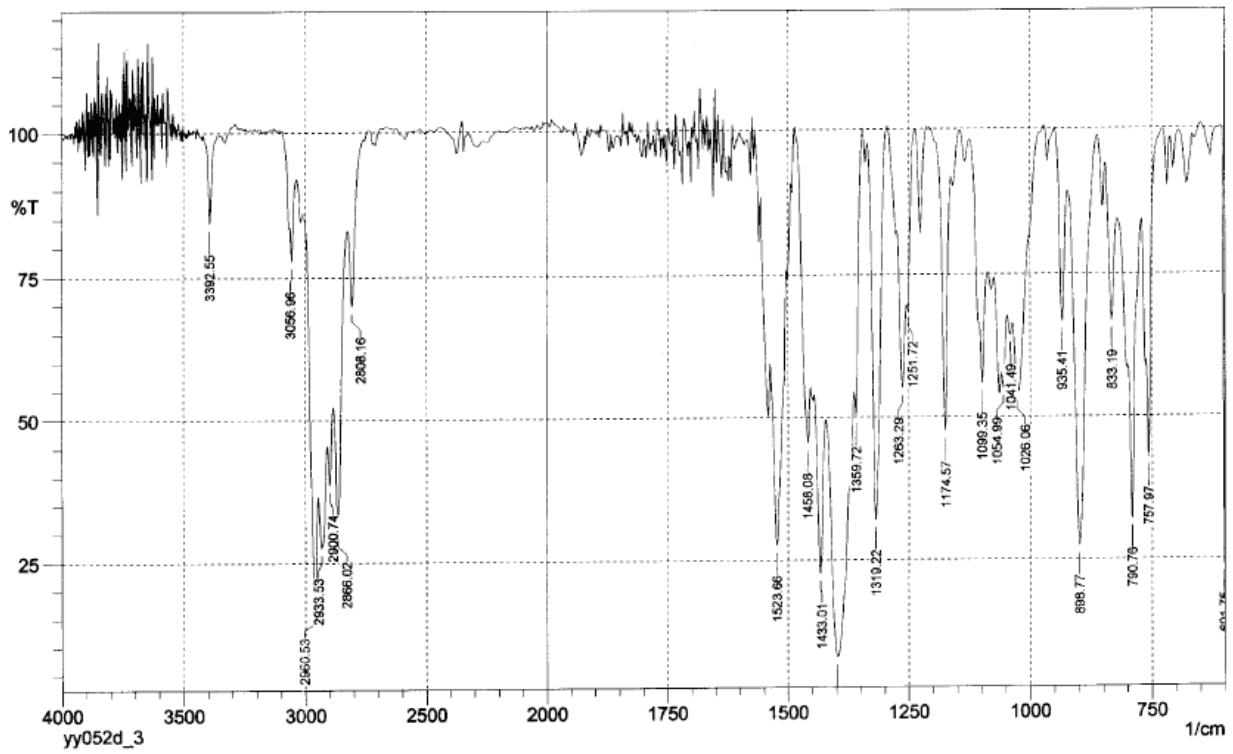


Figure SI.5a. IR spectrum of $L^{Me}Fe(\mu\text{-}NH_2)_2BEt_2$ (**5**).

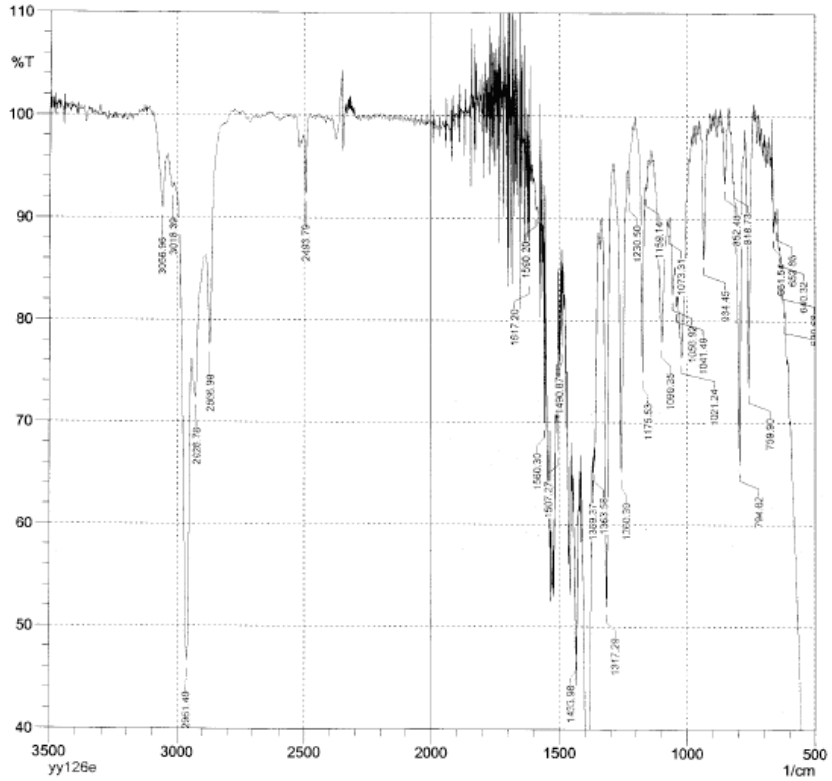


Figure SI.5b. IR spectrum of $L^{Me}Fe(\mu\text{-}ND_2)_2BEt_2$ (**5-*d*$_4$**).

M-H-B Cambridge Data Base Search results.

Table SI.9. Cambridge data base search results for B-H distances in $M(\mu\text{-}H)_2BR_2$

Refcode	B-H distance /Å	Refcode	B-H distance /Å	Refcode	B-H distance /Å
AGEXAL	1.298, 1.281	PIKNAY	1.374, 1.374	WUQQAA	1.192, 1.260
BAJHAW	1.237, 1.272	PUCMOP	1.094, 1.201	WUQQAA	1.187, 1.265
BAJHAW	1.251, 1.330	SURPUQ	1.192, 1.233	WUQQEE	1.263, 1.208
BAJHAW	1.219, 1.265	SURPUQ	1.240, 1.295	ZAZVUR	1.279, 1.252
BAJHEA	1.186, 1.210	SUWROR	1.269, 1.238	ZUBGAE	1.228, 1.236
BAJHEA	1.266, 1.238	SUWRUX	1.269, 1.302	ZUBGAE01	1.228, 1.236
BAJHEA	1.251, 1.211	SUWSAE	1.343, 1.177	LARFEQ	1.197, 1.238
BAJHIE	1.175, 1.201	SUWSEI	1.264, 1.263	LARFEQ	1.240, 1.240
BAJHIE	1.180, 1.234	SUWSIM	1.289, 1.235	LARFIU	1.177, 1.181
BAJHOK	0.556, 1.371	SUWSIM01	1.298, 1.334	LARFIU	1.222, 1.213
BAJHOK	1.164, 1.395	UMOWUO	1.217, 1.097	LARFIU	1.179, 1.228
BAZSIF	1.350, 1.366	UMOXAV	1.149, 1.054	LARFOA	1.202, 1.174
BAZSIF	1.402, 1.404	VAMTIM	1.148, 1.211	LARFOA	1.218, 1.184
BEBPUT	1.285, 1.382	VAMVAG	1.320, 1.193	LARFOA	1.167, 1.242
COQTAD	1.241, 1.186	VAMXIQ	1.150, 1.228	LARFOA	1.247, 1.226
FAPXUQ	1.340, 1.342	WEFZIQ	1.320, 1.320	LARFOA	1.218, 1.214
FOJMEX	1.024, 1.150	WEFZIQ	1.320, 1.320	LARFOA	1.225, 1.226
FOJMEX	1.365, 1.084	WEFZIQ01	1.205, 1.208	NAQVUX	1.346, 1.313
LOCWAB	1.205, 1.206	WEFZIQ01	1.207, 1.215	XALGUN	1.302, 1.296
LOCWEF	1.053, 1.280	WEFZIQ02	1.150, 1.106	XALGUN	1.285, 1.269
LOCWIJ	1.206, 1.171	WEFZIQ02	1.057, 1.142	XALGUN	1.248, 1.302
NULSAO	1.182, 1.186	WEZGUD	1.387, 1.382	XALGUN	1.285, 1.302
NULSES	1.104, 1.203	WEZGUD01	1.261, 1.320		

The average B-H distance based on table SI.9 is 1.24 Å with standard deviation of 0.09 Å.

Analysis used CSD 5.27 (May 2006), ConQuest 1.8, VISTA 2.1c.

Fe-(N_2H_4) Cambridge Data Base Search results

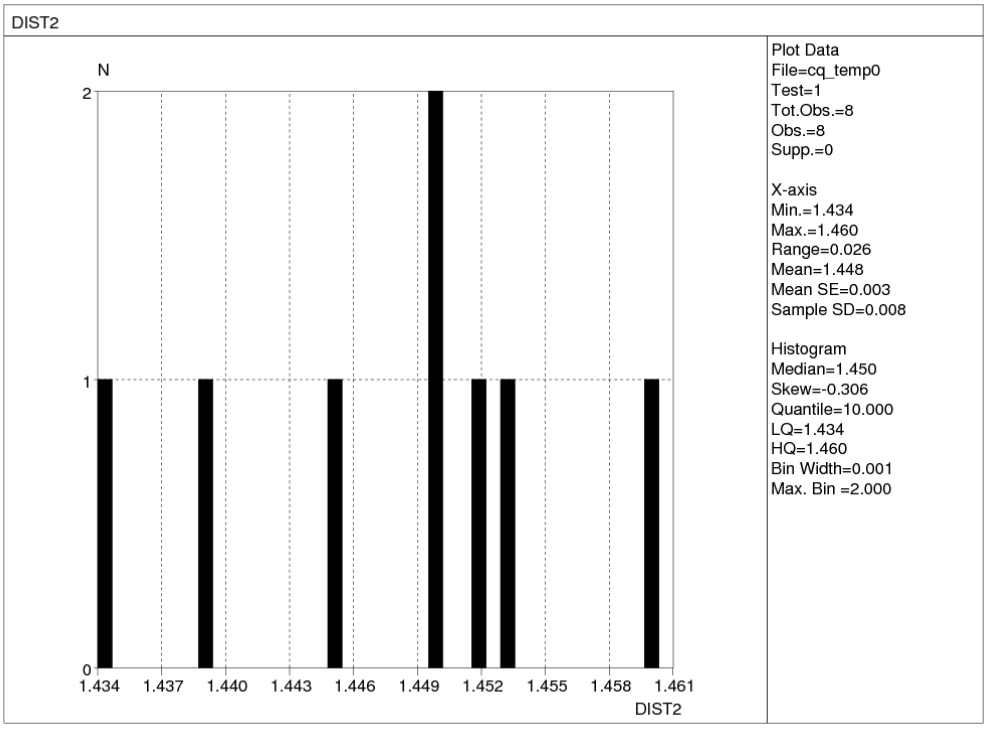


Figure SI.6a. Histogram of N-N distance in Fe-(N_2H_4) complexes.

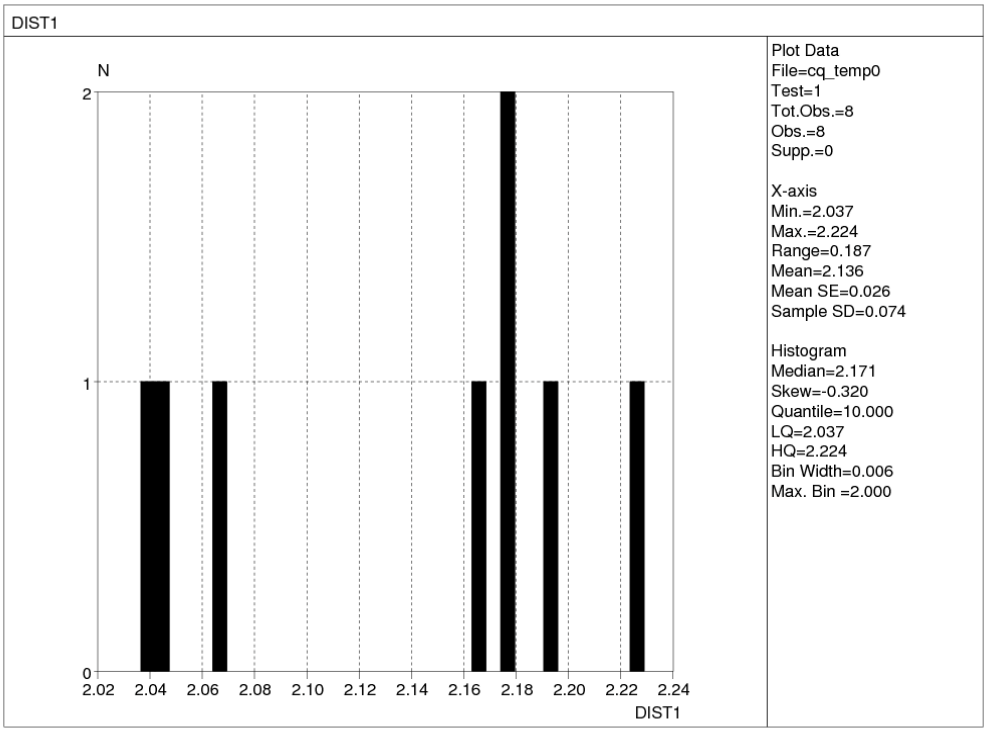


Figure SI.6b. Histogram of Fe-N distance in Fe-(N_2H_4) complexes.

X-ray Crystallography. Single crystals, selected from batches immersed in Paratone-8277, were mounted on glass fibers and placed immediately into a cold nitrogen stream (-80 °C) on a Siemens SMART Platform diffractometer (MoKα radiation, graphite monochromator) equipped with a CCD area detector. For each data collection, a randomly oriented region of reciprocal space was surveyed: four major sections of frames were collected with 0.3° steps in ω at four different φ settings and a detector position of -28° in 2θ.[1] The data were integrated[2] and the intensity data were corrected for absorption.[3] Final cell constants were calculated from the xyz centroids of strong reflections from the actual data collections after integration. Space group assignments were based on statistics related to systematic absences, reflection intensities, and space group frequencies.[4] Each structure was solved by direct methods[5] and was refined by full-matrix least squares on F^2.[4] All non-hydrogen atoms were refined with anisotropic displacement parameters and all hydrogen atoms were placed in appropriated geometrical positions and refined with relative isotropic displacement parameters, except when noted otherwise. A summary of experimental and refinement details can be found in the tables below.

[1]SMART V5.629, Bruker Analytical X-ray System, Madison, WI (2003).
[2]SAINT V7.06A, Bruker Analytical X-ray Systems, Madison, WI (2003).
[3]SADABS V2.10, An empirical correction for absorption anisotropy, R. Blessing, *Acta Cryst.* **A51**, 33-38 (1995).
[4]SHELXTL V6.14, Bruker Analytical X-ray Systems, Madison, WI (2000).
[5]SIR92, A. Altomare, G. Cascarano, C. Giacovazzo, and A. Gualardi, *J. Appl. Cryst.* **26**, 343-350 (1993).

$L^{Me}Fe(\mu\text{-}H)_2BEt_2$ (complex 2a).

Table SI.10a. Crystal data and structure refinement for holyy**2a**.

Identification code	holyy22	
Empirical formula	C33 H53 B Fe N2	
Formula weight	544.43	
Temperature	243(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	*C*2/*c*	
Unit cell dimensions	*a* = 15.0387(15) Å	α = 90°
	b = 10.5584(10) Å	β = 91.965(2)°
	c = 20.980(2) Å	γ = 90°
Volume	3329.4(6) Å^3	
Z	4	
Density (calculated)	1.086 Mg/m^3	
Absorption coefficient	0.474 mm^{-1}	
F(000)	1184	
Crystal color, morphology	red-orange, needle	
Crystal size	0.50 x 0.12 x 0.04 mm^3	
Theta range for data collection	1.94 to 29.57°	
Index ranges	$-20 \le h \le 20, -14 \le k \le 14, -29 \le l \le 29$	
Reflections collected	22469	
Independent reflections	4665 [*R*(int) = 0.0250]	
Observed reflections	3814	
Completeness to theta = 29.57°	99.9%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9813 and 0.7974	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4665 / 0 / 196	
Goodness-of-fit on F^2	1.025	
Final *R* indices [*I*>2sigma(*I*)]	*R*1 = 0.0354, *wR*2 = 0.0981	
R indices (all data)	*R*1 = 0.0459, *wR*2 = 0.1037	
Largest diff. peak and hole	0.274 and -0.218 e.Å^{-3}	

Table SI.10b. Bond lengths [Å] and angles [°] for **2a**.

Fe-H(1)#1	1.744(15)	C(12)-C(62)	1.4034(19)
Fe-N(11)	1.9711(10)	C(12)-C(22)	1.408(2)
Fe-N(11)#1	1.9711(10)	C(22)-C(32)	1.396(2)
Fe-B	2.237(3)	C(22)-C(72)	1.514(3)
Fe-B#1	2.237(3)	C(32)-C(42)	1.374(3)
Fe-H(1)	1.744(15)	C(32)-H(32A)	0.9400
B-H(1)#1	1.214(16)	C(42)-C(52)	1.370(3)
B-C(1)	1.589(6)	C(42)-H(42A)	0.9400
B-C(3)	1.596(5)	C(52)-C(62)	1.398(2)
B-H(1)	1.349(16)	C(52)-H(52A)	0.9400
C(1)-C(2)	1.521(7)	C(62)-C(102)	1.516(2)
C(1)-H(1B)	0.9800	C(72)-C(92)	1.512(3)
C(1)-H(1C)	0.9800	C(72)-C(82)	1.523(3)
C(2)-H(2A)	0.9700	C(72)-H(72A)	0.9900
C(2)-H(2B)	0.9700	C(82)-H(82A)	0.9700
C(2)-H(2C)	0.9700	C(82)-H(82B)	0.9700
C(3)-C(4)	1.482(6)	C(82)-H(82C)	0.9700
C(3)-H(3A)	0.9800	C(92)-H(92A)	0.9700
C(3)-H(3B)	0.9800	C(92)-H(92B)	0.9700
C(4)-H(4A)	0.9700	C(92)-H(92C)	0.9700
C(4)-H(4B)	0.9700	C(102)-C(112)	1.523(3)
C(4)-H(4C)	0.9700	C(102)-C(122)	1.537(2)
N(11)-C(21)	1.3326(16)	C(102)-H(10A)	0.9900
N(11)-C(12)	1.4361(15)	C(112)-H(11G)	0.9700
C(11)-C(21)	1.5099(18)	C(112)-H(11H)	0.9700
C(11)-H(11A)	0.9700	C(112)-H(11I)	0.9700
C(11)-H(11B)	0.9700	C(122)-H(12A)	0.9700
C(11)-H(11C)	0.9700	C(122)-H(12B)	0.9700
C(11)-H(11D)	0.9700	C(122)-H(12C)	0.9700
C(11)-H(11E)	0.9700	H(1)#1-Fe-N(11)	124.2(5)
C(11)-H(11F)	0.9700	H(1)#1-Fe-N(11)#1	123.0(5)
C(21)-C(31)	1.3995(16)	N(11)-Fe-N(11)#1	95.92(6)
C(31)-C(21)#1	1.3995(16)	H(1)#1-Fe-B	32.6(5)
C(31)-H(31A)	0.9400	N(11)-Fe-B	125.53(13)

N(11)#1-Fe-B	138.46(14)	C(21)-C(11)-H(11B)	109.5
H(1)#1-Fe-B#1	37.1(5)	H(11A)-C(11)-H(11B)	109.5
N(11)-Fe-B#1	138.46(14)	C(21)-C(11)-H(11C)	109.5
N(11)#1-Fe-B#1	125.53(13)	H(11A)-C(11)-H(11C)	109.5
B-Fe-B#1	13.80(17)	H(11B)-C(11)-H(11C)	109.5
H(1)#1-Fe-H(1)	68.6(10)	C(21)-C(11)-H(11D)	109.5
N(11)-Fe-H(1)	123.0(5)	H(11A)-C(11)-H(11D)	141.1
N(11)#1-Fe-H(1)	124.2(5)	H(11B)-C(11)-H(11D)	56.3
B-Fe-H(1)	37.1(5)	H(11C)-C(11)-H(11D)	56.3
B#1-Fe-H(1)	32.6(5)	C(21)-C(11)-H(11E)	109.5
H(1)#1-B-C(1)	112.4(8)	H(11A)-C(11)-H(11E)	56.3
H(1)#1-B-C(3)	109.1(9)	H(11B)-C(11)-H(11E)	141.1
C(1)-B-C(3)	114.3(3)	H(11C)-C(11)-H(11E)	56.3
H(1)#1-B-Fe	50.7(7)	H(11D)-C(11)-H(11E)	109.5
C(1)-B-Fe	116.4(3)	C(21)-C(11)-H(11F)	109.5
C(3)-B-Fe	129.3(3)	H(11A)-C(11)-H(11F)	56.3
H(1)#1-B-H(1)	100.0(13)	H(11B)-C(11)-H(11F)	56.3
C(1)-B-H(1)	114.2(9)	H(11C)-C(11)-H(11F)	141.1
C(3)-B-H(1)	105.8(7)	H(11D)-C(11)-H(11F)	109.5
Fe-B-H(1)	51.2(7)	H(11E)-C(11)-H(11F)	109.5
C(2)-C(1)-B	114.4(5)	N(11)-C(21)-C(31)	123.72(13)
C(2)-C(1)-H(1B)	108.7	N(11)-C(21)-C(11)	119.59(12)
B-C(1)-H(1B)	108.7	C(31)-C(21)-C(11)	116.69(13)
C(2)-C(1)-H(1C)	108.7	C(21)-C(31)-C(21)#1	129.56(18)
B-C(1)-H(1C)	108.7	C(21)-C(31)-H(31A)	115.2
H(1B)-C(1)-H(1C)	107.6	C(21)#1-C(31)-H(31A)	115.2
C(4)-C(3)-B	116.7(3)	C(62)-C(12)-C(22)	121.92(13)
C(4)-C(3)-H(3A)	108.1	C(62)-C(12)-N(11)	119.27(12)
B-C(3)-H(3A)	108.1	C(22)-C(12)-N(11)	118.61(12)
C(4)-C(3)-H(3B)	108.1	C(32)-C(22)-C(12)	117.33(16)
B-C(3)-H(3B)	108.1	C(32)-C(22)-C(72)	121.16(16)
H(3A)-C(3)-H(3B)	107.3	C(12)-C(22)-C(72)	121.50(14)
C(21)-N(11)-C(12)	120.59(10)	C(42)-C(32)-C(22)	121.38(17)
C(21)-N(11)-Fe	123.47(8)	C(42)-C(32)-H(32A)	119.3
C(12)-N(11)-Fe	115.87(8)	C(22)-C(32)-H(32A)	119.3
C(21)-C(11)-H(11A)	109.5	C(52)-C(42)-C(32)	120.54(16)

C(52)-C(42)-H(42A)	119.7	H(92A)-C(92)-H(92B)	109.5
C(32)-C(42)-H(42A)	119.7	C(72)-C(92)-H(92C)	109.5
C(42)-C(52)-C(62)	121.16(18)	H(92A)-C(92)-H(92C)	109.5
C(42)-C(52)-H(52A)	119.4	H(92B)-C(92)-H(92C)	109.5
C(62)-C(52)-H(52A)	119.4	C(62)-C(102)-C(112)	110.49(16)
C(52)-C(62)-C(12)	117.65(15)	C(62)-C(102)-C(122)	112.58(15)
C(52)-C(62)-C(102)	120.35(15)	C(112)-C(102)-C(122)	110.45(16)
C(12)-C(62)-C(102)	121.96(12)	C(62)-C(102)-H(10A)	107.7
C(92)-C(72)-C(22)	111.48(18)	C(112)-C(102)-H(10A)	107.7
C(92)-C(72)-C(82)	108.6(2)	C(122)-C(102)-H(10A)	107.7
C(22)-C(72)-C(82)	114.1(2)	C(102)-C(112)-H(11G)	109.5
C(92)-C(72)-H(72A)	107.4	C(102)-C(112)-H(11H)	109.5
C(22)-C(72)-H(72A)	107.4	H(11G)-C(112)-H(11H)	109.5
C(82)-C(72)-H(72A)	107.4	C(102)-C(112)-H(11I)	109.5
C(72)-C(82)-H(82A)	109.5	H(11G)-C(112)-H(11I)	109.5
C(72)-C(82)-H(82B)	109.5	H(11H)-C(112)-H(11I)	109.5
H(82A)-C(82)-H(82B)	109.5	C(102)-C(122)-H(12A)	109.5
C(72)-C(82)-H(82C)	109.5	C(102)-C(122)-H(12B)	109.5
H(82A)-C(82)-H(82C)	109.5	H(12A)-C(122)-H(12B)	109.5
H(82B)-C(82)-H(82C)	109.5	C(102)-C(122)-H(12C)	109.5
C(72)-C(92)-H(92A)	109.5	H(12A)-C(122)-H(12C)	109.5
C(72)-C(92)-H(92B)	109.5	H(12B)-C(122)-H(12C)	109.5

Symmetry transformations used to generate equivalent atoms:

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

$L^{Me}Fe(\mu\text{-}H)_2BPh_2$ (Complex 2b).

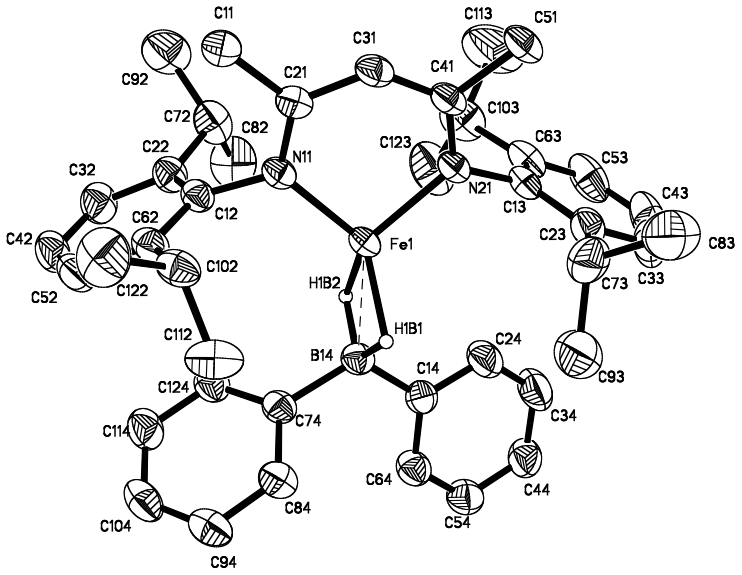


Figure SI.7. Thermal-ellipsoid plot of the molecular structure of $L^{Me}Fe(\mu\text{-}H)_2BPh_2$ **(2b)**

Table SI.11a. Crystal data and structure refinement for **2b**.

Identification code	holyy21	
Empirical formula	C41 H53 B Fe N2	
Formula weight	640.51	
Temperature	180.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	*a* = 11.6217(3) Å	α = 100.311(1)°
	b = 12.3076(3) Å	β = 107.099(1)°
	c = 15.5599(6) Å	γ = 112.180(1)°
Volume	1861.09(10) $Å^3$	
Z	2	
Density (calculated)	1.143 Mg/m^3	
Absorption coefficient	0.434 mm^{-1}	
F(000)	688	
Crystal color, morphology	red-orange, block	

Crystal size	0.28 x 0.28 x 0.22 mm^3
Theta range for data collection	1.45 to 30.03°
Index ranges	$-16 \le h \le 16, -17 \le k \le 17, -21 \le l \le 21$
Reflections collected	29092
Independent reflections	10746 [R(int) = 0.0216]
Observed reflections	9067
Completeness to theta = 30.03°	98.6%
Absorption correction	Multi-scan
Max. and min. transmission	0.9105 and 0.8881
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10746 / 3 / 431
Goodness-of-fit on F^2	1.053
Final R indices [I>2sigma(I)]	$R1$ = 0.0418, $wR2$ = 0.1141
R indices (all data)	$R1$ = 0.0506, $wR2$ = 0.1197
Largest diff. peak and hole	0.540 and -0.223 e.$Å^{-3}$

Table SI.11b. Bond lengths [Å] and angles [°] for **2b**.

Fe(1)-N(11)	1.9626(11)	C(21)-C(31)	1.4020(18)
Fe(1)-N(21)	1.9765(10)	C(31)-C(41)	1.398(2)
Fe(1)-B(14)	2.2391(15)	C(31)-H(31A)	0.9500
Fe(1)-H(1B1)	1.724(16)	C(41)-C(51)	1.5092(19)
Fe(1)-H(1B2)	1.716(17)	C(51)-H(51A)	0.9800
B(14)-C(14)	1.600(2)	C(51)-H(51B)	0.9800
B(14)-C(74)	1.603(2)	C(51)-H(51C)	0.9800
B(14)-H(1B1)	1.277(16)	C(12)-C(62)	1.4057(18)
B(14)-H(1B2)	1.190(16)	C(12)-C(22)	1.4071(19)
N(11)-C(21)	1.3396(16)	C(22)-C(32)	1.398(2)
N(11)-C(12)	1.4456(16)	C(22)-C(72)	1.513(2)
N(21)-C(41)	1.3368(17)	C(32)-C(42)	1.381(2)
N(21)-C(13)	1.4401(17)	C(32)-H(32A)	0.9500
C(11)-C(21)	1.5044(19)	C(42)-C(52)	1.377(3)
C(11)-H(11A)	0.9800	C(42)-H(42A)	0.9500
C(11)-H(11B)	0.9800	C(52)-C(62)	1.394(2)
C(11)-H(11C)	0.9800	C(52)-H(52A)	0.9500

C(62)-C(102)	1.524(2)	C(93)-H(93A)	0.9800
C(72)-C(82)	1.533(3)	C(93)-H(93B)	0.9800
C(72)-C(92)	1.536(3)	C(93)-H(93C)	0.9800
C(72)-H(72A)	1.0000	C(103)-C(123)	1.527(4)
C(82)-H(82A)	0.9800	C(103)-C(113)	1.554(4)
C(82)-H(82B)	0.9800	C(103)-H(10B)	1.0000
C(82)-H(82C)	0.9800	C(113)-H(11G)	0.9800
C(92)-H(92A)	0.9800	C(113)-H(11H)	0.9800
C(92)-H(92B)	0.9800	C(113)-H(11I)	0.9800
C(92)-H(92C)	0.9800	C(123)-H(12D)	0.9800
C(102)-C(112)	1.524(2)	C(123)-H(12E)	0.9800
C(102)-C(122)	1.530(2)	C(123)-H(12F)	0.9800
C(102)-H(10A)	1.0000	C(11')-H(11K)	0.9800
C(112)-H(11D)	0.9800	C(11')-H(11L)	0.9800
C(112)-H(11E)	0.9800	C(11')-H(11M)	0.9800
C(112)-H(11F)	0.9800	C(12')-H(12H)	0.9800
C(122)-H(12A)	0.9800	C(12')-H(12I)	0.9800
C(122)-H(12B)	0.9800	C(12')-H(12J)	0.9800
C(122)-H(12C)	0.9800	C(14)-C(24)	1.387(2)
C(13)-C(23)	1.403(2)	C(14)-C(64)	1.393(2)
C(13)-C(63)	1.407(2)	C(24)-C(34)	1.386(2)
C(23)-C(33)	1.398(2)	C(24)-H(24A)	0.9500
C(23)-C(73)	1.513(2)	C(34)-C(44)	1.377(2)
C(33)-C(43)	1.373(3)	C(34)-H(34A)	0.9500
C(33)-H(33A)	0.9500	C(44)-C(54)	1.378(2)
C(43)-C(53)	1.365(3)	C(44)-H(44A)	0.9500
C(43)-H(43A)	0.9500	C(54)-C(64)	1.387(2)
C(53)-C(63)	1.394(2)	C(54)-H(54A)	0.9500
C(53)-H(53A)	0.9500	C(64)-H(64A)	0.9500
C(63)-C(103)	1.518(3)	C(74)-C(124)	1.385(2)
C(73)-C(93)	1.528(3)	C(74)-C(84)	1.399(2)
C(73)-C(83)	1.534(3)	C(84)-C(94)	1.390(2)
C(73)-H(73A)	1.0000	C(84)-H(84A)	0.9500
C(83)-H(83A)	0.9800	C(94)-C(104)	1.377(3)
C(83)-H(83B)	0.9800	C(94)-H(94A)	0.9500
C(83)-H(83C)	0.9800	C(104)-C(114)	1.376(3)

C(104)-H(10C)	0.9500	N(11)-C(21)-C(31)	123.86(12)
C(114)-C(124)	1.397(2)	N(11)-C(21)-C(11)	119.13(12)
C(114)-H(11J)	0.9500	C(31)-C(21)-C(11)	116.99(11)
C(124)-H(12G)	0.9500	C(41)-C(31)-C(21)	129.74(12)
N(11)-Fe(1)-N(21)	97.12(4)	C(41)-C(31)-H(31A)	115.1
N(11)-Fe(1)-B(14)	130.16(5)	C(21)-C(31)-H(31A)	115.1
N(21)-Fe(1)-B(14)	132.66(5)	N(21)-C(41)-C(31)	123.92(12)
N(11)-Fe(1)-H(1B1)	132.2(5)	N(21)-C(41)-C(51)	119.79(13)
N(21)-Fe(1)-H(1B1)	116.5(6)	C(31)-C(41)-C(51)	116.29(12)
B(14)-Fe(1)-H(1B1)	34.6(5)	C(41)-C(51)-H(51A)	109.5
N(11)-Fe(1)-H(1B2)	119.0(6)	C(41)-C(51)-H(51B)	109.5
N(21)-Fe(1)-H(1B2)	128.0(6)	H(51A)-C(51)-H(51B)	109.5
B(14)-Fe(1)-H(1B2)	31.7(5)	C(41)-C(51)-H(51C)	109.5
H(1B1)-Fe(1)-H(1B2)	66.0(8)	H(51A)-C(51)-H(51C)	109.5
C(14)-B(14)-C(74)	116.09(11)	H(51B)-C(51)-H(51C)	109.5
C(14)-B(14)-Fe(1)	126.93(10)	C(62)-C(12)-C(22)	121.46(12)
C(74)-B(14)-Fe(1)	116.97(9)	C(62)-C(12)-N(11)	119.52(12)
C(14)-B(14)-H(1B1)	109.6(7)	C(22)-C(12)-N(11)	118.88(11)
C(74)-B(14)-H(1B1)	109.9(7)	C(32)-C(22)-C(12)	117.89(14)
Fe(1)-B(14)-H(1B1)	50.0(7)	C(32)-C(22)-C(72)	119.12(13)
C(14)-B(14)-H(1B2)	109.9(8)	C(12)-C(22)-C(72)	122.96(12)
C(74)-B(14)-H(1B2)	111.2(8)	C(42)-C(32)-C(22)	121.30(15)
Fe(1)-B(14)-H(1B2)	49.1(8)	C(42)-C(32)-H(32A)	119.4
H(1B1)-B(14)-H(1B2)	98.7(11)	C(22)-C(32)-H(32A)	119.4
C(21)-N(11)-C(12)	120.22(11)	C(52)-C(42)-C(32)	119.82(14)
C(21)-N(11)-Fe(1)	121.85(9)	C(52)-C(42)-H(42A)	120.1
C(12)-N(11)-Fe(1)	117.87(8)	C(32)-C(42)-H(42A)	120.1
C(41)-N(21)-C(13)	119.68(11)	C(42)-C(52)-C(62)	121.63(15)
C(41)-N(21)-Fe(1)	121.48(9)	C(42)-C(52)-H(52A)	119.2
C(13)-N(21)-Fe(1)	118.83(8)	C(62)-C(52)-H(52A)	119.2
C(21)-C(11)-H(11A)	109.5	C(52)-C(62)-C(12)	117.82(14)
C(21)-C(11)-H(11B)	109.5	C(52)-C(62)-C(102)	120.20(13)
H(11A)-C(11)-H(11B)	109.5	C(12)-C(62)-C(102)	121.97(12)
C(21)-C(11)-H(11C)	109.5	C(22)-C(72)-C(82)	111.72(16)
H(11A)-C(11)-H(11C)	109.5	C(22)-C(72)-C(92)	110.82(15)
H(11B)-C(11)-H(11C)	109.5	C(82)-C(72)-C(92)	110.26(16)

C(22)-C(72)-H(72A)	108.0	C(33)-C(23)-C(13)	117.67(15)
C(82)-C(72)-H(72A)	108.0	C(33)-C(23)-C(73)	119.95(16)
C(92)-C(72)-H(72A)	108.0	C(13)-C(23)-C(73)	122.36(14)
C(72)-C(82)-H(82A)	109.5	C(43)-C(33)-C(23)	121.41(18)
C(72)-C(82)-H(82B)	109.5	C(43)-C(33)-H(33A)	119.3
H(82A)-C(82)-H(82B)	109.5	C(23)-C(33)-H(33A)	119.3
C(72)-C(82)-H(82C)	109.5	C(53)-C(43)-C(33)	120.19(17)
H(82A)-C(82)-H(82C)	109.5	C(53)-C(43)-H(43A)	119.9
H(82B)-C(82)-H(82C)	109.5	C(33)-C(43)-H(43A)	119.9
C(72)-C(92)-H(92A)	109.5	C(43)-C(53)-C(63)	121.56(17)
C(72)-C(92)-H(92B)	109.5	C(43)-C(53)-H(53A)	119.2
H(92A)-C(92)-H(92B)	109.5	C(63)-C(53)-H(53A)	119.2
C(72)-C(92)-H(92C)	109.5	C(53)-C(63)-C(13)	117.78(16)
H(92A)-C(92)-H(92C)	109.5	C(53)-C(63)-C(103)	120.29(15)
H(92B)-C(92)-H(92C)	109.5	C(13)-C(63)-C(103)	121.89(14)
C(62)-C(102)-C(112)	111.04(13)	C(23)-C(73)-C(93)	111.56(17)
C(62)-C(102)-C(122)	112.50(15)	C(23)-C(73)-C(83)	111.82(17)
C(112)-C(102)-C(122)	110.68(15)	C(93)-C(73)-C(83)	109.88(15)
C(62)-C(102)-H(10A)	107.5	C(23)-C(73)-H(73A)	107.8
C(112)-C(102)-H(10A)	107.5	C(93)-C(73)-H(73A)	107.8
C(122)-C(102)-H(10A)	107.5	C(83)-C(73)-H(73A)	107.8
C(102)-C(112)-H(11D)	109.5	C(73)-C(83)-H(83A)	109.5
C(102)-C(112)-H(11E)	109.5	C(73)-C(83)-H(83B)	109.5
H(11D)-C(112)-H(11E)	109.5	H(83A)-C(83)-H(83B)	109.5
C(102)-C(112)-H(11F)	109.5	C(73)-C(83)-H(83C)	109.5
H(11D)-C(112)-H(11F)	109.5	H(83A)-C(83)-H(83C)	109.5
H(11E)-C(112)-H(11F)	109.5	H(83B)-C(83)-H(83C)	109.5
C(102)-C(122)-H(12A)	109.5	C(73)-C(93)-H(93A)	109.5
C(102)-C(122)-H(12B)	109.5	C(73)-C(93)-H(93B)	109.5
H(12A)-C(122)-H(12B)	109.5	H(93A)-C(93)-H(93B)	109.5
C(102)-C(122)-H(12C)	109.5	C(73)-C(93)-H(93C)	109.5
H(12A)-C(122)-H(12C)	109.5	H(93A)-C(93)-H(93C)	109.5
H(12B)-C(122)-H(12C)	109.5	H(93B)-C(93)-H(93C)	109.5
C(23)-C(13)-C(63)	121.38(13)	C(63)-C(103)-C(123)	108.5(2)
C(23)-C(13)-N(21)	120.23(12)	C(63)-C(103)-C(113)	108.5(3)
C(63)-C(13)-N(21)	118.22(12)	C(123)-C(103)-C(113)	109.3(3)

C(63)-C(103)-H(10B)	110.1	C(14)-C(64)-H(64A)	118.9
C(123)-C(103)-H(10B)	110.1	C(124)-C(74)-C(84)	116.31(13)
C(113)-C(103)-H(10B)	110.1	C(124)-C(74)-B(14)	123.73(12)
C(24)-C(14)-C(64)	115.92(14)	C(84)-C(74)-B(14)	119.90(12)
C(24)-C(14)-B(14)	121.81(13)	C(94)-C(84)-C(74)	122.30(15)
C(64)-C(14)-B(14)	122.23(13)	C(94)-C(84)-H(84A)	118.9
C(34)-C(24)-C(14)	122.49(15)	C(74)-C(84)-H(84A)	118.9
C(34)-C(24)-H(24A)	118.8	C(104)-C(94)-C(84)	119.85(15)
C(14)-C(24)-H(24A)	118.8	C(104)-C(94)-H(94A)	120.1
C(44)-C(34)-C(24)	120.23(17)	C(84)-C(94)-H(94A)	120.1
C(44)-C(34)-H(34A)	119.9	C(114)-C(104)-C(94)	119.34(15)
C(24)-C(34)-H(34A)	119.9	C(114)-C(104)-H(10C)	120.3
C(34)-C(44)-C(54)	118.84(16)	C(94)-C(104)-H(10C)	120.3
C(34)-C(44)-H(44A)	120.6	C(104)-C(114)-C(124)	120.36(16)
C(54)-C(44)-H(44A)	120.6	C(104)-C(114)-H(11J)	119.8
C(44)-C(54)-C(64)	120.32(15)	C(124)-C(114)-H(11J)	119.8
C(44)-C(54)-H(54A)	119.8	C(74)-C(124)-C(114)	121.83(15)
C(64)-C(54)-H(54A)	119.8	C(74)-C(124)-H(12G)	119.1
C(54)-C(64)-C(14)	122.19(14)	C(114)-C(124)-H(12G)	119.1
C(54)-C(64)-H(64A)	118.9		

$L^{tBu}Fe(\mu\text{-}H)_2BEt_2$ (Complex 2c)

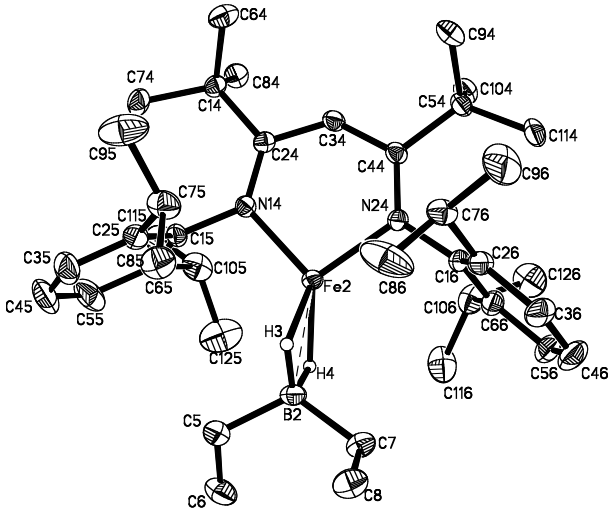


Figure SI.8**.** ORTEP diagram of the molecular structure of $L^{tBu}Fe(\mu\text{-}H)_2BEt_2$

Table SI.12a. Crystal data and structure refinement for **2c**.

Identification code	holyy26	
Empirical formula	C39 H65 B Fe N2	
Formula weight	628.59	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 9.8815(15) Å	α = 90°
	b = 19.289(3) Å	β = 92.644(2)°
	c = 40.693(6) Å	γ = 90°
Volume	7748(2) $Å^3$	
Z	8	
Density (calculated)	1.078 Mg/m^3	
Absorption coefficient	0.416 mm^{-1}	
F(000)	2752	
Crystal color, morphology	dark red, block	
Crystal size	0.48 x 0.28 x 0.12 mm^3	

Theta range for data collection	1.84 to 32.03°
Index ranges	$-14 \le h \le 14, -28 \le k \le 28, -60 \le l \le 60$
Reflections collected	136330
Independent reflections	26979 [R(int) = 0.0342]
Observed reflections	22036
Completeness to theta = 32.03°	99.9%
Absorption correction	Multi-scan
Max. and min. transmission	0.9518 and 0.8255
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	26979 / 0 / 823
Goodness-of-fit on F^2	1.033
Final R indices [I>2sigma(I)]	$R1$ = 0.0416, $wR2$ = 0.1021
R indices (all data)	$R1$ = 0.0545, $wR2$ = 0.1086
Largest diff. peak and hole	0.815 and -0.445 e.Å^{-3}

Table SI.12b. Bond lengths [Å] and angles [°] for **2c**.

Fe(1)-N(11)	1.9691(9)	C(4)-H(4B)	0.9800
Fe(1)-N(21)	1.9714(9)	C(4)-H(4C)	0.9800
Fe(1)-B(1)	2.2323(13)	N(11)-C(21)	1.3344(14)
Fe(1)-H(1)	1.738(16)	N(11)-C(12)	1.4394(14)
Fe(1)-H(2)	1.732(17)	N(14)-C(24)	1.3328(14)
B(1)-C(1)	1.6119(18)	N(14)-C(15)	1.4306(14)
B(1)-C(3)	1.6136(18)	N(14)-Fe(2)	1.9636(10)
B(1)-H(1)	1.256(16)	C(11)-C(81)	1.5316(17)
B(1)-H(2)	1.206(17)	C(11)-C(71)	1.5435(18)
C(1)-C(2)	1.535(2)	C(11)-C(61)	1.5450(18)
C(1)-H(1A)	0.9900	C(11)-C(21)	1.5599(15)
C(1)-H(1B)	0.9900	C(21)-C(31)	1.4091(16)
C(2)-H(2A)	0.9800	C(31)-C(41)	1.4095(15)
C(2)-H(2B)	0.9800	C(31)-H(31)	0.9500
C(2)-H(2C)	0.9800	C(41)-N(21)	1.3377(14)
C(3)-C(4)	1.5278(19)	C(41)-C(51)	1.5619(15)
C(3)-H(3A)	0.9900	C(51)-C(111)	1.5366(17)
C(3)-H(3B)	0.9900	C(51)-C(101)	1.5460(17)
C(4)-H(4A)	0.9800	C(51)-C(91)	1.5456(17)

C(61)-H(61A)	0.9800	C(92)-H(92B)	0.9800
C(61)-H(61B)	0.9800	C(92)-H(92C)	0.9800
C(61)-H(61C)	0.9800	C(102)-C(122)	1.533(2)
C(71)-H(71A)	0.9800	C(102)-C(112)	1.533(2)
C(71)-H(71B)	0.9800	C(102)-H(102)	1.0000
C(71)-H(71C)	0.9800	C(112)-H(11J)	0.9800
C(81)-H(81A)	0.9800	C(112)-H(11K)	0.9800
C(81)-H(81B)	0.9800	C(112)-H(11L)	0.9800
C(81)-H(81C)	0.9800	C(122)-H(12D)	0.9800
C(91)-H(91A)	0.9800	C(122)-H(12E)	0.9800
C(91)-H(91B)	0.9800	C(122)-H(12F)	0.9800
C(91)-H(91C)	0.9800	C(13)-C(63)	1.4127(15)
C(101)-H(10A)	0.9800	C(13)-C(23)	1.4110(15)
C(101)-H(10B)	0.9800	C(13)-N(21)	1.4334(14)
C(101)-H(10C)	0.9800	C(23)-C(33)	1.3951(16)
C(111)-H(11A)	0.9800	C(23)-C(73)	1.5245(16)
C(111)-H(11B)	0.9800	C(33)-C(43)	1.3888(18)
C(111)-H(11C)	0.9800	C(33)-H(33)	0.9500
C(12)-C(22)	1.4105(16)	C(43)-C(53)	1.3825(19)
C(12)-C(62)	1.4118(16)	C(43)-H(43)	0.9500
C(22)-C(32)	1.3997(17)	C(53)-C(63)	1.3954(16)
C(22)-C(72)	1.5213(18)	C(53)-H(53)	0.9500
C(32)-C(42)	1.386(2)	C(63)-C(103)	1.5249(16)
C(32)-H(32)	0.9500	C(73)-C(93)	1.5318(17)
C(42)-C(52)	1.381(2)	C(73)-C(83)	1.5349(19)
C(42)-H(42)	0.9500	C(73)-H(18)	1.0000
C(52)-C(62)	1.3954(19)	C(83)-H(20A)	0.9800
C(52)-H(52)	0.9500	C(83)-H(20B)	0.9800
C(62)-C(102)	1.522(2)	C(83)-H(20C)	0.9800
C(72)-C(92)	1.5296(19)	C(93)-H(19A)	0.9800
C(72)-C(82)	1.5357(18)	C(93)-H(19B)	0.9800
C(72)-H(72)	1.0000	C(93)-H(19C)	0.9800
C(82)-H(82A)	0.9800	C(103)-C(113)	1.5336(17)
C(82)-H(82B)	0.9800	C(103)-C(123)	1.5333(17)
C(82)-H(82C)	0.9800	C(103)-H(103)	1.0000
C(92)-H(92A)	0.9800	C(113)-H(11G)	0.9800

C(113)-H(11H)	0.9800	C(54)-C(104)	1.5421(18)
C(113)-H(11I)	0.9800	C(54)-C(94)	1.5431(18)
C(123)-H(12A)	0.9800	C(64)-H(64A)	0.9800
C(123)-H(12B)	0.9800	C(64)-H(64B)	0.9800
C(123)-H(12C)	0.9800	C(64)-H(64C)	0.9800
Fe(2)-N(24)	1.9681(10)	C(74)-H(74A)	0.9800
Fe(2)-B(2)	2.2210(13)	C(74)-H(74B)	0.9800
Fe(2)-H(3)	1.757(17)	C(74)-H(74C)	0.9800
Fe(2)-H(4)	1.756(16)	C(84)-H(84A)	0.9800
B(2)-C(7)	1.6089(19)	C(84)-H(84B)	0.9800
B(2)-C(5)	1.6134(19)	C(84)-H(84C)	0.9800
B(2)-H(3)	1.232(16)	C(94)-H(94A)	0.9800
B(2)-H(4)	1.188(17)	C(94)-H(94B)	0.9800
C(5)-C(6)	1.536(2)	C(94)-H(94C)	0.9800
C(5)-H(5A)	0.9900	C(104)-H(10D)	0.9800
C(5)-H(5B)	0.9900	C(104)-H(10E)	0.9800
C(6)-H(6A)	0.9800	C(104)-H(10F)	0.9800
C(6)-H(6B)	0.9800	C(114)-H(11D)	0.9800
C(6)-H(6C)	0.9800	C(114)-H(11E)	0.9800
C(7)-C(8)	1.5270(18)	C(114)-H(11F)	0.9800
C(7)-H(7A)	0.9900	C(15)-C(65)	1.4045(18)
C(7)-H(7B)	0.9900	C(15)-C(25)	1.4158(17)
C(8)-H(8A)	0.9800	C(25)-C(35)	1.3910(19)
C(8)-H(8B)	0.9800	C(25)-C(75)	1.532(2)
C(8)-H(8C)	0.9800	C(35)-C(45)	1.374(3)
N(24)-C(44)	1.3376(14)	C(35)-H(35)	0.9500
N(24)-C(16)	1.4359(14)	C(45)-C(55)	1.382(3)
C(14)-C(74)	1.5355(17)	C(45)-H(45)	0.9500
C(14)-C(84)	1.5435(16)	C(55)-C(65)	1.4031(19)
C(14)-C(64)	1.5462(17)	C(55)-H(55)	0.9500
C(14)-C(24)	1.5589(15)	C(65)-C(105)	1.522(2)
C(24)-C(34)	1.4097(16)	C(75)-C(85)	1.521(2)
C(34)-C(44)	1.4088(16)	C(75)-C(95)	1.528(2)
C(34)-H(34)	0.9500	C(75)-H(75)	1.0000
C(44)-C(54)	1.5562(16)	C(85)-H(85A)	0.9800
C(54)-C(114)	1.5365(18)	C(85)-H(85B)	0.9800

C(85)-H(85C)	0.9800	C(116)-H(11M)	0.9800
C(95)-H(95A)	0.9800	C(116)-H(11N)	0.9800
C(95)-H(95B)	0.9800	C(116)-H(11O)	0.9800
C(95)-H(95C)	0.9800	C(126)-H(12G)	0.9800
C(105)-C(115)	1.535(2)	C(126)-H(12H)	0.9800
C(105)-C(125)	1.531(2)	C(126)-H(12I)	0.9800
C(105)-H(105)	1.0000		
C(115)-H(11P)	0.9800	N(11)-Fe(1)-N(21)	97.35(4)
C(115)-H(11Q)	0.9800	N(11)-Fe(1)-B(1)	132.27(4)
C(115)-H(11R)	0.9800	N(21)-Fe(1)-B(1)	130.37(4)
C(125)-H(12J)	0.9800	N(11)-Fe(1)-H(1)	123.8(5)
C(125)-H(12K)	0.9800	N(21)-Fe(1)-H(1)	121.7(5)
C(125)-H(12L)	0.9800	B(1)-Fe(1)-H(1)	34.1(5)
C(16)-C(66)	1.4096(17)	N(11)-Fe(1)-H(2)	125.4(5)
C(16)-C(26)	1.4115(16)	N(21)-Fe(1)-H(2)	123.1(5)
C(26)-C(36)	1.3968(17)	B(1)-Fe(1)-H(2)	32.4(6)
C(26)-C(76)	1.5232(18)	H(1)-Fe(1)-H(2)	66.5(8)
C(36)-C(46)	1.383(2)	C(1)-B(1)-C(3)	117.86(10)
C(36)-H(36)	0.9500	C(1)-B(1)-Fe(1)	121.58(8)
C(46)-C(56)	1.382(2)	C(3)-B(1)-Fe(1)	120.55(8)
C(46)-H(46)	0.9500	C(1)-B(1)-H(1)	108.6(7)
C(56)-C(66)	1.3975(18)	C(3)-B(1)-H(1)	108.6(7)
C(56)-H(56)	0.9500	Fe(1)-B(1)-H(1)	50.9(7)
C(66)-C(106)	1.5203(18)	C(1)-B(1)-H(2)	109.1(8)
C(76)-C(86)	1.520(2)	C(3)-B(1)-H(2)	110.1(8)
C(76)-C(96)	1.5291(19)	Fe(1)-B(1)-H(2)	50.3(8)
C(76)-H(76)	1.0000	H(1)-B(1)-H(2)	101.2(11)
C(86)-H(86A)	0.9800	C(2)-C(1)-B(1)	113.46(11)
C(86)-H(86B)	0.9800	C(2)-C(1)-H(1A)	108.9
C(86)-H(86C)	0.9800	B(1)-C(1)-H(1A)	108.9
C(96)-H(96A)	0.9800	C(2)-C(1)-H(1B)	108.9
C(96)-H(96B)	0.9800	B(1)-C(1)-H(1B)	108.9
C(96)-H(96C)	0.9800	H(1A)-C(1)-H(1B)	107.7
C(106)-C(126)	1.532(2)	C(1)-C(2)-H(2A)	109.5
C(106)-C(116)	1.531(2)	C(1)-C(2)-H(2B)	109.5
C(106)-H(106)	1.0000	H(2A)-C(2)-H(2B)	109.5

C(1)-C(2)-H(2C)	109.5	C(111)-C(51)-C(101)	106.77(10)
H(2A)-C(2)-H(2C)	109.5	C(111)-C(51)-C(91)	106.21(10)
H(2B)-C(2)-H(2C)	109.5	C(101)-C(51)-C(91)	109.57(10)
C(4)-C(3)-B(1)	113.18(11)	C(111)-C(51)-C(41)	117.51(9)
C(4)-C(3)-H(3A)	108.9	C(101)-C(51)-C(41)	107.55(9)
B(1)-C(3)-H(3A)	108.9	C(91)-C(51)-C(41)	109.08(9)
C(4)-C(3)-H(3B)	108.9	C(11)-C(61)-H(61A)	109.5
B(1)-C(3)-H(3B)	108.9	C(11)-C(61)-H(61B)	109.5
H(3A)-C(3)-H(3B)	107.8	H(61A)-C(61)-H(61B)	109.5
C(3)-C(4)-H(4A)	109.5	C(11)-C(61)-H(61C)	109.5
C(3)-C(4)-H(4B)	109.5	H(61A)-C(61)-H(61C)	109.5
H(4A)-C(4)-H(4B)	109.5	H(61B)-C(61)-H(61C)	109.5
C(3)-C(4)-H(4C)	109.5	C(11)-C(71)-H(71A)	109.5
H(4A)-C(4)-H(4C)	109.5	C(11)-C(71)-H(71B)	109.5
H(4B)-C(4)-H(4C)	109.5	H(71A)-C(71)-H(71B)	109.5
C(21)-N(11)-C(12)	129.28(9)	C(11)-C(71)-H(71C)	109.5
C(21)-N(11)-Fe(1)	123.13(7)	H(71A)-C(71)-H(71C)	109.5
C(12)-N(11)-Fe(1)	107.57(7)	H(71B)-C(71)-H(71C)	109.5
C(24)-N(14)-C(15)	127.60(10)	C(11)-C(81)-H(81A)	109.5
C(24)-N(14)-Fe(2)	123.67(8)	C(11)-C(81)-H(81B)	109.5
C(15)-N(14)-Fe(2)	108.73(7)	H(81A)-C(81)-H(81B)	109.5
C(81)-C(11)-C(71)	106.96(10)	C(11)-C(81)-H(81C)	109.5
C(81)-C(11)-C(61)	106.44(10)	H(81A)-C(81)-H(81C)	109.5
C(71)-C(11)-C(61)	109.39(11)	H(81B)-C(81)-H(81C)	109.5
C(81)-C(11)-C(21)	116.67(10)	C(51)-C(91)-H(91A)	109.5
C(71)-C(11)-C(21)	108.19(9)	C(51)-C(91)-H(91B)	109.5
C(61)-C(11)-C(21)	109.02(10)	H(91A)-C(91)-H(91B)	109.5
N(11)-C(21)-C(31)	121.52(10)	C(51)-C(91)-H(91C)	109.5
N(11)-C(21)-C(11)	125.20(10)	H(91A)-C(91)-H(91C)	109.5
C(31)-C(21)-C(11)	113.28(10)	H(91B)-C(91)-H(91C)	109.5
C(21)-C(31)-C(41)	133.35(10)	C(51)-C(101)-H(10A)	109.5
C(21)-C(31)-H(31)	113.3	C(51)-C(101)-H(10B)	109.5
C(41)-C(31)-H(31)	113.3	H(10A)-C(101)-H(10B)	109.5
N(21)-C(41)-C(31)	121.04(10)	C(51)-C(101)-H(10C)	109.5
N(21)-C(41)-C(51)	125.45(10)	H(10A)-C(101)-H(10C)	109.5
C(31)-C(41)-C(51)	113.50(9)	H(10B)-C(101)-H(10C)	109.5

C(51)-C(111)-H(11A)	109.5	C(72)-C(92)-H(92A)	109.5
C(51)-C(111)-H(11B)	109.5	C(72)-C(92)-H(92B)	109.5
H(11A)-C(111)-H(11B)	109.5	H(92A)-C(92)-H(92B)	109.5
C(51)-C(111)-H(11C)	109.5	C(72)-C(92)-H(92C)	109.5
H(11A)-C(111)-H(11C)	109.5	H(92A)-C(92)-H(92C)	109.5
H(11B)-C(111)-H(11C)	109.5	H(92B)-C(92)-H(92C)	109.5
C(22)-C(12)-C(62)	121.19(11)	C(62)-C(102)-C(122)	111.23(14)
C(22)-C(12)-N(11)	119.35(10)	C(62)-C(102)-C(112)	112.05(13)
C(62)-C(12)-N(11)	118.91(10)	C(122)-C(102)-C(112)	109.28(12)
C(32)-C(22)-C(12)	118.04(12)	C(62)-C(102)-H(102)	108.0
C(32)-C(22)-C(72)	119.68(11)	C(122)-C(102)-H(102)	108.0
C(12)-C(22)-C(72)	122.28(10)	C(112)-C(102)-H(102)	108.0
C(42)-C(32)-C(22)	121.33(13)	C(102)-C(112)-H(11J)	109.5
C(42)-C(32)-H(32)	119.3	C(102)-C(112)-H(11K)	109.5
C(22)-C(32)-H(32)	119.3	H(11J)-C(112)-H(11K)	109.5
C(52)-C(42)-C(32)	119.74(12)	C(102)-C(112)-H(11L)	109.5
C(52)-C(42)-H(42)	120.1	H(11J)-C(112)-H(11L)	109.5
C(32)-C(42)-H(42)	120.1	H(11K)-C(112)-H(11L)	109.5
C(42)-C(52)-C(62)	121.58(13)	C(102)-C(122)-H(12D)	109.5
C(42)-C(52)-H(52)	119.2	C(102)-C(122)-H(12E)	109.5
C(62)-C(52)-H(52)	119.2	H(12D)-C(122)-H(12E)	109.5
C(52)-C(62)-C(12)	118.10(12)	C(102)-C(122)-H(12F)	109.5
C(52)-C(62)-C(102)	119.70(12)	H(12D)-C(122)-H(12F)	109.5
C(12)-C(62)-C(102)	122.20(11)	H(12E)-C(122)-H(12F)	109.5
C(22)-C(72)-C(92)	111.28(11)	C(63)-C(13)-C(23)	121.06(10)
C(22)-C(72)-C(82)	112.61(12)	C(63)-C(13)-N(21)	118.95(9)
C(92)-C(72)-C(82)	108.86(11)	C(23)-C(13)-N(21)	119.53(9)
C(22)-C(72)-H(72)	108.0	C(33)-C(23)-C(13)	118.12(10)
C(92)-C(72)-H(72)	108.0	C(33)-C(23)-C(73)	119.73(10)
C(82)-C(72)-H(72)	108.0	C(13)-C(23)-C(73)	122.14(10)
C(72)-C(82)-H(82A)	109.5	C(43)-C(33)-C(23)	121.34(11)
C(72)-C(82)-H(82B)	109.5	C(43)-C(33)-H(33)	119.3
H(82A)-C(82)-H(82B)	109.5	C(23)-C(33)-H(33)	119.3
C(72)-C(82)-H(82C)	109.5	C(53)-C(43)-C(33)	119.86(11)
H(82A)-C(82)-H(82C)	109.5	C(53)-C(43)-H(43)	120.1
H(82B)-C(82)-H(82C)	109.5	C(33)-C(43)-H(43)	120.1

C(43)-C(53)-C(63)	121.25(11)	C(103)-C(123)-H(12A)	109.5
C(43)-C(53)-H(53)	119.4	C(103)-C(123)-H(12B)	109.5
C(63)-C(53)-H(53)	119.4	H(12A)-C(123)-H(12B)	109.5
C(53)-C(63)-C(13)	118.29(10)	C(103)-C(123)-H(12C)	109.5
C(53)-C(63)-C(103)	119.51(10)	H(12A)-C(123)-H(12C)	109.5
C(13)-C(63)-C(103)	122.20(10)	H(12B)-C(123)-H(12C)	109.5
C(23)-C(73)-C(93)	112.20(10)	N(14)-Fe(2)-N(24)	97.47(4)
C(23)-C(73)-C(83)	110.81(11)	N(14)-Fe(2)-B(2)	129.48(5)
C(93)-C(73)-C(83)	109.57(11)	N(24)-Fe(2)-B(2)	132.99(5)
C(23)-C(73)-H(18)	108.0	N(14)-Fe(2)-H(3)	118.5(5)
C(93)-C(73)-H(18)	108.0	N(24)-Fe(2)-H(3)	126.6(5)
C(83)-C(73)-H(18)	108.0	B(2)-Fe(2)-H(3)	33.6(5)
C(73)-C(83)-H(20A)	109.5	N(14)-Fe(2)-H(4)	124.9(5)
C(73)-C(83)-H(20B)	109.5	N(24)-Fe(2)-H(4)	124.5(5)
H(20A)-C(83)-H(20B)	109.5	B(2)-Fe(2)-H(4)	32.1(5)
C(73)-C(83)-H(20C)	109.5	H(3)-Fe(2)-H(4)	65.7(8)
H(20A)-C(83)-H(20C)	109.5	C(7)-B(2)-C(5)	118.21(10)
H(20B)-C(83)-H(20C)	109.5	C(7)-B(2)-Fe(2)	117.94(9)
C(73)-C(93)-H(19A)	109.5	C(5)-B(2)-Fe(2)	123.85(9)
C(73)-C(93)-H(19B)	109.5	C(7)-B(2)-H(3)	107.7(8)
H(19A)-C(93)-H(19B)	109.5	C(5)-B(2)-H(3)	108.9(8)
C(73)-C(93)-H(19C)	109.5	Fe(2)-B(2)-H(3)	52.1(8)
H(19A)-C(93)-H(19C)	109.5	C(7)-B(2)-H(4)	107.7(8)
H(19B)-C(93)-H(19C)	109.5	C(5)-B(2)-H(4)	109.6(8)
C(63)-C(103)-C(113)	111.12(10)	Fe(2)-B(2)-H(4)	51.8(8)
C(63)-C(103)-C(123)	112.38(10)	H(3)-B(2)-H(4)	103.9(11)
C(113)-C(103)-C(123)	109.61(10)	C(6)-C(5)-B(2)	112.51(11)
C(63)-C(103)-H(103)	107.9	C(6)-C(5)-H(5A)	109.1
C(113)-C(103)-H(103)	107.9	B(2)-C(5)-H(5A)	109.1
C(123)-C(103)-H(103)	107.9	C(6)-C(5)-H(5B)	109.1
C(103)-C(113)-H(11G)	109.5	B(2)-C(5)-H(5B)	109.1
C(103)-C(113)-H(11H)	109.5	H(5A)-C(5)-H(5B)	107.8
H(11G)-C(113)-H(11H)	109.5	C(5)-C(6)-H(6A)	109.5
C(103)-C(113)-H(11I)	109.5	C(5)-C(6)-H(6B)	109.5
H(11G)-C(113)-H(11I)	109.5	H(6A)-C(6)-H(6B)	109.5
H(11H)-C(113)-H(11I)	109.5	C(5)-C(6)-H(6C)	109.5

H(6A)-C(6)-H(6C)	109.5	C(114)-C(54)-C(94)	106.41(10)
H(6B)-C(6)-H(6C)	109.5	C(104)-C(54)-C(94)	110.02(10)
C(8)-C(7)-B(2)	112.03(11)	C(114)-C(54)-C(44)	117.83(10)
C(8)-C(7)-H(7A)	109.2	C(104)-C(54)-C(44)	107.40(9)
B(2)-C(7)-H(7A)	109.2	C(94)-C(54)-C(44)	108.58(10)
C(8)-C(7)-H(7B)	109.2	C(14)-C(64)-H(64A)	109.5
B(2)-C(7)-H(7B)	109.2	C(14)-C(64)-H(64B)	109.5
H(7A)-C(7)-H(7B)	107.9	H(64A)-C(64)-H(64B)	109.5
C(7)-C(8)-H(8A)	109.5	C(14)-C(64)-H(64C)	109.5
C(7)-C(8)-H(8B)	109.5	H(64A)-C(64)-H(64C)	109.5
H(8A)-C(8)-H(8B)	109.5	H(64B)-C(64)-H(64C)	109.5
C(7)-C(8)-H(8C)	109.5	C(14)-C(74)-H(74A)	109.5
H(8A)-C(8)-H(8C)	109.5	C(14)-C(74)-H(74B)	109.5
H(8B)-C(8)-H(8C)	109.5	H(74A)-C(74)-H(74B)	109.5
C(41)-N(21)-C(13)	127.80(9)	C(14)-C(74)-H(74C)	109.5
C(41)-N(21)-Fe(1)	123.38(7)	H(74A)-C(74)-H(74C)	109.5
C(13)-N(21)-Fe(1)	108.80(7)	H(74B)-C(74)-H(74C)	109.5
C(44)-N(24)-C(16)	127.50(9)	C(14)-C(84)-H(84A)	109.5
C(44)-N(24)-Fe(2)	122.84(8)	C(14)-C(84)-H(84B)	109.5
C(16)-N(24)-Fe(2)	109.65(7)	H(84A)-C(84)-H(84B)	109.5
C(74)-C(14)-C(84)	106.77(10)	C(14)-C(84)-H(84C)	109.5
C(74)-C(14)-C(64)	106.37(10)	H(84A)-C(84)-H(84C)	109.5
C(84)-C(14)-C(64)	109.25(10)	H(84B)-C(84)-H(84C)	109.5
C(74)-C(14)-C(24)	117.27(9)	C(54)-C(94)-H(94A)	109.5
C(84)-C(14)-C(24)	107.61(9)	C(54)-C(94)-H(94B)	109.5
C(64)-C(14)-C(24)	109.37(9)	H(94A)-C(94)-H(94B)	109.5
N(14)-C(24)-C(34)	120.97(10)	C(54)-C(94)-H(94C)	109.5
N(14)-C(24)-C(14)	125.51(10)	H(94A)-C(94)-H(94C)	109.5
C(34)-C(24)-C(14)	113.52(9)	H(94B)-C(94)-H(94C)	109.5
C(44)-C(34)-C(24)	133.22(10)	C(54)-C(104)-H(10D)	109.5
C(44)-C(34)-H(34)	113.4	C(54)-C(104)-H(10E)	109.5
C(24)-C(34)-H(34)	113.4	H(10D)-C(104)-H(10E)	109.5
N(24)-C(44)-C(34)	121.59(10)	C(54)-C(104)-H(10F)	109.5
N(24)-C(44)-C(54)	125.30(10)	H(10D)-C(104)-H(10F)	109.5
C(34)-C(44)-C(54)	113.11(10)	H(10E)-C(104)-H(10F)	109.5
C(114)-C(54)-C(104)	106.48(11)	C(54)-C(114)-H(11D)	109.5

C(54)-C(114)-H(11E)	109.5	C(75)-C(95)-H(95B)	109.5
H(11D)-C(114)-H(11E)	109.5	H(95A)-C(95)-H(95B)	109.5
C(54)-C(114)-H(11F)	109.5	C(75)-C(95)-H(95C)	109.5
H(11D)-C(114)-H(11F)	109.5	H(95A)-C(95)-H(95C)	109.5
H(11E)-C(114)-H(11F)	109.5	H(95B)-C(95)-H(95C)	109.5
C(65)-C(15)-C(25)	122.27(11)	C(65)-C(105)-C(115)	113.13(14)
C(65)-C(15)-N(14)	119.52(11)	C(65)-C(105)-C(125)	110.40(13)
C(25)-C(15)-N(14)	117.90(11)	C(115)-C(105)-C(125)	109.45(13)
C(35)-C(25)-C(15)	117.57(13)	C(65)-C(105)-H(105)	107.9
C(35)-C(25)-C(75)	120.37(13)	C(115)-C(105)-H(105)	107.9
C(15)-C(25)-C(75)	122.06(11)	C(125)-C(105)-H(105)	107.9
C(45)-C(35)-C(25)	121.26(15)	C(105)-C(115)-H(11P)	109.5
C(45)-C(35)-H(35)	119.4	C(105)-C(115)-H(11Q)	109.5
C(25)-C(35)-H(35)	119.4	H(11P)-C(115)-H(11Q)	109.5
C(35)-C(45)-C(55)	120.39(14)	C(105)-C(115)-H(11R)	109.5
C(35)-C(45)-H(45)	119.8	H(11P)-C(115)-H(11R)	109.5
C(55)-C(45)-H(45)	119.8	H(11Q)-C(115)-H(11R)	109.5
C(45)-C(55)-C(65)	121.52(15)	C(105)-C(125)-H(12J)	109.5
C(45)-C(55)-H(55)	119.2	C(105)-C(125)-H(12K)	109.5
C(65)-C(55)-H(55)	119.2	H(12J)-C(125)-H(12K)	109.5
C(55)-C(65)-C(15)	116.84(14)	C(105)-C(125)-H(12L)	109.5
C(55)-C(65)-C(105)	121.07(13)	H(12J)-C(125)-H(12L)	109.5
C(15)-C(65)-C(105)	122.09(11)	H(12K)-C(125)-H(12L)	109.5
C(85)-C(75)-C(95)	109.61(12)	C(66)-C(16)-C(26)	121.29(10)
C(85)-C(75)-C(25)	112.09(12)	C(66)-C(16)-N(24)	119.30(10)
C(95)-C(75)-C(25)	112.69(14)	C(26)-C(16)-N(24)	119.02(10)
C(85)-C(75)-H(75)	107.4	C(36)-C(26)-C(16)	117.90(12)
C(95)-C(75)-H(75)	107.4	C(36)-C(26)-C(76)	120.55(11)
C(25)-C(75)-H(75)	107.4	C(16)-C(26)-C(76)	121.55(10)
C(75)-C(85)-H(85A)	109.5	C(46)-C(36)-C(26)	121.47(13)
C(75)-C(85)-H(85B)	109.5	C(46)-C(36)-H(36)	119.3
H(85A)-C(85)-H(85B)	109.5	C(26)-C(36)-H(36)	119.3
C(75)-C(85)-H(85C)	109.5	C(36)-C(46)-C(56)	119.93(12)
H(85A)-C(85)-H(85C)	109.5	C(36)-C(46)-H(46)	120.0
H(85B)-C(85)-H(85C)	109.5	C(56)-C(46)-H(46)	120.0
C(75)-C(95)-H(95A)	109.5	C(46)-C(56)-C(66)	121.26(13)

C(46)-C(56)-H(56)	119.4	H(96A)-C(96)-H(96C)	109.5
C(66)-C(56)-H(56)	119.4	H(96B)-C(96)-H(96C)	109.5
C(56)-C(66)-C(16)	118.15(12)	C(66)-C(106)-C(126)	112.08(12)
C(56)-C(66)-C(106)	119.87(12)	C(66)-C(106)-C(116)	111.33(13)
C(16)-C(66)-C(106)	121.98(11)	C(126)-C(106)-C(116)	109.43(12)
C(86)-C(76)-C(26)	111.48(11)	C(66)-C(106)-H(106)	107.9
C(86)-C(76)-C(96)	109.85(13)	C(126)-C(106)-H(106)	107.9
C(26)-C(76)-C(96)	112.38(12)	C(116)-C(106)-H(106)	107.9
C(86)-C(76)-H(76)	107.6	C(106)-C(116)-H(11M)	109.5
C(26)-C(76)-H(76)	107.6	C(106)-C(116)-H(11N)	109.5
C(96)-C(76)-H(76)	107.6	H(11M)-C(116)-H(11N)	109.5
C(76)-C(86)-H(86A)	109.5	C(106)-C(116)-H(11O)	109.5
C(76)-C(86)-H(86B)	109.5	H(11M)-C(116)-H(11O)	109.5
H(86A)-C(86)-H(86B)	109.5	H(11N)-C(116)-H(11O)	109.5
C(76)-C(86)-H(86C)	109.5	C(106)-C(126)-H(12G)	109.5
H(86A)-C(86)-H(86C)	109.5	C(106)-C(126)-H(12H)	109.5
H(86B)-C(86)-H(86C)	109.5	H(12G)-C(126)-H(12H)	109.5
C(76)-C(96)-H(96A)	109.5	C(106)-C(126)-H(12I)	109.5
C(76)-C(96)-H(96B)	109.5	H(12G)-C(126)-H(12I)	109.5
H(96A)-C(96)-H(96B)	109.5	H(12H)-C(126)-H(12I)	109.5
C(76)-C(96)-H(96C)	109.5		

$L^{Me}FePh$ (Complex 3b)

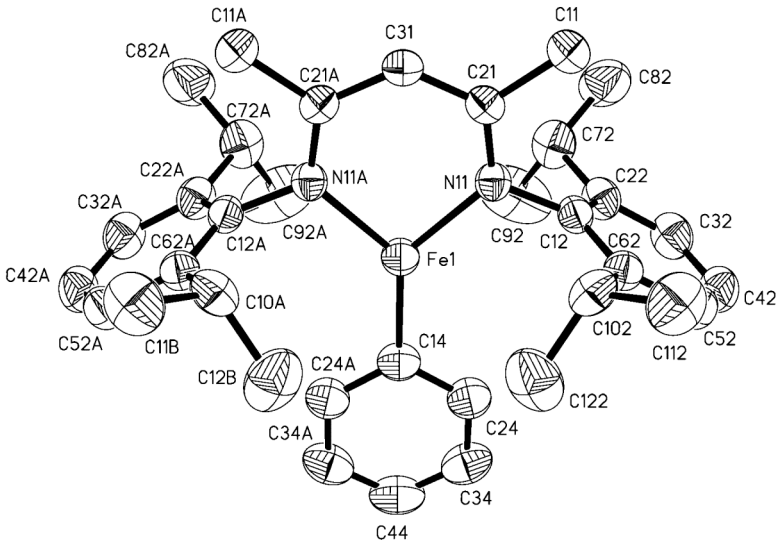


Table SI.13a. Crystal data and structure refinement for **3b**.

Identification code	holjs76	
Empirical formula	C35 H46 Fe N2	
Formula weight	550.59	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/m$ 1	
Unit cell dimensions	a = 8.3804(5) Å	α = 90°
	b = 20.8589(12) Å	β = 104.136(1)°
	c = 9.4280(6) Å	γ = 90°
Volume	1598.16(17) $Å^3$	
Z	2	
Density (calculated)	1.144 Mg/m^3	
Absorption coefficient	0.496 mm^{-1}	
F(000)	592	
Crystal color, morphology	yellow-green, block	
Crystal size	0.28 x 0.24 x 0.14 mm^3	
Theta range for data collection	2.23 to 26.02°	
Index ranges	$-8 \le h \le 10, -25 \le k \le 16, -11 \le l \le 10$	
Reflections collected	8690	

Independent reflections	3184 [R(int) = 0.0255]
Observed reflections	2583
Completeness to theta = 26.02°	98.0%
Absorption correction	Multi-scan
Max. and min. transmission	0.9339 and 0.8737
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3184 / 0 / 183
Goodness-of-fit on F^2	1.045
Final R indices [I>2sigma(I)]	$R1$ = 0.0367, $wR2$ = 0.0970
R indices (all data)	$R1$ = 0.0488, $wR2$ = 0.1009
Largest diff. peak and hole	0.328 and -0.255 e.Å^{-3}

Table SI.13b. Bond lengths [A] and angles [deg] for **3b**.

Fe(1)-N(11)#1	1.9724(14)
Fe(1)-N(11)	1.9724(14)
Fe(1)-C(14)	2.025(3)
N(11)-C(21)	1.336(2)
N(11)-C(12)	1.440(2)
C(14)-C(24)#1	1.400(2)
C(14)-C(24)	1.400(2)
C(24)-C(34)	1.388(3)
C(24)-H(24A)	0.9500
C(34)-C(44)	1.375(3)
C(34)-H(34A)	0.9500
C(44)-C(34)#1	1.375(3)
C(44)-H(44A)	0.9500
C(11)-C(21)	1.511(2)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(21)-C(31)	1.399(2)
C(31)-C(21)#1	1.399(2)
C(31)-H(31A)	0.9500
C(12)-C(62)	1.409(2)

C(12)-C(22)	1.410(2)
C(22)-C(32)	1.394(3)
C(22)-C(72)	1.526(3)
C(32)-C(42)	1.376(3)
C(32)-H(32A)	0.9500
C(42)-C(52)	1.382(3)
C(42)-H(42A)	0.9500
C(52)-C(62)	1.394(2)
C(52)-H(52A)	0.9500
C(62)-C(102)	1.518(2)
C(72)-C(82)	1.516(3)
C(72)-C(92)	1.534(4)
C(72)-H(72A)	1.0000
C(82)-H(82A)	0.9800
C(82)-H(82B)	0.9800
C(82)-H(82C)	0.9800
C(92)-H(92A)	0.9800
C(92)-H(92B)	0.9800
C(92)-H(92C)	0.9800
C(102)-C(122)	1.527(3)
C(102)-C(112)	1.527(3)
C(102)-H(10A)	1.0000
C(112)-H(11D)	0.9800
C(112)-H(11E)	0.9800
C(112)-H(11F)	0.9800
C(122)-H(12A)	0.9800
C(122)-H(12B)	0.9800
C(122)-H(12C)	0.9800
N(11)#1-Fe(1)-N(11)	92.92(8)
N(11)#1-Fe(1)-C(14)	133.54(4)
N(11)-Fe(1)-C(14)	133.54(4)
C(21)-N(11)-C(12)	121.08(14)
C(21)-N(11)-Fe(1)	126.25(11)
C(12)-N(11)-Fe(1)	112.67(11)
C(24)#1-C(14)-C(24)	115.4(2)
C(24)#1-C(14)-Fe(1)	122.29(12)

C(24)-C(14)-Fe(1)	122.29(12)
C(34)-C(24)-C(14)	122.4(2)
C(34)-C(24)-H(24A)	118.8
C(14)-C(24)-H(24A)	118.8
C(44)-C(34)-C(24)	120.4(2)
C(44)-C(34)-H(34A)	119.8
C(24)-C(34)-H(34A)	119.8
C(34)#1-C(44)-C(34)	119.2(3)
C(34)#1-C(44)-H(44A)	120.4
C(34)-C(44)-H(44A)	120.4
C(21)-C(11)-H(11A)	109.5
C(21)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(21)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
N(11)-C(21)-C(31)	123.05(16)
N(11)-C(21)-C(11)	119.04(15)
C(31)-C(21)-C(11)	117.91(16)
C(21)#1-C(31)-C(21)	128.5(2)
C(21)#1-C(31)-H(31A)	115.8
C(21)-C(31)-H(31A)	115.8
C(62)-C(12)-C(22)	121.35(16)
C(62)-C(12)-N(11)	119.42(15)
C(22)-C(12)-N(11)	118.92(15)
C(32)-C(22)-C(12)	117.99(17)
C(32)-C(22)-C(72)	120.32(17)
C(12)-C(22)-C(72)	121.68(16)
C(42)-C(32)-C(22)	121.36(18)
C(42)-C(32)-H(32A)	119.3
C(22)-C(32)-H(32A)	119.3
C(32)-C(42)-C(52)	120.04(18)
C(32)-C(42)-H(42A)	120.0
C(52)-C(42)-H(42A)	120.0
C(42)-C(52)-C(62)	121.40(18)
C(42)-C(52)-H(52A)	119.3

C(62)-C(52)-H(52A)	119.3
C(52)-C(62)-C(12)	117.85(16)
C(52)-C(62)-C(102)	121.15(16)
C(12)-C(62)-C(102)	121.00(15)
C(82)-C(72)-C(22)	113.04(18)
C(82)-C(72)-C(92)	109.6(2)
C(22)-C(72)-C(92)	110.0(2)
C(82)-C(72)-H(72A)	108.0
C(22)-C(72)-H(72A)	108.0
C(92)-C(72)-H(72A)	108.0
C(72)-C(82)-H(82A)	109.5
C(72)-C(82)-H(82B)	109.5
H(82A)-C(82)-H(82B)	109.5
C(72)-C(82)-H(82C)	109.5
H(82A)-C(82)-H(82C)	109.5
H(82B)-C(82)-H(82C)	109.5
C(72)-C(92)-H(92A)	109.5
C(72)-C(92)-H(92B)	109.5
H(92A)-C(92)-H(92B)	109.5
C(72)-C(92)-H(92C)	109.5
H(92A)-C(92)-H(92C)	109.5
H(92B)-C(92)-H(92C)	109.5
C(62)-C(102)-C(122)	110.47(17)
C(62)-C(102)-C(112)	113.41(17)
C(122)-C(102)-C(112)	109.91(18)
C(62)-C(102)-H(10A)	107.6
C(122)-C(102)-H(10A)	107.6
C(112)-C(102)-H(10A)	107.6
C(102)-C(112)-H(11D)	109.5
C(102)-C(112)-H(11E)	109.5
H(11D)-C(112)-H(11E)	109.5
C(102)-C(112)-H(11F)	109.5
H(11D)-C(112)-H(11F)	109.5
H(11E)-C(112)-H(11F)	109.5
C(102)-C(122)-H(12A)	109.5
C(102)-C(122)-H(12B)	109.5

H(12A)-C(122)-H(12B)	109.5
C(102)-C(122)-H(12C)	109.5
H(12A)-C(122)-H(12C)	109.5
H(12B)-C(122)-H(12C)	109.5

Symmetry transformations used to generate equivalent atoms:

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

$L^{Me}Fe(H_2NNH_2)(\mu\text{-}H)_2BEt_2$ (Complex 4).

Table SI.14a. Crystal data and structure refinement for holyy18.

Identification code	holyy18	
Empirical formula	C33 H57 B Fe N4	
Formula weight	576.49	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 8.8057(4) Å	α = 73.571(1)°
	b = 11.8380(5) Å	β = 76.110(1)°
	c = 16.5524(8) Å	γ = 87.915(1)°
Volume	1605.69(13) Å^3	
Z	2	
Density (calculated)	1.192 Mg/m^3	
Absorption coefficient	0.497 mm^{-1}	
F(000)	628	
Crystal color, morphology	yellow, needle	
Crystal size	0.38 x 0.15 x 0.15 mm^3	
Theta range for data collection	1.90 to 29.57°	
Index ranges	$-12 \le h \le 12, -16 \le k \le 16, -22 \le l \le 22$	
Reflections collected	19734	
Independent reflections	8850 [R(int) = 0.0301]	
Observed reflections	6912	
Completeness to theta = 29.57°	98.2%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9292 and 0.8336	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8850 / 0 / 388	
Goodness-of-fit on F^2	1.024	
Final R indices [I>2sigma(I)]	R1 = 0.0435, wR2 = 0.1019	
R indices (all data)	R1 = 0.0643, wR2 = 0.1098	
Largest diff. peak and hole	1.256 and -0.422 e.Å^{-3}	

Table SI.14b. Bond lengths [Å] and angles [°] for **4**.

Fe-N(11)	2.0075(14)	C(11)-H(11C)	0.9800
Fe-N(21)	2.0235(14)	C(21)-C(31)	1.406(2)
Fe-N(15)	2.2139(16)	C(31)-C(41)	1.409(2)
Fe-B	2.350(2)	C(31)-H(31)	0.9500
Fe-H(1)	1.91(2)	C(41)-C(51)	1.514(2)
Fe-H(2)	1.82(2)	C(51)-H(51A)	0.9800
B-C(24)	1.601(3)	C(51)-H(51B)	0.9800
B-C(34)	1.646(3)	C(51)-H(51C)	0.9800
B-H(1)	1.22(2)	C(12)-C(62)	1.411(2)
B-H(2)	1.22(2)	C(12)-C(22)	1.412(2)
C(14)-C(24)	1.513(3)	C(22)-C(32)	1.398(2)
C(14)-H(14A)	0.9800	C(22)-C(72)	1.519(2)
C(14)-H(14B)	0.9800	C(32)-C(42)	1.380(3)
C(14)-H(14C)	0.9800	C(32)-H(32)	0.9500
C(24)-H(24A)	0.9900	C(42)-C(52)	1.386(3)
C(24)-H(24B)	0.9900	C(42)-H(42)	0.9500
C(34)-C(44)	1.509(3)	C(52)-C(62)	1.395(2)
C(34)-H(34A)	0.9900	C(52)-H(52)	0.9500
C(34)-H(34B)	0.9900	C(62)-C(102)	1.525(2)
C(44)-H(44A)	0.9800	C(72)-C(82)	1.529(3)
C(44)-H(44B)	0.9800	C(72)-C(92)	1.539(2)
C(44)-H(44C)	0.9800	C(72)-H(72)	1.0000
N(15)-N(25)	1.441(2)	C(82)-H(82A)	0.9800
N(15)-H(15A)	0.88(3)	C(82)-H(82B)	0.9800
N(15)-H(15B)	0.89(2)	C(82)-H(82C)	0.9800
N(25)-H(25A)	0.83(3)	C(92)-H(92A)	0.9800
N(25)-H(25B)	0.79(3)	C(92)-H(92B)	0.9800
N(11)-C(21)	1.332(2)	C(92)-H(92C)	0.9800
N(11)-C(12)	1.443(2)	C(102)-C(112)	1.531(2)
N(21)-C(41)	1.328(2)	C(102)-C(122)	1.536(3)
N(21)-C(13)	1.441(2)	C(102)-H(102)	1.0000
C(11)-C(21)	1.515(2)	C(112)-H(11D)	0.9800
C(11)-H(11A)	0.9800	C(112)-H(11E)	0.9800
C(11)-H(11B)	0.9800	C(112)-H(11F)	0.9800

C(122)-H(12A)	0.9800	N(11)-Fe-B	130.35(7)
C(122)-H(12B)	0.9800	N(21)-Fe-B	121.38(7)
C(122)-H(12C)	0.9800	N(15)-Fe-B	108.57(7)
C(13)-C(23)	1.400(2)	N(11)-Fe-H(1)	111.0(7)
C(13)-C(63)	1.413(2)	N(21)-Fe-H(1)	105.3(7)
C(23)-C(33)	1.400(2)	N(15)-Fe-H(1)	139.5(7)
C(23)-C(73)	1.519(2)	B-Fe-H(1)	31.0(7)
C(33)-C(43)	1.380(3)	N(11)-Fe-H(2)	130.5(7)
C(33)-H(33)	0.9500	N(21)-Fe-H(2)	137.0(7)
C(43)-C(53)	1.383(3)	N(15)-Fe-H(2)	79.2(7)
C(43)-H(43)	0.9500	B-Fe-H(2)	30.9(7)
C(53)-C(63)	1.393(2)	H(1)-Fe-H(2)	61.2(9)
C(53)-H(53)	0.9500	C(24)-B-C(34)	115.37(16)
C(63)-C(103)	1.522(3)	C(24)-B-Fe	133.48(14)
C(73)-C(83)	1.531(3)	C(34)-B-Fe	110.94(13)
C(73)-C(93)	1.536(2)	C(24)-B-H(1)	110.1(10)
C(73)-H(73)	1.0000	C(34)-B-H(1)	110.9(10)
C(83)-H(83A)	0.9800	Fe-B-H(1)	54.3(10)
C(83)-H(83B)	0.9800	C(24)-B-H(2)	110.0(10)
C(83)-H(83C)	0.9800	C(34)-B-H(2)	106.8(10)
C(93)-H(93A)	0.9800	Fe-B-H(2)	50.1(10)
C(93)-H(93B)	0.9800	H(1)-B-H(2)	102.9(14)
C(93)-H(93C)	0.9800	C(24)-C(14)-H(14A)	109.5
C(103)-C(113)	1.518(3)	C(24)-C(14)-H(14B)	109.5
C(103)-C(123)	1.518(3)	H(14A)-C(14)-H(14B)	109.5
C(103)-H(103)	1.0000	C(24)-C(14)-H(14C)	109.5
C(113)-H(11G)	0.9800	H(14A)-C(14)-H(14C)	109.5
C(113)-H(11H)	0.9800	H(14B)-C(14)-H(14C)	109.5
C(113)-H(11I)	0.9800	C(14)-C(24)-B	116.31(17)
C(123)-H(12D)	0.9800	C(14)-C(24)-H(24A)	108.2
C(123)-H(12E)	0.9800	B-C(24)-H(24A)	108.2
C(123)-H(12F)	0.9800	C(14)-C(24)-H(24B)	108.2
		B-C(24)-H(24B)	108.2
N(11)-Fe-N(21)	92.44(6)	H(24A)-C(24)-H(24B)	107.4
N(11)-Fe-N(15)	100.69(6)	C(44)-C(34)-B	114.48(18)
N(21)-Fe-N(15)	97.49(6)	C(44)-C(34)-H(34A)	108.6

B-C(34)-H(34A)	108.6	C(41)-C(31)-H(31)	115.8
C(44)-C(34)-H(34B)	108.6	N(21)-C(41)-C(31)	123.21(15)
B-C(34)-H(34B)	108.6	N(21)-C(41)-C(51)	120.07(15)
H(34A)-C(34)-H(34B)	107.6	C(31)-C(41)-C(51)	116.73(15)
C(34)-C(44)-H(44A)	109.5	C(41)-C(51)-H(51A)	109.5
C(34)-C(44)-H(44B)	109.5	C(41)-C(51)-H(51B)	109.5
H(44A)-C(44)-H(44B)	109.5	H(51A)-C(51)-H(51B)	109.5
C(34)-C(44)-H(44C)	109.5	C(41)-C(51)-H(51C)	109.5
H(44A)-C(44)-H(44C)	109.5	H(51A)-C(51)-H(51C)	109.5
H(44B)-C(44)-H(44C)	109.5	H(51B)-C(51)-H(51C)	109.5
N(25)-N(15)-Fe	114.35(13)	C(62)-C(12)-C(22)	121.05(15)
N(25)-N(15)-H(15A)	110.5(17)	C(62)-C(12)-N(11)	118.43(14)
Fe-N(15)-H(15A)	108.8(17)	C(22)-C(12)-N(11)	120.47(15)
N(25)-N(15)-H(15B)	107.9(15)	C(32)-C(22)-C(12)	118.25(16)
Fe-N(15)-H(15B)	109.0(15)	C(32)-C(22)-C(72)	119.50(15)
H(15A)-N(15)-H(15B)	106(2)	C(12)-C(22)-C(72)	122.23(15)
N(15)-N(25)-H(25A)	110.4(17)	C(42)-C(32)-C(22)	121.18(16)
N(15)-N(25)-H(25B)	109(2)	C(42)-C(32)-H(32)	119.4
H(25A)-N(25)-H(25B)	111(3)	C(22)-C(32)-H(32)	119.4
C(21)-N(11)-C(12)	118.72(14)	C(32)-C(42)-C(52)	120.02(16)
C(21)-N(11)-Fe	122.44(11)	C(32)-C(42)-H(42)	120.0
C(12)-N(11)-Fe	118.74(10)	C(52)-C(42)-H(42)	120.0
C(41)-N(21)-C(13)	119.18(14)	C(42)-C(52)-C(62)	121.29(17)
C(41)-N(21)-Fe	122.94(11)	C(42)-C(52)-H(52)	119.4
C(13)-N(21)-Fe	117.87(10)	C(62)-C(52)-H(52)	119.4
C(21)-C(11)-H(11A)	109.5	C(52)-C(62)-C(12)	118.16(16)
C(21)-C(11)-H(11B)	109.5	C(52)-C(62)-C(102)	121.16(15)
H(11A)-C(11)-H(11B)	109.5	C(12)-C(62)-C(102)	120.67(14)
C(21)-C(11)-H(11C)	109.5	C(22)-C(72)-C(82)	110.51(14)
H(11A)-C(11)-H(11C)	109.5	C(22)-C(72)-C(92)	111.91(15)
H(11B)-C(11)-H(11C)	109.5	C(82)-C(72)-C(92)	109.41(15)
N(11)-C(21)-C(31)	123.98(15)	C(22)-C(72)-H(72)	108.3
N(11)-C(21)-C(11)	119.75(14)	C(82)-C(72)-H(72)	108.3
C(31)-C(21)-C(11)	116.26(14)	C(92)-C(72)-H(72)	108.3
C(21)-C(31)-C(41)	128.33(15)	C(72)-C(82)-H(82A)	109.5
C(21)-C(31)-H(31)	115.8	C(72)-C(82)-H(82B)	109.5

H(82A)-C(82)-H(82B)	109.5	C(23)-C(33)-H(33)	119.5
C(72)-C(82)-H(82C)	109.5	C(33)-C(43)-C(53)	120.08(16)
H(82A)-C(82)-H(82C)	109.5	C(33)-C(43)-H(43)	120.0
H(82B)-C(82)-H(82C)	109.5	C(53)-C(43)-H(43)	120.0
C(72)-C(92)-H(92A)	109.5	C(43)-C(53)-C(63)	121.19(17)
C(72)-C(92)-H(92B)	109.5	C(43)-C(53)-H(53)	119.4
H(92A)-C(92)-H(92B)	109.5	C(63)-C(53)-H(53)	119.4
C(72)-C(92)-H(92C)	109.5	C(53)-C(63)-C(13)	118.15(16)
H(92A)-C(92)-H(92C)	109.5	C(53)-C(63)-C(103)	120.38(16)
H(92B)-C(92)-H(92C)	109.5	C(13)-C(63)-C(103)	121.47(15)
C(62)-C(102)-C(112)	113.35(14)	C(23)-C(73)-C(83)	110.96(14)
C(62)-C(102)-C(122)	112.75(14)	C(23)-C(73)-C(93)	111.93(14)
C(112)-C(102)-C(122)	108.89(15)	C(83)-C(73)-C(93)	109.57(15)
C(62)-C(102)-H(102)	107.2	C(23)-C(73)-H(73)	108.1
C(112)-C(102)-H(102)	107.2	C(83)-C(73)-H(73)	108.1
C(122)-C(102)-H(102)	107.2	C(93)-C(73)-H(73)	108.1
C(102)-C(112)-H(11D)	109.5	C(73)-C(83)-H(83A)	109.5
C(102)-C(112)-H(11E)	109.5	C(73)-C(83)-H(83B)	109.5
H(11D)-C(112)-H(11E)	109.5	H(83A)-C(83)-H(83B)	109.5
C(102)-C(112)-H(11F)	109.5	C(73)-C(83)-H(83C)	109.5
H(11D)-C(112)-H(11F)	109.5	H(83A)-C(83)-H(83C)	109.5
H(11E)-C(112)-H(11F)	109.5	H(83B)-C(83)-H(83C)	109.5
C(102)-C(122)-H(12A)	109.5	C(73)-C(93)-H(93A)	109.5
C(102)-C(122)-H(12B)	109.5	C(73)-C(93)-H(93B)	109.5
H(12A)-C(122)-H(12B)	109.5	H(93A)-C(93)-H(93B)	109.5
C(102)-C(122)-H(12C)	109.5	C(73)-C(93)-H(93C)	109.5
H(12A)-C(122)-H(12C)	109.5	H(93A)-C(93)-H(93C)	109.5
H(12B)-C(122)-H(12C)	109.5	H(93B)-C(93)-H(93C)	109.5
C(23)-C(13)-C(63)	121.16(15)	C(113)-C(103)-C(123)	109.29(17)
C(23)-C(13)-N(21)	120.97(15)	C(113)-C(103)-C(63)	112.88(17)
C(63)-C(13)-N(21)	117.77(15)	C(123)-C(103)-C(63)	111.61(15)
C(13)-C(23)-C(33)	118.36(16)	C(113)-C(103)-H(103)	107.6
C(13)-C(23)-C(73)	122.48(15)	C(123)-C(103)-H(103)	107.6
C(33)-C(23)-C(73)	119.15(16)	C(63)-C(103)-H(103)	107.6
C(43)-C(33)-C(23)	121.03(17)	C(103)-C(113)-H(11G)	109.5
C(43)-C(33)-H(33)	119.5	C(103)-C(113)-H(11H)	109.5

H(11G)-C(113)-H(11H)	109.5	C(103)-C(123)-H(12E)	109.5
C(103)-C(113)-H(11I)	109.5	H(12D)-C(123)-H(12E)	109.5
H(11G)-C(113)-H(11I)	109.5	C(103)-C(123)-H(12F)	109.5
H(11H)-C(113)-H(11I)	109.5	H(12D)-C(123)-H(12F)	109.5
C(103)-C(123)-H(12D)	109.5	H(12E)-C(123)-H(12F)	109.5

$L^{Me}Fe(\mu\text{-}NH_2)_2BEt_2$ (Complex 5).

Table SI.15a. Crystal data and structure refinement for 5.

Identification code	holyy15	
Empirical formula	C33 H55 B Fe N4	
Formula weight	574.47	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	*C*2/*c*	
Unit cell dimensions	*a* = 14.669(2) Å	α = 90°
	b = 11.1121(16) Å	β = 90.674(2)°
	c = 20.749(3) Å	γ = 90°
Volume	3381.9(8) Å^3	
Z	4	
Density (calculated)	1.128 Mg/m^3	
Absorption coefficient	0.472 mm^{-1}	
F(000)	1248	
Crystal color, morphology	orange, block	
Crystal size	0.46 x 0.31 x 0.22 mm^3	
Theta range for data collection	1.96 to 29.57°	
Index ranges	$-20 \le h \le 20, -15 \le k \le 15, -28 \le l \le 28$	
Reflections collected	23588	
Independent reflections	4724 [*R*(int) = 0.0209]	
Observed reflections	4251	
Completeness to theta = 29.57°	99.5%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9033 and 0.8122	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4724 / 3 / 224	
Goodness-of-fit on F^2	1.051	
Final *R* indices [*I*>2sigma(*I*)]	*R*1 = 0.0369, *wR*2 = 0.1011	
R indices (all data)	*R*1 = 0.0418, *wR*2 = 0.1050	
Largest diff. peak and hole	0.498 and -0.403 e.Å^{-3}	

Table SI.15b. Bond lengths [Å] and angles [°] for **5**.

Fe-N(11)	1.9925(10)	C(11)-H(11B)	0.9800
Fe-N(11)#1	1.9925(10)	C(11)-H(11C)	0.9800
Fe-N(1)	2.0639(15)	C(21)-C(31)	1.4092(14)
Fe-N(1)#1	2.0639(14)	C(31)-C(21)#1	1.4092(14)
N(1)-B	1.509(15)	C(31)-H(31A)	0.9500
N(1)-B#1	1.644(13)	C(12)-C(62)	1.4094(17)
N(1)-H(1)	0.9200	C(12)-C(22)	1.4131(18)
N(1)-H(2)	0.9200	C(22)-C(32)	1.406(2)
C(2)-C(1)	1.534(5)	C(22)-C(72)	1.516(2)
C(2)-H(2A)	0.9800	C(32)-C(42)	1.381(3)
C(2)-H(2B)	0.9800	C(32)-H(32A)	0.9500
C(2)-H(2C)	0.9800	C(42)-C(52)	1.377(3)
C(1)-B	1.616(11)	C(42)-H(42A)	0.9500
C(1)-H(1A)	0.9900	C(52)-C(62)	1.4011(18)
C(1)-H(1B)	0.9900	C(52)-H(52A)	0.9500
B-C(3)	1.624(16)	C(62)-C(102)	1.522(2)
B-N(1)#1	1.644(13)	C(72)-C(92)	1.529(3)
B-C(3')	1.68(2)	C(72)-C(82)	1.540(2)
C(3)-C(4)	1.518(8)	C(72)-H(72A)	1.0000
C(3)-H(3A)	0.9900	C(82)-H(82A)	0.9800
C(3)-H(3B)	0.9900	C(82)-H(82B)	0.9800
C(4)-H(4A)	0.9800	C(82)-H(82C)	0.9800
C(4)-H(4B)	0.9800	C(92)-H(92A)	0.9800
C(4)-H(4C)	0.9800	C(92)-H(92B)	0.9800
C(3')-C(4')	1.52(2)	C(92)-H(92C)	0.9800
C(3')-H(3C)	0.9601	C(102)-C(122)	1.512(3)
C(3')-H(3D)	0.9600	C(102)-C(112)	1.546(6)
C(4')-H(4D)	0.9800	C(102)-H(10A)	1.0000
C(4')-H(4E)	0.9800	C(112)-H(11D)	0.9800
C(4')-H(4F)	0.9800	C(112)-H(11E)	0.9800
N(11)-C(21)	1.3329(15)	C(112)-H(11F)	0.9800
N(11)-C(12)	1.4333(14)	C(122)-H(12A)	0.9800
C(11)-C(21)	1.5133(16)	C(122)-H(12B)	0.9800
C(11)-H(11A)	0.9800	C(122)-H(12C)	0.9800

C(11')-H(11G)	0.9800	C(4)-C(3)-B	112.2(7)
C(11')-H(11H)	0.9800	C(4)-C(3)-H(3A)	109.2
C(11')-H(11I)	0.9800	B-C(3)-H(3A)	109.2
C(12')-H(12D)	0.9800	C(4)-C(3)-H(3B)	109.2
C(12')-H(12E)	0.9800	B-C(3)-H(3B)	109.2
C(12')-H(12F)	0.9800	H(3A)-C(3)-H(3B)	107.9
N(11)-Fe-N(11)#1	93.05(6)	C(4')-C(3')-B	121.0(12)
N(11)-Fe-N(1)	125.02(6)	C(4')-C(3')-H(3C)	106.9
N(11)#1-Fe-N(1)	122.10(5)	B-C(3')-H(3C)	106.9
N(11)-Fe-N(1)#1	122.10(5)	C(4')-C(3')-H(3D)	107.2
N(11)#1-Fe-N(1)#1	125.02(6)	B-C(3')-H(3D)	107.4
N(1)-Fe-N(1)#1	73.12(9)	H(3C)-C(3')-H(3D)	106.8
B-N(1)-Fe	93.9(4)	C(21)-N(11)-C(12)	121.80(10)
B#1-N(1)-Fe	90.0(4)	C(21)-N(11)-Fe	125.90(8)
B-N(1)-H(1)	112.9	C(12)-N(11)-Fe	112.23(7)
B#1-N(1)-H(1)	123.2	C(21)-C(11)-H(11A)	109.5
Fe-N(1)-H(1)	112.9	C(21)-C(11)-H(11B)	109.5
B-N(1)-H(2)	112.9	H(11A)-C(11)-H(11B)	109.5
B#1-N(1)-H(2)	106.0	C(21)-C(11)-H(11C)	109.5
Fe-N(1)-H(2)	112.9	H(11A)-C(11)-H(11C)	109.5
H(1)-N(1)-H(2)	110.4	H(11B)-C(11)-H(11C)	109.5
C(2)-C(1)-B	116.2(5)	N(11)-C(21)-C(31)	123.13(11)
C(2)-C(1)-H(1A)	108.2	N(11)-C(21)-C(11)	120.24(10)
B-C(1)-H(1A)	108.2	C(31)-C(21)-C(11)	116.62(11)
C(2)-C(1)-H(1B)	108.2	C(21)#1-C(31)-C(21)	128.79(16)
B-C(1)-H(1B)	108.2	C(21)#1-C(31)-H(31A)	115.6
H(1A)-C(1)-H(1B)	107.4	C(21)-C(31)-H(31A)	115.6
N(1)-B-C(1)	113.6(11)	C(62)-C(12)-C(22)	120.72(12)
N(1)-B-C(3)	98.5(9)	C(62)-C(12)-N(11)	120.04(11)
C(1)-B-C(3)	117.0(4)	C(22)-C(12)-N(11)	118.93(11)
N(1)-B-N(1)#1	102.5(3)	C(32)-C(22)-C(12)	117.94(14)
C(1)-B-N(1)#1	112.8(9)	C(32)-C(22)-C(72)	121.36(14)
C(3)-B-N(1)#1	110.7(9)	C(12)-C(22)-C(72)	120.69(13)
N(1)-B-C(3')	119.9(11)	C(42)-C(32)-C(22)	121.57(15)
C(1)-B-C(3')	108.2(7)	C(42)-C(32)-H(32A)	119.2
N(1)#1-B-C(3')	98.8(10)	C(22)-C(32)-H(32A)	119.2

C(52)-C(42)-C(32)	119.82(14)	H(82A)-C(82)-H(82B)	109.5
C(52)-C(42)-H(42A)	120.1	C(72)-C(82)-H(82C)	109.5
C(32)-C(42)-H(42A)	120.1	H(82A)-C(82)-H(82C)	109.5
C(42)-C(52)-C(62)	121.31(15)	H(82B)-C(82)-H(82C)	109.5
C(42)-C(52)-H(52A)	119.3	C(72)-C(92)-H(92A)	109.5
C(62)-C(52)-H(52A)	119.3	C(72)-C(92)-H(92B)	109.5
C(52)-C(62)-C(12)	118.63(13)	H(92A)-C(92)-H(92B)	109.5
C(52)-C(62)-C(102)	119.13(13)	C(72)-C(92)-H(92C)	109.5
C(12)-C(62)-C(102)	122.24(11)	H(92A)-C(92)-H(92C)	109.5
C(22)-C(72)-C(92)	110.46(15)	H(92B)-C(92)-H(92C)	109.5
C(22)-C(72)-C(82)	113.11(15)	C(122)-C(102)-C(62)	116.9(2)
C(92)-C(72)-C(82)	109.52(15)	C(122)-C(102)-C(112)	109.8(4)
C(22)-C(72)-H(72A)	107.9	C(62)-C(102)-C(112)	112.9(4)
C(92)-C(72)-H(72A)	107.9	C(122)-C(102)-H(10A)	105.4
C(82)-C(72)-H(72A)	107.9	C(62)-C(102)-H(10A)	105.4
C(72)-C(82)-H(82A)	109.5	C(112)-C(102)-H(10A)	105.4
C(72)-C(82)-H(82B)	109.5		

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+3/2