Electronic Supplementary Material (ESI) for Chemical Communications

Supporting Information

The Elusive Tripodal Tris(2-pyridyl)borate Ligand: A Strongly Coordinating Tetraarylborate

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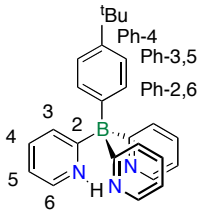
Materials and General Methods. Mg, 2-bromopyridine, and NEt_3 were purchased from Fisher Scientific and $FeCl_2$ (anhydrous) from Sigma-Aldrich. Solvents were purchased from Pharmco and used as received unless noted otherwise. Ether solvents were distilled from Na/benzophenone prior to use. Hydrocarbon and chlorinated solvents were purified using a solvent purification system (Innovative Technologies; alumina/copper columns for hydrocarbon solvents). Chlorinated solvents were distilled from CaH_2 and degassed via several freeze-pump-thaw cycles. 4-*t*-Butylphenyl dibromoborane was prepared according to a literature procedure (Y. Qin, I. Kiburu, S. Shah and F. Jäkle, *Org Lett*, 2006, **8**, 5227-5230). Reactions and manipulations involving boron halide species were carried out under an atmosphere of prepurified nitrogen using either Schlenk techniques or an inert-atmosphere glove box (Innovative Technologies). All other procedures were carried out under ambient conditions.

The 499.9 MHz ^{1}H, 125.7 MHz ^{13}C, and 160.4 MHz ^{11}B NMR spectra were recorded on a Varian INOVA 500 MHz spectrometer equipped with a boron-free probe. All ^{1}H and ^{13}C NMR spectra were referenced internally to the solvent peaks and ^{11}B NMR spectra to BF_3•Et_2O (δ = 0) in C_6D_6. The assignments are based on the numbering scheme shown here.



The MALDI TOF measurements were performed on an Applied Biosystems 4800 Proteomics Analyzer in reflectron (+) or (–)-mode with delayed extraction. For data acquisition in (+)-mode benzo[α]pyrene was used as the matrix (20 mg/mL in toluene) and in (–)-mode α-cyano-4-hydroxycinnamic acid (50% acetonitrile, 0.1% TFA in deionized water). The sample was dissolved in toluene or MeOH (ca. 10 mg/mL), mixed with the matrix in a 1:10 ratio, and then spotted on the wells of a sample plate.

Cyclic voltammetry (CV) experiments were carried out on a CV-50W analyzer from BAS. The three-electrode system consisted of an Au disk as working electrode, a Pt wire as secondary electrode and an Ag wire as a pseudo-reference electrode. The voltammograms were recorded with ca. 10^{-3} to 10^{-4} M solution in CH_2Cl_2 containing $Bu_4N[PF_6]$ (0.1 M) as the supporting electrolyte. The scans were referenced after the addition of a small amount of ferrocene (Fc) as internal standard. The potentials are reported relative to the $Fc^{0/+}$ couple. UV-vis absorption data were acquired on a Varian Cary 500 UV-Vis / NIR spectrophotometer. Elemental analyses were performed by Quantitative Technologies, Inc., Whitehouse, NJ.

Single crystal X-ray diffraction intensities were collected on a Smart Apex2 CCD diffractometer at 100 K using Cu Kα (1.54178 Å) radiation and details of the X-ray diffraction experiments and crystal structure refinements are provided at the end of the Supporting Information. Crystallographic data for the structures of $(PyMgCl)_2(THF)_4$, **1**, **2**, and [**2**$^+$]$FeCl_4$ have been deposited with the Cambridge Crystallographic Data Center as supplementary publications CCDC 878726-878729, respectively. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: (+44) 1223-336-033; email: deposit@ccdc.cam.ac.uk).

Synthetic Procedures

Synthesis of 2-Pyridyl Grignard Reagent. To a freshly prepared and filtered solution of *i*-PrMgCl in tetrahydrofuran (400 mL, 345 mmol), neat 2-bromopyridine (30.0 mL, 313 mmol) was added through a syringe. The resulting dark red reaction mixture was kept stirring for 5 h and then connected to vacuum to evaporate the solvent until a dense yellow slurry formed suddenly. The slurry was carefully transferred under nitrogen protection to a fritted addition

funnel and anhydrous tetrahydrofuran (ca. 150 mL) was used to help complete the transfer of the solids. Anhydrous tetrahydrofuran was continuously passed through the filter cake until it was white and the filtrate colorless. The solid was dried under high vacuum at room temperature for 6 h and then further dried under high vacuum at 65 °C for 12 h. Yield of $(PyMgCl)_2$*$(THF)_4$: 63 g (71%). ^{1}H NMR (499.973 MHz, CD_2Cl_2) δ = 8.60 (br), 7.87 (br), 7.45 (br), 7.01 (br), 3.76 (br m, thf), 1.84 (br m, thf). Single crystals for X-ray diffraction analysis were obtained by recrystallization from hot THF.

Synthesis of *t*-Butylphenyltris(2-pyridyl)borate Free Acid (1). *t*-Butylphenyl dibromoborane (5.00 g, 16.5 mmol) in CH_2Cl_2 (30 mL) was added drop-wise to a solution of pyridyl Grignard (14.5 g, 25.7 mmol) in CH_2Cl_2 (50 mL). The resulting dark red mixture was kept stirring for 5 h. The reaction mixture was poured into an aqueous Na_2CO_3 solution (30 g in 250 mL H_2O) to give a slurry which was stirred for 30 min. Extraction with CH_2Cl_2 (3×200 mL) gave a brown organic phase that was dried over Na_2SO_4. The solvents were removed under vacuum to give an oil that was redissolved in acetone (100 mL), filtered and brought to dryness. The product was further purified by chromatography on silica gel with a 1:1 mixture of hexanes and acetone containing 1% (v/v) triethylamine as the eluent. The product was dried under high vacuum at 60 °C for 10 h to give a white solid. Yield: 3.4 g (54%). ^{1}H NMR (499.973 MHz, $CDCl_3$) δ = 19.5 (br s, 1H, pyridyl N-H), 8.49 (d, ^{3}J = 5.0 Hz, 3H, pyridyl-H6), 7.58 (pst, ^{3}J = 7.5 Hz, 3H, pyridyl-H4), 7.40 (d, ^{3}J = 7.5 Hz, 3H, pyridyl-H3), 7.16 (d, ^{3}J = 7.5 Hz, 2H, tPh-H3,5), 7.10 (pst, ^{3}J = 6.3 Hz, 3H, pyridyl-H5), 6.96 (br d, ^{3}J = 6.0 Hz, 2H, tPh-H2,6), 1.27 (s, 9H, *t*-Bu). ^{13}C NMR (125.718 MHz, $CDCl_3$) δ = 184.2 (q, $^1J_{C\text{-}B}$ = 53.1 Hz, pyridyl-C2), 152.3 (q, $^1J_{C\text{-}B}$ = 50.0 Hz, tPh-C1), 146.9 (tPh-C4), 143.6 (pyridyl-C6), 136.3 (pyridyl-C4), 134.2 (pyridyl-C3), 131.8 (tPh-C2,6), 124.2 (tPh-C3,5), 119.8 (pyridyl-C5), 34.3 ($C(CH_3)_3$), 31.7 ($C(CH_3)_3$). ^{11}B NMR (160.386 MHz, $CDCl_3$) δ = –10.8 ($w_{1/2}$ = 13 Hz). MALDI-TOF MS (benzo[α]pyrene): m/z = 380.2333 (MH^+, calcd for $^{12}C_{25}{}^1H_{27}{}^{11}B_1{}^{14}N_3$ 380.3130). Elemental analysis: calcd for $C_{25}H_{26}B_1N_3$: C 79.16, H 6.91, N 11.08%; found C 78.92, H 6.94, N 11.08%. Single crystals for X-ray diffraction analysis were obtained by slow evaporation of a toluene solution.

Synthesis of Bis(t-butylphenyltris(2-pyridyl)borate) Iron(II) (2). A 100 mL Schlenk flask was charged with anhydrous $FeCl_2$ powder (0.10 g, 0.79 mmol) and anhydrous tetrahydrofuran (50 mL). A solution of *t*-butylphenyltris(2-pyridyl)borate free acid (0.30 g, 0.79 mmol) and triethylamine (2 mL, 14.3 mmol) in methanol (10 mL) was then added. The reaction mixture was kept stirring for 3 h and subsequently filtered to give a red solution. The volatile components were removed on a rotary evaporator to give a red solid, which was purified by column chromatography on silica gel with hexanes as the eluent. Solvent evaporation gave the product as a red solid, which was dried under high vacuum at RT for 1 h. Yield: 0.22 g (68%). ^{1}H NMR (499.973 MHz, $CDCl_3$) δ = 8.09 (d, ^{3}J = 7.5 Hz, 4H, tPh-H2,6), 7.60 (d, ^{3}J = 8.0 Hz, 4H, tPh-H3,5), 7.59 (d, ^{3}J = 9.0 Hz, 6H, pyridyl-H3), 7.27 (pst, ^{3}J = 7.5 Hz, 6H, pyridyl-H4), 7.11 (d, ^{3}J = 5.5 Hz, 6H, pyridyl-H6), 6.44 (pst, ^{3}J = 6.5 Hz, 6H, pyridyl-H5), 1.52 (s, 18H, *t*-Bu). ^{13}C NMR (125.718 MHz, $CDCl_3$) δ = 188.0 (q, $^1J_{C\text{-}B}$ = 49.6 Hz, pyridyl-C2), 158.3 (pyridyl-C6), 149.2 (q, $^1J_{C\text{-}B}$ = 57.3 Hz, tPh-C1), 147.4 (tPh-C4), 136.7 (tPh-C2,6), 132.0 (pyridyl-C4), 125.7 (pyridyl-C3), 124.5 (tPh-C3,5), 119.7 (pyridyl-C5), 34.7 ($C(CH_3)_3$), 32.0 ($C(CH_3)_3$). ^{11}B NMR (160.411 MHz, $CDCl_3$) δ = –7.5 ($w_{1/2}$ = 21 Hz). UV-Vis (25 °C, CH_2Cl_2): λ_{max} = 480 nm (ε = 16400 $M^{-1}cm^{-1}$), 425 (shoulder, ε = 11000 $M^{-1}cm^{-1}$). Cyclic voltammetry: $E_{1/2}$ = –350 mV, ΔE_p = 84 mV (1 mM, CH_2Cl_2 containing 0.1 M $[Bu_4N]PF_6$ as the supporting electrolyte; scan rate 100 mV/s). MALDI-TOF MS (benzo[α]pyrene): m/z = 812.3564 (M^+, calcd for $^{12}C_{50}{}^1H_{50}{}^{11}B_2{}^{56}Fe^{14}N_6$ 812.4392). Elemental analysis for crystals obtained from toluene: calcd for $C_{50}H_{50}B_2FeN_6$•C_7H_8:

C 75.68, H 6.46, N 9.29%; found C 75.61, H 6.46, N 9.24%. Single crystals of the Fe(II) complex for X-ray diffraction analysis were obtained by slow evaporation of a solution in toluene.

Synthesis of Bis(t-butylphenyltris(2-pyridyl)borate) Iron(III) Tetrachloroferrate(III) ([2$^+$]FeCl$_4$). A solution of **2**•toluene (0.20 g, 0.22 mmol) in CH_2Cl_2 (10 mL) was layered with a solution of $FeCl_3$ (0.12 g, 0.74 mmol) in H_2O (10 mL). The reaction mixture was shaken vigorously for 5 min. The organic layer was collected and dried over Na_2SO_4. A dark purple solid was obtained after solvent evaporation. The product was purified by repeated precipitation from dichloromethane solution into diethyl ether and then dried under high vacuum at 60 ºC. Yield: 0.18 g (81%). ^{1}H NMR (499.973 MHz, $CDCl_3$) δ = 22.8 (br, 4H, tPh-H), 21.9 (br, 6H, pyridyl-H), 13.5 (br, 4H, tPh-H), 4.37 (s, 9H, *t*-Bu), –6.91 (br, 6H, pyridyl-H), –8.06 (br, 6H, pyridyl-H), –79.1 (br, 6H, pyridyl-H). ^{11}B NMR (160.411 MHz, $CDCl_3$) δ = 30 ($w_{1/2}$ = 160 Hz). UV-Vis (25 °C, CH_2Cl_2): λ_{max} = 574 nm (ε = 370 M^{-1} cm^{-1}). Single crystals for X-ray diffraction analysis were obtained from $CDCl_3$ solution.

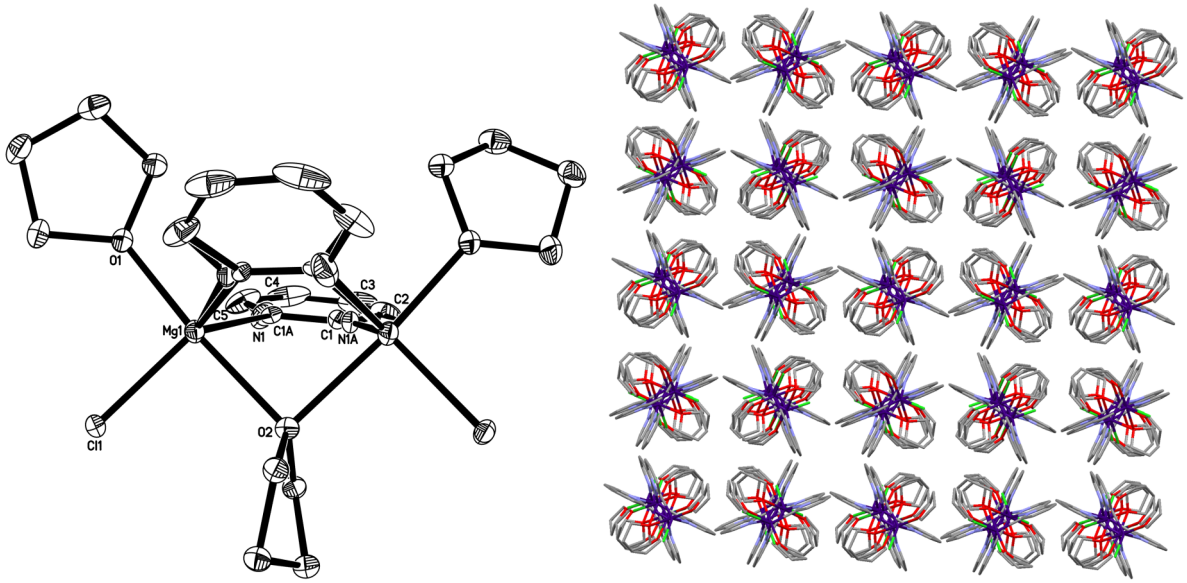


Figure S1. (left) ORTEP plot of the structure of the Grignard reagent $(PyMgCl)_2(THF)_4$. Note that 1 molecule of disordered THF per Grignard dimer that is located in channels along the crystallographic c-axis is omitted. Note also that N1 and C1 show positional disorder with occupancies of 0.50. (right) View along the crystallographic c-axis (slightly offset to show multiple layers). Selected bond lengths (Å) and angles (deg): Mg1-C1 2.1312(18), Mg1-N1 2.1461(18), Mg1-Cl1 2.3378(7), Mg1-O1 2.0904(14), Mg1-O2 2.3444(13), N1-C1 1.390(2), N1 C5 1.383(3); O1-Mg1-C1 93.40(6), O1-Mg1-N1 93.79(6), C1-Mg1-N1 114.27(7), O1-Mg1-Cl1 95.22(4), C1-Mg1-Cl1 121.20(5), N1-Mg1-Cl1 122.96(5), O1-Mg1-O2 174.87(5), C1-Mg1-O2 83.44(5), N1-Mg1-O2 83.88(5), Cl1-Mg1-O2 89.88(4), C5-N1-C1 116.73(18), C5-N1-Mg1 125.07(16), C1-N1-Mg1 118.20(12), C2-C1-N1 119.13(18), C2-C1-Mg1 125.34(16), N1-C1-Mg1 115.35(12).

Table S1. Selected bond lengths (Å) and angles (deg) for **1**, **2** and [**2**$^{+}$]$FeCl_4$.

	1 (Molecules A, B)	**2**	[**2**$^{+}$]$FeCl_4$
Fe-N		1.9880(13)	1.996(3), 2.011(3)
Fe-N		1.9902(13)	1.966(3), 1.991(3)
Fe-N		1.9685(13)	1.990(3), 1.990(2)
B-C(Ph)	1.628(2), 1.635(2)	1.634(2)	1.613(5), 1.621(5)
B-C(Py)	1.641(2), 1.638(2)	1.638(2)	1.636(5), 1.637(5)
B-C(Py)	1.641(2), 1.642(2)	1.641(2)	1.633(5), 1.635(5)
B-C(Py)	1.638(2), 1.643(2)	1.642(2)	1.632(5), 1.622(5)
N-C(B)	1.349(2), 1.340(2)	1.363(2)	1.361(4), 1.356(4)
N-C(B)	1.349(2), 1.356(2)	1.365(2)	1.354(4), 1.360(4)
N-C(B)	1.354(2), 1.354(2)	1.361(2)	1.357(4), 1.355(4)
N-Fe-N(trans)		180	179.40(12)
N-Fe-N(trans)		180	178.81(13)
N-Fe-N(trans)		180	179.32(11)
N-Fe-N		89.82(5)	90.65(12), 89.18(11)
N-Fe-N		90.18(5)	90.16(11), 89.60(11)
N-Fe-N		90.27(5)	91.35(11), 89.80(12)
N-Fe-N		89.73(5)	90.07(11), 90.25(10)
N-Fe-N		90.06(5)	90.23(11), 89.49(11)
N-Fe-N		89.94(5)	88.80(11), 90.44(11)
C(Py)-B-C(Ph)	107.77(10), 108.15(11)	115.56(13)	117.4(3), 118.8(3)
C(Py)-B-C(Ph)	111.13(11), 113.53(12)	115.09(13)	107.6(3), 106.4(3)
C(Py)-B-C(Ph)	113.47(11), 106.44(11)	107.99(13)	114.8(3), 114.1(3)
C(Py)-B-C(Py)	107.42(11), 106.20 (11)	101.76(13)	107.3(3), 106.6(3)
C(Py)-B-C(Py)	112.97(11), 112.23(12)	109.33(13)	99.4(3), 100.8(3)
C(Py)-B-C(Py)	103.92(10), 110.38(11)	106.64(13)	109.9(3), 109.7(3)

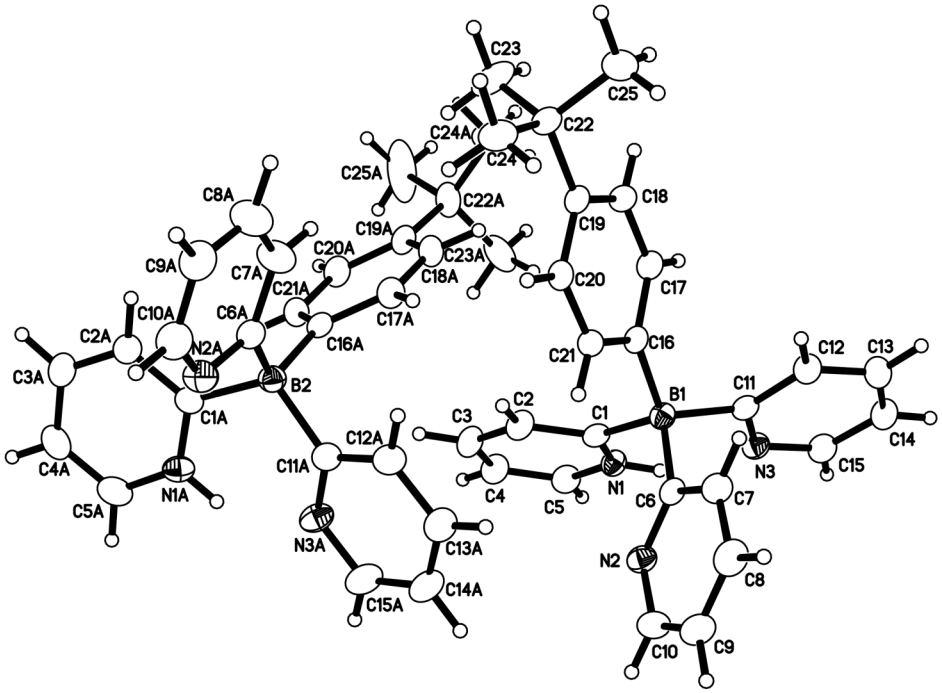


Figure S2. ORTEP plot of the structures of Molecules **A** and **B** of ligand **1**.

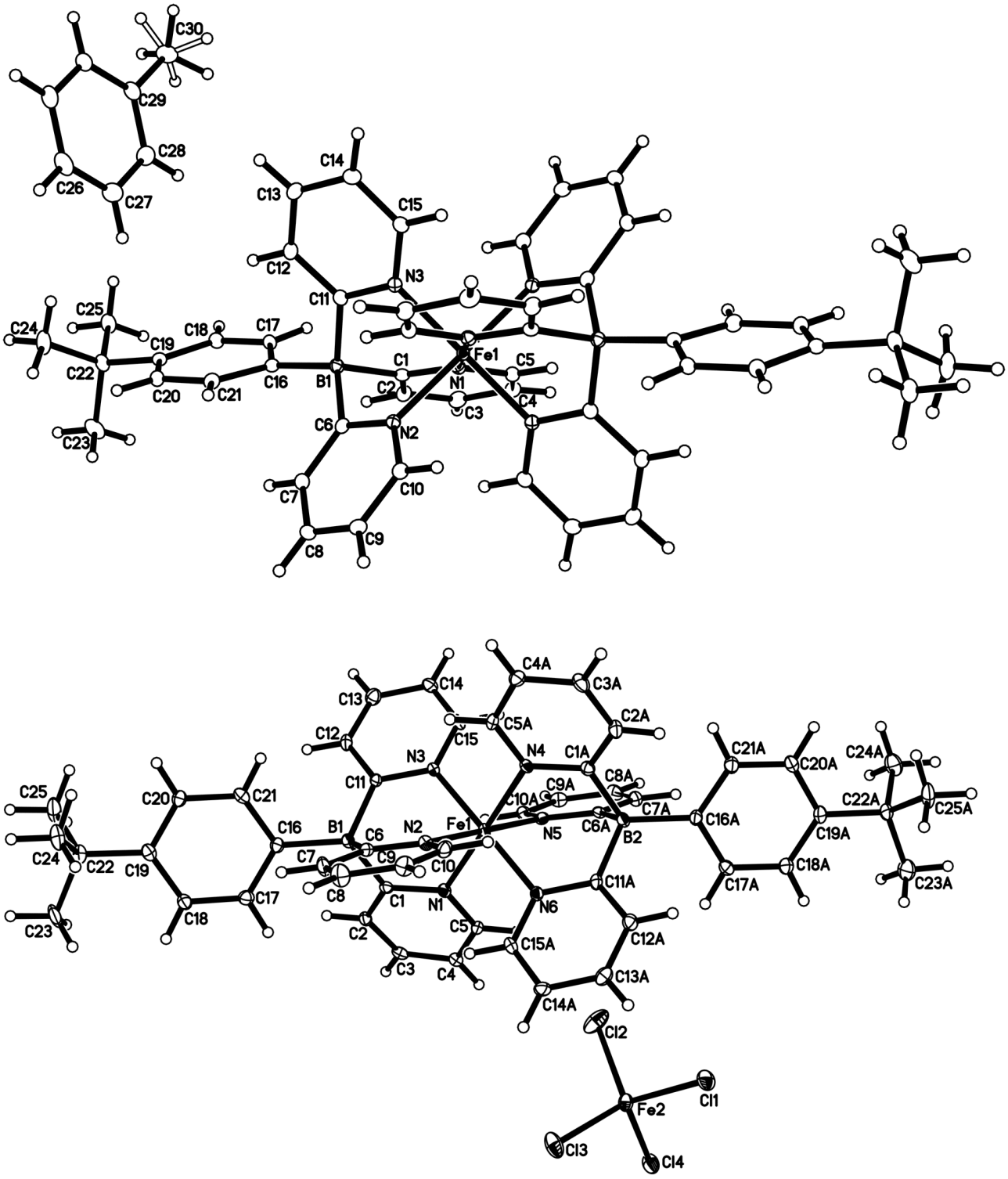
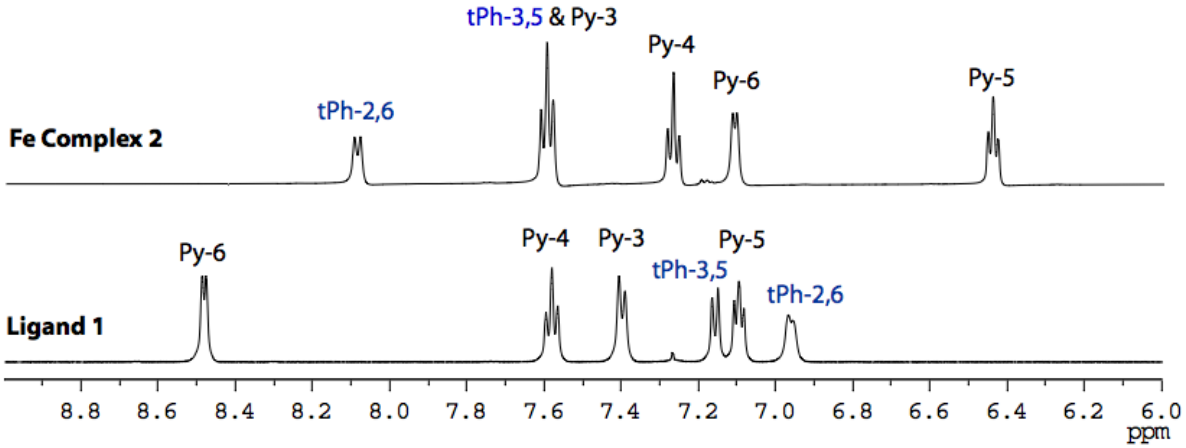


Figure S3. ORTEP plots of the structures of Fe complexes **2** (top) and [**2**$^{+}$]$FeCl_4$ (bottom).

Table S2. ^{1}H NMR assignments of tris(pyridyl)borate ligand **1** and iron complex **2** ($CDCl_3$, RT).

	NH/ Py	**H6/ Py**	**H4/ Py**	**H3/ Py**	**H5/ Py**	**H3,5/ Ph**	**H2,6/ Ph**	**tBu/ Ph**
1	19.5	8.49	7.58	7.40	7.10	7.16	6.96	1.27
2-Fe		7.11	7.27	7.59	6.44	7.60	8.09	1.52



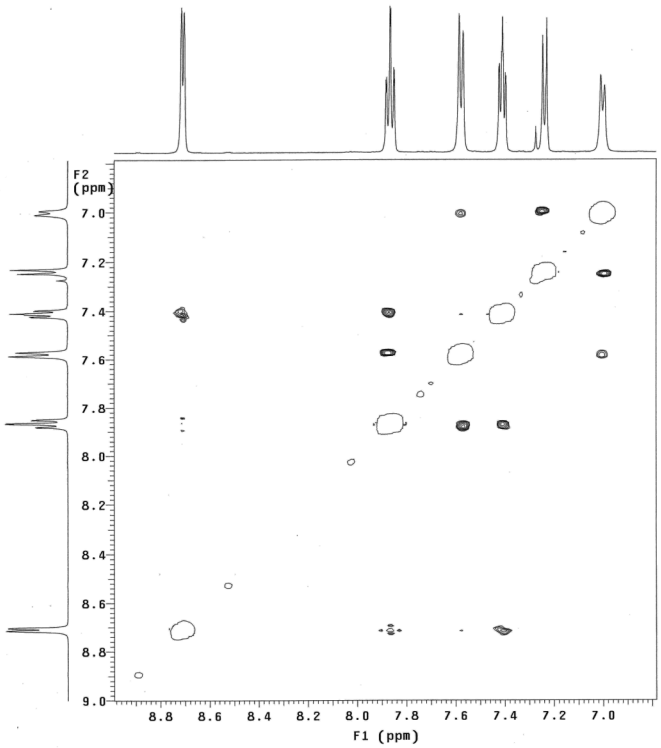


Figure S4. (a) Overlay of aromatic region of the ^{1}H NMR spectra of ligand **1** and the Fe complex **2** and (b) Aromatic Region of NOESY NMR spectrum of ligand **1** in $CDCl_3$.

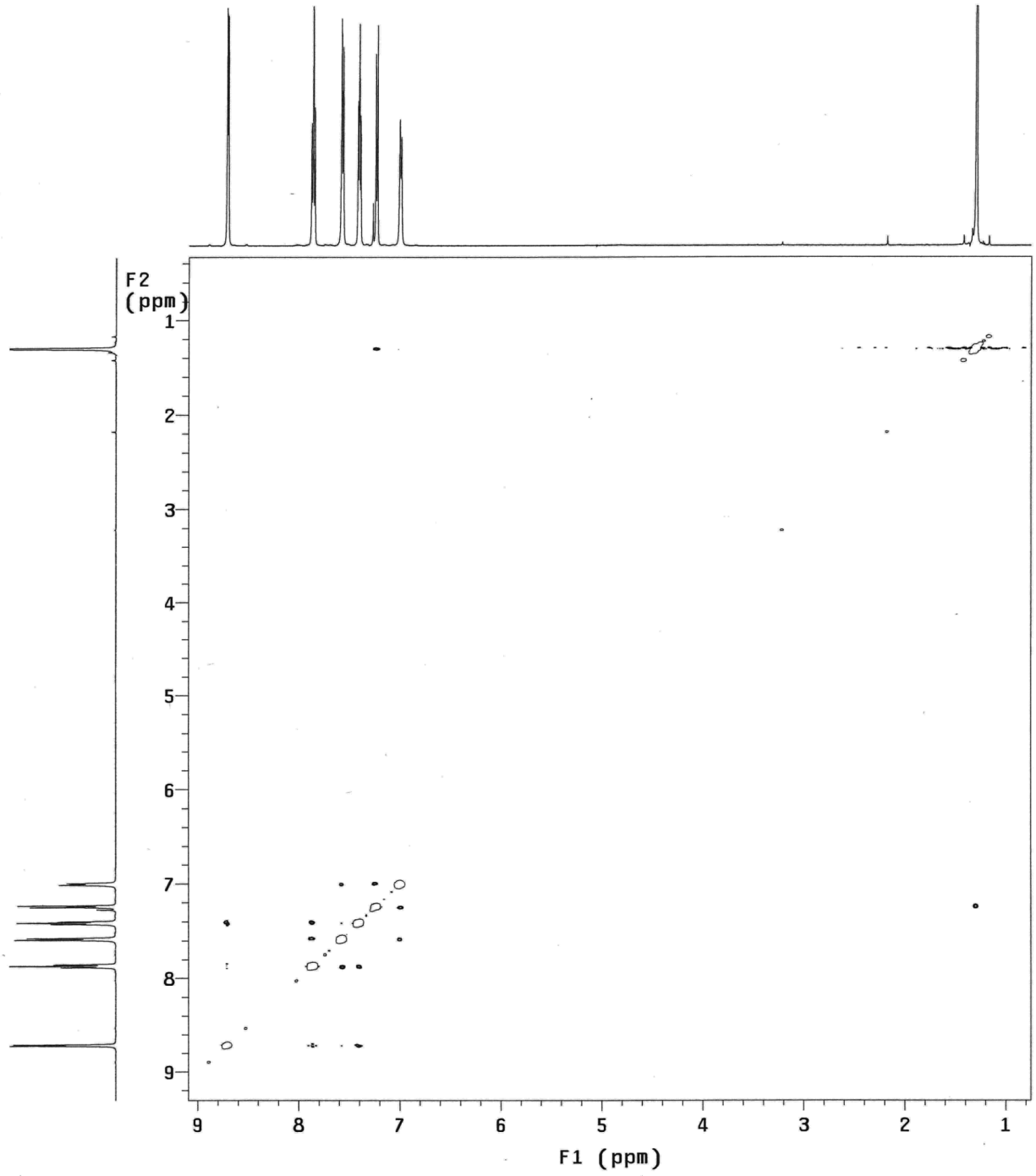


Figure S5. Full NOESY NMR spectrum of ligand **1** in $CDCl_3$.

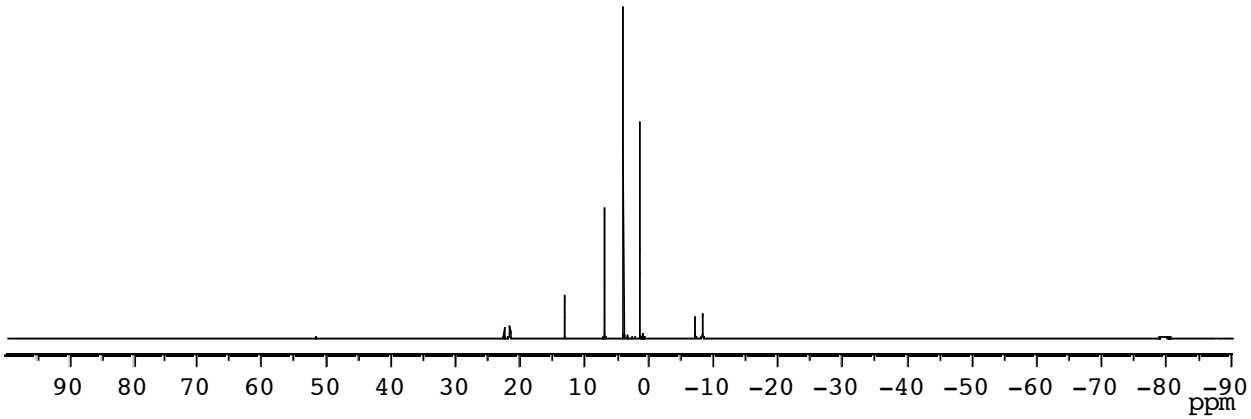


Figure S6. ^{1}H NMR spectrum of $\mathbf{2}^{+}$ in $CDCl_3$.

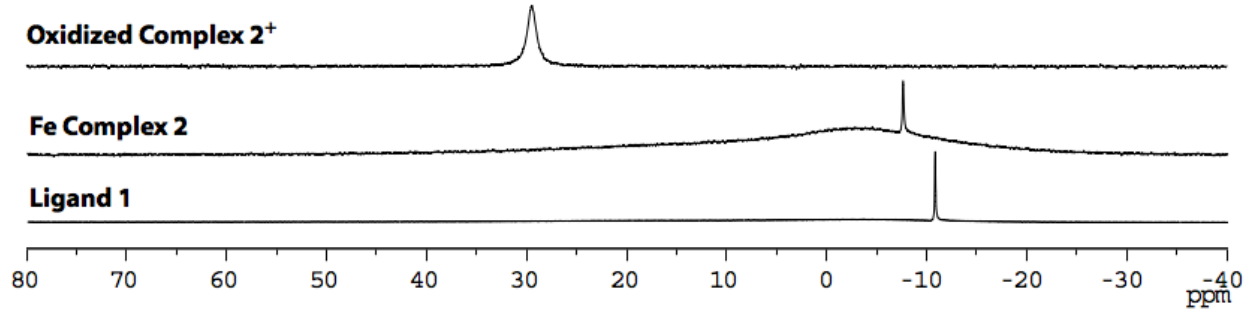


Figure S7. Overlay of ^{11}B NMR spectra of **1**, **2**, and $\mathbf{2}^{+}$ in $CDCl_3$.

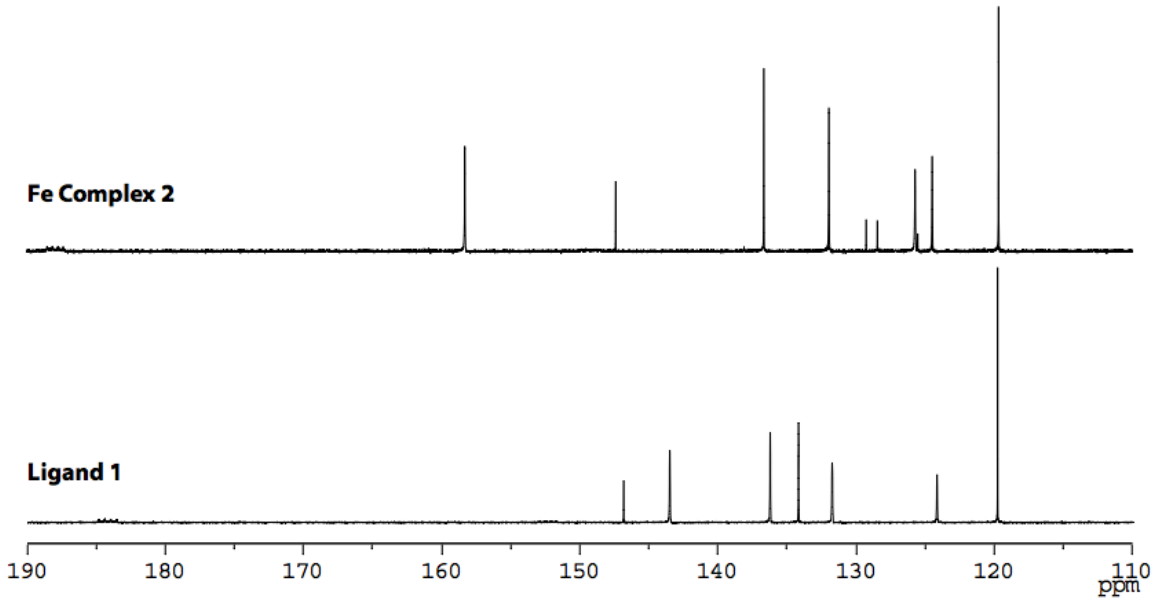


Figure S8. Overlay of aromatic region of the ^{13}C NMR spectra of ligand **1** and the Fe complex **2** in $CDCl_3$ (the Fe complex **2** contains cocrystallized toluene)

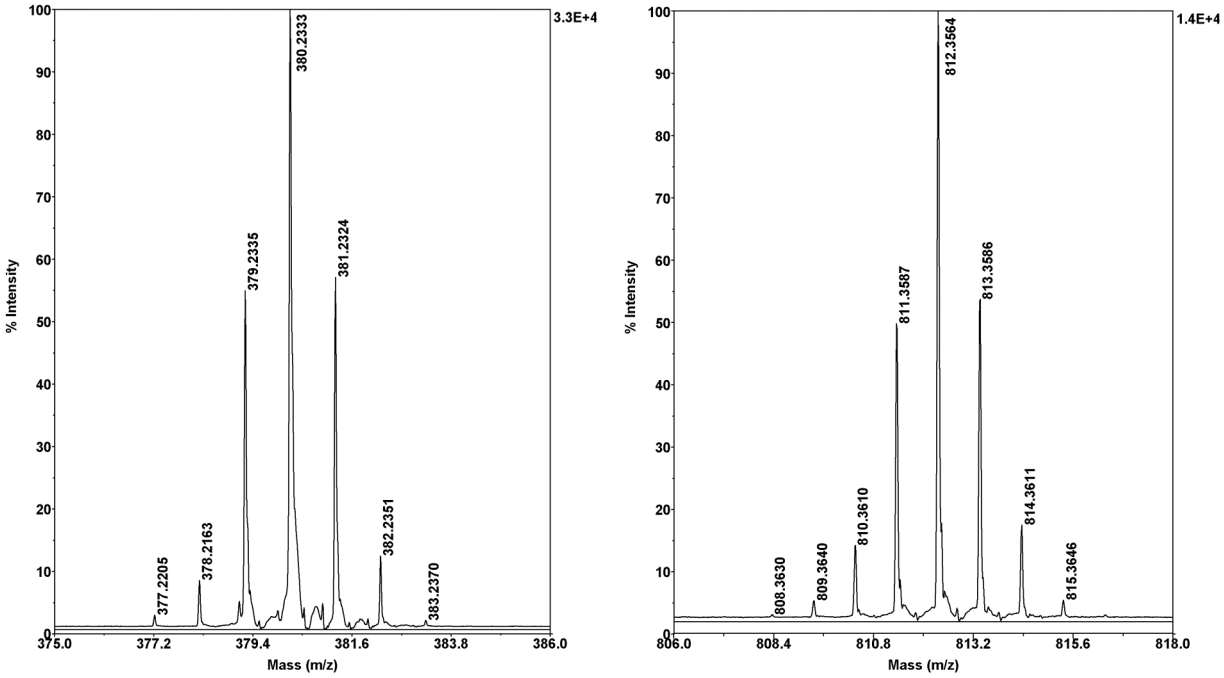


Figure S9. MALDI-TOF-MS Data of a) free ligand **1** (cinnamic acid/MeOH) and b) the iron complex **2** (benzo[α]pyrene/toluene).

Experimental

Crystal data

$C_{22}H_{32}Cl_2Mg_2N_2O_3$
$M_r = 492.02$
Tetragonal, *P*4/*ncc*
$a = 17.1131$ (2) Å
$c = 18.5626$ (3) Å
$V = 5436.21$ (13) Å^3
$Z = 8$
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
$\mu = 2.79$ mm^{-1}
$T = 100$ K
0.48 × 0.31 × 0.30 mm

Data collection

Bruker SMART CCD Apex-II area-detector diffractometer
Absorption correction: Numerical *SADABS* (Sheldrick, 2008a)
$T_{min} = 0.348$, $T_{max} = 0.488$
2706 measured reflections
2706 independent reflections
2550 reflections with $I > 2\sigma(I)$
$R_{int} = 0.000$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.122$
$S = 1.10$
2706 reflections
142 parameters
0 restraints
H-atom parameters constrained
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

Data collection: *APEX* 2 (Bruker, 2006); cell refinement: *APEX* 2; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008b); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

References

Bruker (2005). *SAINT* Version 7.23a. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (2006). *APEX 2* Version 2.0-2. Bruker AXS Inc., Madison, Wisconsin, USA.

Sheldrick, G. M. (2008*a*). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (2008*b*). *Acta Cryst.*A**64**, 112—122.

Refinement

All H atoms for (I) were found in electron density difference maps. The methylene and aromatic Hs were placed in geometrically idealized positions and constrained to ride on their parent C atoms with C—H distances of 0.99 and 0.95 Å, respectively, and $U_{iso}(H) = 1.2U_{eq}(C)$. The occupancy of the pyridine C1 and N1 atoms was refined to be 50/50, and was fixed to be 0.50. Disordered solvent (THF) molecules were not determined, but SQUEEZE found that there were approximately 3.5-4.0 such disordered solvent molecules per cell, which are located in channels along the crystallographic c axis.

(pyMgCl)2.(THF)4

Crystal data

$C_{22}H_{32}Cl_2Mg_2N_2O_3$	$D_x = 1.202$ Mg m^{-3}
$M_r = 492.02$	Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Tetragonal, $P4/ncc$	Cell parameters from 9782 reflections
Hall symbol: -P 4a 2ac	$\theta = 4.8–67.7°$
$a = 17.1131$ (2) Å	$\mu = 2.79$ mm^{-1}
$c = 18.5626$ (3) Å	$T = 100$ K
$V = 5436.21$ (13) Å^3	Parallelepiped, Colourless
$Z = 8$	0.48 × 0.31 × 0.30 mm
$F(000) = 2080$	

Data collection

Bruker SMART CCD Apex-II area-detector diffractometer	2706 independent reflections
Radiation source: fine-focus sealed tube	2550 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.000$
φ and ω scans	$\theta_{max} = 74.1°$, $\theta_{min} = 4.8°$
Absorption correction: Numerical *SADABS* (Sheldrick, 2008a)	$h = 0\rightarrow15$
$T_{min} = 0.348$, $T_{max} = 0.488$	$k = 0\rightarrow21$
2706 measured reflections	$l = 0\rightarrow22$

Refinement

Refinement on F^2	Primary atom site location: Structure-invariant direct methods
Least-squares matrix: Full	Secondary atom site location: Difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.043$	Hydrogen site location: Inferred from neighbouring sites
$wR(F^2) = 0.122$	H-atom parameters constrained
$S = 1.10$	$w = 1/[\sigma^2(F_o^2) + (0.0659P)^2 + 3.3738P]$ where $P = (F_o^2 + 2F_c^2)/3$
2706 reflections	$(\Delta/\sigma)_{max} < 0.001$
142 parameters	$\Delta\rho_{max} = 0.47$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.34$ e Å^{-3}

Special details

Experimental. 'crystal mounted on a Cryoloop using Paratone-N'

Geometry. 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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR 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 $F^2 > 2\text{sigma}(F^2)$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Mg1	0.03496 (3)	0.02747 (3)	0.32975 (3)	0.02481 (19)
Cl1	−0.00183 (3)	0.12790 (3)	0.40809 (2)	0.03442 (18)
O1	0.12550 (8)	−0.01422 (8)	0.39484 (8)	0.0308 (3)
O2	−0.06458 (7)	0.06458 (7)	0.2500	0.0251 (4)
N1	0.10955 (10)	0.04586 (10)	0.23837 (10)	0.0360 (4)
C1	0.08175 (10)	0.02488 (9)	0.17074 (9)	0.0230 (3)
C2	0.12749 (14)	0.03848 (12)	0.11135 (13)	0.0436 (5)
H2	0.1080	0.0228	0.0656	0.052*
C3	0.19864 (15)	0.07285 (14)	0.11397 (18)	0.0571 (7)
H3	0.2274	0.0828	0.0712	0.068*
C4	0.22806 (13)	0.09287 (15)	0.1803 (2)	0.0635 (9)
H4	0.2780	0.1166	0.1843	0.076*
C5	0.18373 (12)	0.07785 (13)	0.24112 (15)	0.0476 (6)
H5	0.2053	0.0901	0.2869	0.057*
C6	0.17202 (11)	−0.07997 (11)	0.37087 (11)	0.0337 (4)
H6A	0.2228	−0.0621	0.3514	0.040*
H6B	0.1442	−0.1099	0.3331	0.040*
C7	0.18384 (13)	−0.12937 (12)	0.43751 (13)	0.0422 (5)
H7A	0.2324	−0.1607	0.4342	0.051*
H7B	0.1390	−0.1648	0.4457	0.051*
C8	0.18965 (12)	−0.06802 (14)	0.49636 (11)	0.0427 (5)
H8A	0.1743	−0.0899	0.5436	0.051*
H8B	0.2434	−0.0471	0.4999	0.051*
C9	0.13334 (14)	−0.00577 (14)	0.47256 (12)	0.0431 (5)
H9A	0.0821	−0.0128	0.4964	0.052*
H9B	0.1537	0.0467	0.4848	0.052*
C10	−0.14381 (10)	0.05622 (11)	0.27946 (10)	0.0284 (4)
H10A	−0.1420	0.0329	0.3282	0.034*
H10B	−0.1760	0.0224	0.2480	0.034*
C11	−0.17724 (11)	0.13790 (11)	0.28237 (11)	0.0345 (4)
H11A	−0.1633	0.1644	0.3280	0.041*
H11B	−0.2348	0.1373	0.2771	0.041*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg1	0.0298 (3)	0.0245 (3)	0.0201 (3)	−0.0003 (2)	−0.0001 (2)	−0.0010 (2)
Cl1	0.0490 (3)	0.0318 (3)	0.0225 (3)	0.01345 (18)	−0.00381 (17)	−0.00570 (16)
O1	0.0333 (7)	0.0349 (7)	0.0241 (7)	0.0058 (5)	−0.0024 (5)	−0.0011 (5)
O2	0.0242 (5)	0.0242 (5)	0.0268 (9)	−0.0003 (6)	0.0034 (5)	0.0034 (5)
N1	0.0314 (8)	0.0348 (8)	0.0419 (10)	0.0007 (6)	−0.0008 (7)	0.0083 (7)
C1	0.0233 (8)	0.0208 (8)	0.0250 (8)	0.0029 (6)	0.0051 (6)	0.0015 (6)

C2	0.0578 (14)	0.0329 (10)	0.0401 (12)	0.0073 (9)	0.0222 (10)	0.0043 (9)
C3	0.0467 (13)	0.0432 (12)	0.0813 (19)	0.0127 (10)	0.0370 (14)	0.0242 (12)
C4	0.0245 (10)	0.0417 (12)	0.124 (3)	0.0022 (9)	0.0108 (13)	0.0396 (15)
C5	0.0336 (10)	0.0406 (11)	0.0685 (16)	−0.0081 (8)	−0.0182 (10)	0.0209 (11)
C6	0.0315 (9)	0.0353 (10)	0.0342 (10)	0.0048 (7)	−0.0002 (8)	−0.0017 (8)
C7	0.0381 (10)	0.0400 (11)	0.0485 (13)	0.0065 (8)	0.0039 (9)	0.0135 (9)
C8	0.0371 (10)	0.0613 (14)	0.0296 (10)	0.0071 (9)	−0.0003 (8)	0.0115 (9)
C9	0.0517 (13)	0.0508 (12)	0.0267 (11)	0.0079 (10)	−0.0090 (9)	−0.0022 (8)
C10	0.0234 (8)	0.0332 (9)	0.0285 (9)	−0.0002 (7)	0.0039 (7)	0.0002 (7)
C11	0.0303 (9)	0.0381 (10)	0.0350 (10)	0.0068 (7)	0.0014 (8)	−0.0028 (8)

Geometric parameters (Å, º)

Mg1—O1	2.0904 (14)	C4—H4	0.9500
Mg1—C1^{i}	2.1312 (18)	C5—H5	0.9500
Mg1—N1	2.1461 (18)	C6—C7	1.512 (3)
Mg1—Cl1	2.3378 (7)	C6—H6A	0.9900
Mg1—O2	2.3444 (13)	C6—H6B	0.9900
Mg1—Mg1^{i}	3.3237 (11)	C7—C8	1.518 (3)
O1—C6	1.448 (2)	C7—H7A	0.9900
O1—C9	1.456 (3)	C7—H7B	0.9900
O2—C10	1.4689 (19)	C8—C9	1.503 (3)
O2—C10^{i}	1.4689 (19)	C8—H8A	0.9900
O2—Mg1^{i}	2.3444 (13)	C8—H8B	0.9900
N1—C5	1.383 (3)	C9—H9A	0.9900
N1—C1	1.390 (2)	C9—H9B	0.9900
C1—C2	1.372 (3)	C10—C11	1.511 (2)
C1—Mg1^{i}	2.1312 (18)	C10—H10A	0.9900
C2—C3	1.353 (4)	C10—H10B	0.9900
C2—H2	0.9500	C11—C11^{i}	1.533 (4)
C3—C4	1.373 (4)	C11—H11A	0.9900
C3—H3	0.9500	C11—H11B	0.9900
C4—C5	1.385 (4)		

O1—Mg1—C1^{i}	93.40 (6)	N1—C5—C4	123.1 (2)
O1—Mg1—N1	93.79 (6)	N1—C5—H5	118.4
C1^{i}—Mg1—N1	114.27 (7)	C4—C5—H5	118.4
O1—Mg1—Cl1	95.22 (4)	O1—C6—C7	104.87 (16)
C1^{i}—Mg1—Cl1	121.20 (5)	O1—C6—H6A	110.8
N1—Mg1—Cl1	122.96 (5)	C7—C6—H6A	110.8
O1—Mg1—O2	174.87 (5)	O1—C6—H6B	110.8
C1^{i}—Mg1—O2	83.44 (5)	C7—C6—H6B	110.8
N1—Mg1—O2	83.88 (5)	H6A—C6—H6B	108.8
Cl1—Mg1—O2	89.88 (4)	C6—C7—C8	102.17 (17)
O1—Mg1—Mg1^{i}	130.05 (4)	C6—C7—H7A	111.3
C1^{i}—Mg1—Mg1^{i}	63.89 (5)	C8—C7—H7A	111.3
N1—Mg1—Mg1^{i}	62.24 (5)	C6—C7—H7B	111.3
Cl1—Mg1—Mg1^{i}	134.737 (17)	C8—C7—H7B	111.3
O2—Mg1—Mg1^{i}	44.86 (3)	H7A—C7—H7B	109.2
C6—O1—C9	109.33 (14)	C9—C8—C7	103.69 (17)
C6—O1—Mg1	119.67 (11)	C9—C8—H8A	111.0
C9—O1—Mg1	127.37 (12)	C7—C8—H8A	111.0
C10—O2—C10^{i}	108.56 (17)	C9—C8—H8B	111.0
C10—O2—Mg1^{i}	114.48 (8)	C7—C8—H8B	111.0
C10^{i}—O2—Mg1^{i}	114.16 (8)	H8A—C8—H8B	109.0

C10—O2—Mg1	114.16 (8)	O1—C9—C8	106.25 (17)
C10^{i}—O2—Mg1	114.48 (8)	O1—C9—H9A	110.5
Mg1^{i}—O2—Mg1	90.29 (6)	C8—C9—H9A	110.5
C5—N1—C1	116.73 (18)	O1—C9—H9B	110.5
C5—N1—Mg1	125.07 (16)	C8—C9—H9B	110.5
C1—N1—Mg1	118.20 (12)	H9A—C9—H9B	108.7
C2—C1—N1	119.13 (18)	O2—C10—C11	105.82 (14)
C2—C1—Mg1^{i}	125.34 (16)	O2—C10—H10A	110.6
N1—C1—Mg1^{i}	115.35 (12)	C11—C10—H10A	110.6
C3—C2—C1	123.9 (3)	O2—C10—H10B	110.6
C3—C2—H2	118.0	C11—C10—H10B	110.6
C1—C2—H2	118.0	H10A—C10—H10B	108.7
C2—C3—C4	118.1 (2)	C10—C11—C11^{i}	102.23 (11)
C2—C3—H3	121.0	C10—C11—H11A	111.3
C4—C3—H3	121.0	C11^{i}—C11—H11A	111.3
C3—C4—C5	118.9 (2)	C10—C11—H11B	111.3
C3—C4—H4	120.5	C11^{i}—C11—H11B	111.3
C5—C4—H4	120.5	H11A—C11—H11B	109.2

C1^{i}—Mg1—O1—C6	58.90 (14)	Mg1^{i}—Mg1—N1—C5	−176.20 (18)
N1—Mg1—O1—C6	−55.71 (14)	O1—Mg1—N1—C1	138.30 (13)
Cl1—Mg1—O1—C6	−179.32 (12)	C1^{i}—Mg1—N1—C1	42.84 (13)
O2—Mg1—O1—C6	7.1 (6)	Cl1—Mg1—N1—C1	−122.99 (12)
Mg1^{i}—Mg1—O1—C6	0.64 (16)	O2—Mg1—N1—C1	−37.12 (13)
C1^{i}—Mg1—O1—C9	−97.21 (16)	Mg1^{i}—Mg1—N1—C1	4.36 (11)
N1—Mg1—O1—C9	148.17 (16)	C5—N1—C1—C2	−1.6 (3)
Cl1—Mg1—O1—C9	24.56 (16)	Mg1—N1—C1—C2	177.91 (14)
O2—Mg1—O1—C9	−149.1 (5)	C5—N1—C1—Mg1^{i}	173.84 (14)
Mg1^{i}—Mg1—O1—C9	−155.47 (15)	Mg1—N1—C1—Mg1^{i}	−6.67 (17)
O1—Mg1—O2—C10	110.2 (5)	N1—C1—C2—C3	−1.2 (3)
C1^{i}—Mg1—O2—C10	57.98 (10)	Mg1^{i}—C1—C2—C3	−176.17 (16)
N1—Mg1—O2—C10	173.35 (11)	C1—C2—C3—C4	2.4 (3)
Cl1—Mg1—O2—C10	−63.46 (10)	C2—C3—C4—C5	−0.6 (3)
Mg1^{i}—Mg1—O2—C10	117.15 (10)	C1—N1—C5—C4	3.3 (3)
O1—Mg1—O2—C10^{i}	−123.8 (5)	Mg1—N1—C5—C4	−176.10 (17)
C1^{i}—Mg1—O2—C10^{i}	−176.03 (11)	C3—C4—C5—N1	−2.3 (3)
N1—Mg1—O2—C10^{i}	−60.67 (11)	C9—O1—C6—C7	20.8 (2)
Cl1—Mg1—O2—C10^{i}	62.52 (10)	Mg1—O1—C6—C7	−139.22 (13)
Mg1^{i}—Mg1—O2—C10^{i}	−116.87 (10)	O1—C6—C7—C8	−34.74 (19)
O1—Mg1—O2—Mg1^{i}	−7.0 (5)	C6—C7—C8—C9	35.6 (2)
C1^{i}—Mg1—O2—Mg1^{i}	−59.17 (5)	C6—O1—C9—C8	2.0 (2)
N1—Mg1—O2—Mg1^{i}	56.20 (5)	Mg1—O1—C9—C8	160.07 (14)
Cl1—Mg1—O2—Mg1^{i}	179.39 (3)	C7—C8—C9—O1	−23.8 (2)
O1—Mg1—N1—C5	−42.26 (17)	C10^{i}—O2—C10—C11	−12.54 (9)
C1^{i}—Mg1—N1—C5	−137.72 (16)	Mg1^{i}—O2—C10—C11	−141.38 (12)
Cl1—Mg1—N1—C5	56.45 (18)	Mg1—O2—C10—C11	116.49 (13)
O2—Mg1—N1—C5	142.33 (16)	O2—C10—C11—C11^{i}	32.0 (2)

Symmetry code: (i) −*y*, −*x*, −*z*+1/2.

Experimental

Crystal data

$C_{25}H_{26}BN_3$
$M_r = 379.30$
Triclinic, $P\overline{1}$
$a = 9.5834$ (2) Å
$b = 13.3508$ (3) Å
$c = 17.3829$ (4) Å
$\alpha = 86.769$ (1)°
$\beta = 86.723$ (1)°
$\gamma = 70.469$ (1)°
$V = 2091.03$ (8) Å^3
$Z = 4$
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
$\mu = 0.54$ mm^{-1}
$T = 100$ K
0.50 × 0.15 × 0.10 mm

Data collection

Bruker SMART CCD Apex-II area-detector diffractometer
Absorption correction: Numerical *SADABS* (Sheldrick, 2008a)
$T_{min} = 0.774$, $T_{max} = 0.948$
14577 measured reflections
7078 independent reflections
6431 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.111$
$S = 1.02$
7078 reflections
529 parameters
0 restraints
H-atom parameters constrained
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

Data collection: *APEX* 2 (Bruker, 2006); cell refinement: *APEX* 2; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008b); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

References

Bruker (2005). *SAINT* Version 7.23a. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (2006). *APEX 2* Version 2.0-2. Bruker AXS Inc., Madison, Wisconsin, USA.

Sheldrick, G. M. (2008*a*). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (2008*b*). *Acta Cryst.*A**64**, 112—122.

Refinement

All H atoms for (I) were found in electron density difference maps. The methyl H atoms were put in ideally staggered positions with C—H distances of 0.98 Å and $U_{iso}(H) = 1.5U_{eq}(C)$. The pyridinium and aromatic Hs were placed in geometrically idealized positions and constrained to ride on their parent C or N atoms with distances of 0.88 and 0.95 Å, respectively, and $U_{iso}(H) = 1.2U_{eq}(C)$.

(ligand1)

Crystal data

$C_{25}H_{26}BN_3$	$Z = 4$
$M_r = 379.30$	$F(000) = 808$
Triclinic, $P\overline{1}$	$D_x = 1.205$ Mg m^{-3}
Hall symbol: -P 1	Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
$a = 9.5834$ (2) Å	Cell parameters from 9977 reflections
$b = 13.3508$ (3) Å	$\theta = 3.7$–$68.3°$
$c = 17.3829$ (4) Å	$\mu = 0.54$ mm^{-1}
$\alpha = 86.769$ (1)°	$T = 100$ K
$\beta = 86.723$ (1)°	Needle, Colourless
$\gamma = 70.469$ (1)°	0.50 × 0.15 × 0.10 mm
$V = 2091.03$ (8) Å^3	

Data collection

Bruker SMART CCD Apex-II area-detector diffractometer	7078 independent reflections
Radiation source: fine-focus sealed tube	6431 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.020$
φ and ω scans	$\theta_{max} = 68.0°$, $\theta_{min} = 2.6°$
Absorption correction: Numerical *SADABS* (Sheldrick, 2008a)	$h = -11 \rightarrow 11$
$T_{min} = 0.774$, $T_{max} = 0.948$	$k = -16 \rightarrow 14$
14577 measured reflections	$l = -20 \rightarrow 20$

Refinement

Refinement on F^2	Primary atom site location: Structure-invariant direct methods
Least-squares matrix: Full	Secondary atom site location: Difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.041$	Hydrogen site location: Inferred from neighbouring sites
$wR(F^2) = 0.111$	H-atom parameters constrained
$S = 1.02$	$w = 1/[\sigma^2(F_o^2) + (0.057P)^2 + 0.8759P]$ where $P = (F_o^2 + 2F_c^2)/3$
7078 reflections	$(\Delta/\sigma)_{max} < 0.001$
529 parameters	$\Delta\rho_{max} = 0.31$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.19$ e Å^{-3}

Special details

Experimental. 'crystal mounted on a Cryoloop using Paratone-N'

Geometry. 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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR 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 $F^2 > 2\text{sigma}(F^2)$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
B1	0.68573 (17)	0.82247 (13)	0.39062 (8)	0.0209 (3)
N1	0.43378 (13)	0.88183 (9)	0.46892 (6)	0.0228 (2)
H1	0.4860	0.8902	0.5065	0.027*
N2	0.59858 (13)	1.02326 (9)	0.35286 (6)	0.0250 (3)
N3	0.68790 (13)	0.85327 (9)	0.53491 (6)	0.0239 (3)
C1	0.50632 (15)	0.84713 (11)	0.40159 (8)	0.0215 (3)
C2	0.41843 (16)	0.83629 (12)	0.34301 (8)	0.0269 (3)
H2	0.4636	0.8136	0.2941	0.032*
C3	0.26791 (17)	0.85786 (13)	0.35480 (9)	0.0298 (3)
H3	0.2106	0.8490	0.3145	0.036*
C4	0.20028 (16)	0.89274 (12)	0.42610 (9)	0.0290 (3)
H4	0.0967	0.9080	0.4353	0.035*
C5	0.28675 (16)	0.90450 (12)	0.48254 (8)	0.0271 (3)
H5	0.2431	0.9287	0.5315	0.033*
C6	0.71142 (15)	0.93002 (11)	0.35145 (7)	0.0208 (3)
C7	0.85113 (16)	0.92746 (12)	0.32005 (8)	0.0268 (3)
H7	0.9303	0.8617	0.3184	0.032*
C8	0.87448 (18)	1.01941 (13)	0.29157 (9)	0.0326 (3)
H8	0.9690	1.0174	0.2706	0.039*
C9	0.75786 (18)	1.11451 (12)	0.29412 (9)	0.0328 (3)
H9	0.7702	1.1794	0.2755	0.039*
C10	0.62325 (18)	1.11182 (12)	0.32464 (8)	0.0298 (3)
H10	0.5426	1.1768	0.3258	0.036*
C11	0.76820 (15)	0.80456 (11)	0.47273 (7)	0.0213 (3)
C12	0.92049 (16)	0.75138 (12)	0.47925 (8)	0.0257 (3)
H12	0.9775	0.7154	0.4364	0.031*
C13	0.98867 (16)	0.75071 (12)	0.54747 (8)	0.0290 (3)
H13	1.0920	0.7147	0.5516	0.035*
C14	0.90432 (17)	0.80323 (12)	0.60962 (8)	0.0286 (3)
H14	0.9484	0.8052	0.6568	0.034*
C15	0.75479 (17)	0.85248 (12)	0.60095 (8)	0.0275 (3)
H15	0.6960	0.8876	0.6436	0.033*
C16	0.75231 (14)	0.72252 (11)	0.33436 (7)	0.0206 (3)
C17	0.79488 (15)	0.61581 (11)	0.36142 (7)	0.0227 (3)
H17	0.7903	0.6008	0.4154	0.027*
C18	0.84324 (15)	0.53158 (11)	0.31229 (8)	0.0237 (3)
H18	0.8715	0.4609	0.3336	0.028*
C19	0.85153 (14)	0.54803 (11)	0.23224 (8)	0.0219 (3)
C20	0.80788 (14)	0.65338 (11)	0.20458 (7)	0.0217 (3)
H20	0.8104	0.6682	0.1505	0.026*
C21	0.76066 (14)	0.73734 (11)	0.25422 (8)	0.0215 (3)
H21	0.7328	0.8079	0.2327	0.026*
C22	0.90839 (16)	0.45416 (11)	0.17862 (8)	0.0259 (3)
C23	0.8071 (2)	0.38623 (15)	0.18730 (11)	0.0448 (4)

H23A	0.8049	0.3598	0.2409	0.067*
H23B	0.8450	0.3259	0.1534	0.067*
H23C	0.7067	0.4295	0.1730	0.067*
C24	0.9158 (2)	0.49185 (13)	0.09446 (9)	0.0369 (4)
H24A	0.8159	0.5333	0.0783	0.055*
H24B	0.9570	0.4301	0.0622	0.055*
H24C	0.9792	0.5364	0.0889	0.055*
C25	1.06638 (18)	0.38572 (13)	0.20019 (9)	0.0364 (4)
H25A	1.1311	0.4293	0.1952	0.055*
H25B	1.1040	0.3263	0.1656	0.055*
H25C	1.0647	0.3580	0.2535	0.055*
B2	0.26399 (17)	0.79272 (13)	0.08985 (9)	0.0230 (3)
N1A	−0.00814 (13)	0.91557 (10)	0.07815 (7)	0.0265 (3)
H1A	0.0193	0.9593	0.1049	0.032*
N2A	0.35020 (14)	0.80551 (10)	−0.05011 (7)	0.0298 (3)
N3A	0.18349 (14)	0.97875 (10)	0.14787 (7)	0.0281 (3)
C1A	0.09480 (15)	0.82228 (11)	0.06136 (7)	0.0229 (3)
C2A	0.04550 (17)	0.75365 (13)	0.02073 (8)	0.0297 (3)
H2A	0.1135	0.6864	0.0070	0.036*
C3A	−0.10002 (17)	0.78193 (13)	0.00036 (9)	0.0327 (3)
H3A	−0.1323	0.7335	−0.0258	0.039*
C4A	−0.19930 (17)	0.88140 (13)	0.01816 (8)	0.0317 (3)
H4A	−0.2992	0.9025	0.0032	0.038*
C5A	−0.15057 (17)	0.94796 (13)	0.05740 (9)	0.0322 (3)
H5A	−0.2161	1.0165	0.0700	0.039*
C6A	0.37378 (15)	0.74306 (11)	0.01540 (8)	0.0241 (3)
C7A	0.48306 (19)	0.64332 (13)	0.01373 (9)	0.0373 (4)
H7A	0.5010	0.5990	0.0593	0.045*
C8A	0.5664 (2)	0.60735 (15)	−0.05342 (10)	0.0439 (4)
H8A	0.6412	0.5394	−0.0538	0.053*
C9A	0.53902 (17)	0.67146 (14)	−0.11912 (9)	0.0347 (4)
H9A	0.5930	0.6491	−0.1662	0.042*
C10A	0.43096 (18)	0.76892 (13)	−0.11432 (9)	0.0329 (3)
H10A	0.4119	0.8137	−0.1597	0.039*
C11A	0.29729 (16)	0.89712 (11)	0.11903 (7)	0.0245 (3)
C12A	0.44157 (17)	0.90162 (12)	0.12047 (9)	0.0303 (3)
H12A	0.5224	0.8458	0.0993	0.036*
C13A	0.46768 (18)	0.98624 (13)	0.15223 (9)	0.0344 (4)
H13A	0.5657	0.9881	0.1537	0.041*
C14A	0.34896 (19)	1.06806 (13)	0.18173 (9)	0.0333 (4)
H14A	0.3635	1.1269	0.2041	0.040*
C15A	0.20960 (19)	1.06159 (13)	0.17769 (8)	0.0321 (3)
H15A	0.1275	1.1183	0.1968	0.039*
C16A	0.28432 (15)	0.70924 (11)	0.16449 (7)	0.0217 (3)
C17A	0.42232 (16)	0.66376 (12)	0.19772 (8)	0.0260 (3)
H17A	0.5047	0.6807	0.1751	0.031*
C18A	0.44375 (16)	0.59517 (12)	0.26206 (8)	0.0280 (3)
H18A	0.5399	0.5663	0.2821	0.034*
C19A	0.32753 (17)	0.56749 (12)	0.29811 (8)	0.0265 (3)
C20A	0.18877 (16)	0.61348 (12)	0.26711 (8)	0.0277 (3)
H20A	0.1061	0.5979	0.2907	0.033*
C21A	0.16867 (16)	0.68198 (12)	0.20212 (8)	0.0263 (3)
H21A	0.0722	0.7114	0.1826	0.032*
C22A	0.35210 (18)	0.49543 (13)	0.37173 (8)	0.0325 (4)

C23A	0.3424 (2)	0.56647 (16)	0.43994 (9)	0.0443 (4)
H23E	0.4212	0.5982	0.4337	0.066*
H23D	0.3540	0.5234	0.4882	0.066*
H23F	0.2457	0.6230	0.4413	0.066*
C24A	0.5057 (2)	0.40986 (13)	0.36890 (9)	0.0435 (4)
H24D	0.5180	0.3698	0.3220	0.065*
H24E	0.5154	0.3613	0.4142	0.065*
H24F	0.5821	0.4437	0.3686	0.065*
C25A	0.2352 (3)	0.4417 (2)	0.38433 (14)	0.0840 (10)
H25E	0.1371	0.4959	0.3900	0.126*
H25D	0.2554	0.3956	0.4311	0.126*
H25F	0.2377	0.3989	0.3400	0.126*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
B1	0.0208 (7)	0.0228 (8)	0.0197 (7)	−0.0077 (6)	0.0013 (6)	−0.0039 (6)
N1	0.0231 (6)	0.0247 (6)	0.0217 (5)	−0.0089 (5)	0.0005 (4)	−0.0042 (4)
N2	0.0283 (6)	0.0231 (6)	0.0236 (6)	−0.0084 (5)	0.0010 (5)	−0.0044 (5)
N3	0.0273 (6)	0.0243 (6)	0.0205 (5)	−0.0088 (5)	0.0005 (5)	−0.0038 (4)
C1	0.0245 (7)	0.0183 (7)	0.0225 (6)	−0.0084 (6)	0.0015 (5)	−0.0028 (5)
C2	0.0273 (7)	0.0312 (8)	0.0242 (7)	−0.0120 (7)	0.0022 (6)	−0.0072 (6)
C3	0.0281 (7)	0.0345 (9)	0.0303 (7)	−0.0140 (7)	−0.0023 (6)	−0.0069 (6)
C4	0.0227 (7)	0.0330 (8)	0.0338 (8)	−0.0127 (7)	0.0026 (6)	−0.0051 (6)
C5	0.0258 (7)	0.0295 (8)	0.0259 (7)	−0.0094 (6)	0.0050 (6)	−0.0052 (6)
C6	0.0246 (7)	0.0231 (7)	0.0157 (6)	−0.0084 (6)	−0.0003 (5)	−0.0058 (5)
C7	0.0259 (7)	0.0269 (8)	0.0281 (7)	−0.0094 (6)	0.0017 (6)	−0.0041 (6)
C8	0.0323 (8)	0.0390 (9)	0.0312 (8)	−0.0190 (7)	0.0041 (6)	−0.0015 (6)
C9	0.0440 (9)	0.0284 (8)	0.0308 (8)	−0.0187 (7)	−0.0023 (7)	0.0027 (6)
C10	0.0357 (8)	0.0224 (8)	0.0303 (7)	−0.0083 (7)	−0.0016 (6)	−0.0011 (6)
C11	0.0246 (7)	0.0198 (7)	0.0215 (6)	−0.0101 (6)	0.0011 (5)	−0.0025 (5)
C12	0.0248 (7)	0.0299 (8)	0.0228 (7)	−0.0095 (6)	0.0017 (5)	−0.0052 (6)
C13	0.0249 (7)	0.0336 (8)	0.0288 (7)	−0.0098 (7)	−0.0026 (6)	−0.0013 (6)
C14	0.0343 (8)	0.0329 (8)	0.0211 (7)	−0.0138 (7)	−0.0051 (6)	−0.0012 (6)
C15	0.0332 (8)	0.0296 (8)	0.0202 (6)	−0.0107 (7)	0.0000 (6)	−0.0047 (5)
C16	0.0175 (6)	0.0238 (7)	0.0218 (6)	−0.0081 (6)	0.0000 (5)	−0.0049 (5)
C17	0.0240 (7)	0.0265 (7)	0.0194 (6)	−0.0107 (6)	0.0005 (5)	−0.0026 (5)
C18	0.0247 (7)	0.0216 (7)	0.0265 (7)	−0.0097 (6)	−0.0012 (5)	−0.0018 (5)
C19	0.0181 (6)	0.0245 (7)	0.0246 (7)	−0.0085 (6)	−0.0004 (5)	−0.0064 (5)
C20	0.0193 (6)	0.0272 (7)	0.0189 (6)	−0.0079 (6)	−0.0003 (5)	−0.0039 (5)
C21	0.0204 (6)	0.0211 (7)	0.0230 (6)	−0.0068 (6)	−0.0018 (5)	−0.0022 (5)
C22	0.0286 (7)	0.0234 (7)	0.0263 (7)	−0.0086 (6)	−0.0003 (6)	−0.0073 (6)
C23	0.0519 (11)	0.0401 (10)	0.0519 (10)	−0.0266 (9)	0.0122 (8)	−0.0234 (8)
C24	0.0486 (10)	0.0291 (9)	0.0278 (8)	−0.0047 (8)	0.0000 (7)	−0.0103 (6)
C25	0.0369 (9)	0.0310 (9)	0.0353 (8)	−0.0015 (7)	−0.0018 (7)	−0.0106 (7)
B2	0.0238 (8)	0.0214 (8)	0.0230 (7)	−0.0065 (7)	−0.0005 (6)	−0.0017 (6)
N1A	0.0260 (6)	0.0215 (6)	0.0302 (6)	−0.0057 (5)	0.0034 (5)	−0.0037 (5)
N2A	0.0332 (7)	0.0280 (7)	0.0270 (6)	−0.0093 (6)	0.0026 (5)	−0.0007 (5)
N3A	0.0338 (7)	0.0263 (7)	0.0259 (6)	−0.0129 (6)	0.0071 (5)	−0.0061 (5)
C1A	0.0261 (7)	0.0217 (7)	0.0185 (6)	−0.0051 (6)	0.0012 (5)	0.0004 (5)
C2A	0.0279 (7)	0.0288 (8)	0.0290 (7)	−0.0036 (7)	−0.0031 (6)	−0.0077 (6)
C3A	0.0309 (8)	0.0388 (9)	0.0275 (7)	−0.0089 (7)	−0.0036 (6)	−0.0081 (6)
C4A	0.0243 (7)	0.0383 (9)	0.0280 (7)	−0.0048 (7)	−0.0022 (6)	0.0035 (6)
C5A	0.0269 (8)	0.0272 (8)	0.0372 (8)	−0.0033 (7)	0.0036 (6)	0.0015 (6)
C6A	0.0245 (7)	0.0244 (7)	0.0249 (7)	−0.0097 (6)	−0.0012 (5)	−0.0026 (5)

C7A	0.0413 (9)	0.0317 (9)	0.0293 (8)	0.0000 (8)	0.0011 (7)	−0.0009 (6)
C8A	0.0395 (9)	0.0390 (10)	0.0392 (9)	0.0058 (8)	0.0031 (7)	−0.0085 (7)
C9A	0.0288 (8)	0.0438 (10)	0.0302 (8)	−0.0102 (8)	0.0071 (6)	−0.0112 (7)
C10A	0.0369 (8)	0.0372 (9)	0.0259 (7)	−0.0150 (8)	0.0035 (6)	−0.0009 (6)
C11A	0.0307 (7)	0.0234 (7)	0.0196 (6)	−0.0097 (6)	0.0003 (5)	0.0004 (5)
C12A	0.0301 (8)	0.0265 (8)	0.0339 (8)	−0.0090 (7)	−0.0001 (6)	−0.0023 (6)
C13A	0.0353 (8)	0.0343 (9)	0.0378 (8)	−0.0169 (7)	−0.0035 (7)	−0.0009 (7)
C14A	0.0464 (9)	0.0316 (9)	0.0281 (7)	−0.0210 (8)	0.0018 (7)	−0.0060 (6)
C15A	0.0414 (9)	0.0299 (8)	0.0278 (7)	−0.0161 (7)	0.0105 (6)	−0.0083 (6)
C16A	0.0251 (7)	0.0207 (7)	0.0204 (6)	−0.0084 (6)	−0.0008 (5)	−0.0045 (5)
C17A	0.0232 (7)	0.0305 (8)	0.0260 (7)	−0.0113 (6)	0.0000 (5)	−0.0012 (6)
C18A	0.0258 (7)	0.0322 (8)	0.0275 (7)	−0.0110 (6)	−0.0064 (6)	0.0001 (6)
C19A	0.0329 (8)	0.0286 (8)	0.0221 (7)	−0.0150 (7)	−0.0060 (6)	−0.0002 (6)
C20A	0.0282 (7)	0.0327 (8)	0.0268 (7)	−0.0166 (7)	−0.0023 (6)	0.0015 (6)
C21A	0.0242 (7)	0.0279 (8)	0.0284 (7)	−0.0104 (6)	−0.0053 (6)	0.0002 (6)
C22A	0.0349 (8)	0.0415 (9)	0.0258 (7)	−0.0191 (7)	−0.0097 (6)	0.0084 (6)
C23A	0.0384 (9)	0.0532 (11)	0.0240 (8)	0.0079 (8)	−0.0049 (7)	−0.0002 (7)
C24A	0.0671 (12)	0.0268 (9)	0.0294 (8)	−0.0065 (9)	−0.0028 (8)	0.0034 (6)
C25A	0.0942 (17)	0.125 (2)	0.0683 (14)	−0.0880 (18)	−0.0529 (13)	0.0704 (15)

Geometric parameters (Å, º)

B1—C16	1.628 (2)	B2—C1A	1.635 (2)
B1—C11	1.6380 (19)	B2—C16A	1.6384 (19)
B1—C1	1.6407 (19)	B2—C6A	1.642 (2)
B1—C6	1.6410 (19)	B2—C11A	1.643 (2)
N1—C5	1.3483 (18)	N1A—C1A	1.3402 (19)
N1—C1	1.3491 (18)	N1A—C5A	1.351 (2)
N1—H1	0.8800	N1A—H1A	0.8800
N2—C10	1.3426 (19)	N2A—C10A	1.339 (2)
N2—C6	1.3490 (19)	N2A—C6A	1.3564 (18)
N3—C15	1.3443 (18)	N3A—C15A	1.3487 (19)
N3—C11	1.3539 (18)	N3A—C11A	1.354 (2)
C1—C2	1.4013 (19)	C1A—C2A	1.401 (2)
C2—C3	1.379 (2)	C2A—C3A	1.379 (2)
C2—H2	0.9500	C2A—H2A	0.9500
C3—C4	1.394 (2)	C3A—C4A	1.390 (2)
C3—H3	0.9500	C3A—H3A	0.9500
C4—C5	1.368 (2)	C4A—C5A	1.362 (2)
C4—H4	0.9500	C4A—H4A	0.9500
C5—H5	0.9500	C5A—H5A	0.9500
C6—C7	1.4071 (19)	C6A—C7A	1.393 (2)
C7—C8	1.380 (2)	C7A—C8A	1.390 (2)
C7—H7	0.9500	C7A—H7A	0.9500
C8—C9	1.384 (2)	C8A—C9A	1.371 (2)
C8—H8	0.9500	C8A—H8A	0.9500
C9—C10	1.377 (2)	C9A—C10A	1.369 (2)
C9—H9	0.9500	C9A—H9A	0.9500
C10—H10	0.9500	C10A—H10A	0.9500
C11—C12	1.4014 (19)	C11A—C12A	1.406 (2)
C12—C13	1.384 (2)	C12A—C13A	1.385 (2)
C12—H12	0.9500	C12A—H12A	0.9500
C13—C14	1.385 (2)	C13A—C14A	1.384 (2)
C13—H13	0.9500	C13A—H13A	0.9500
C14—C15	1.375 (2)	C14A—C15A	1.373 (2)

C14—H14	0.9500	C14A—H14A	0.9500
C15—H15	0.9500	C15A—H15A	0.9500
C16—C21	1.3975 (18)	C16A—C21A	1.3959 (19)
C16—C17	1.4053 (19)	C16A—C17A	1.4008 (19)
C17—C18	1.3868 (19)	C17A—C18A	1.384 (2)
C17—H17	0.9500	C17A—H17A	0.9500
C18—C19	1.3984 (19)	C18A—C19A	1.393 (2)
C18—H18	0.9500	C18A—H18A	0.9500
C19—C20	1.392 (2)	C19A—C20A	1.391 (2)
C19—C22	1.5341 (19)	C19A—C22A	1.5373 (19)
C20—C21	1.3897 (19)	C20A—C21A	1.393 (2)
C20—H20	0.9500	C20A—H20A	0.9500
C21—H21	0.9500	C21A—H21A	0.9500
C22—C24	1.526 (2)	C22A—C25A	1.520 (2)
C22—C23	1.531 (2)	C22A—C24A	1.532 (2)
C22—C25	1.539 (2)	C22A—C23A	1.539 (2)
C23—H23A	0.9800	C23A—H23E	0.9800
C23—H23B	0.9800	C23A—H23D	0.9800
C23—H23C	0.9800	C23A—H23F	0.9800
C24—H24A	0.9800	C24A—H24D	0.9800
C24—H24B	0.9800	C24A—H24E	0.9800
C24—H24C	0.9800	C24A—H24F	0.9800
C25—H25A	0.9800	C25A—H25E	0.9800
C25—H25B	0.9800	C25A—H25D	0.9800
C25—H25C	0.9800	C25A—H25F	0.9800

C16—B1—C11	113.47 (11)	C1A—B2—C16A	108.15 (11)
C16—B1—C1	107.77 (10)	C1A—B2—C6A	106.20 (11)
C11—B1—C1	112.97 (11)	C16A—B2—C6A	113.53 (12)
C16—B1—C6	111.13 (11)	C1A—B2—C11A	112.23 (12)
C11—B1—C6	103.92 (10)	C16A—B2—C11A	106.44 (11)
C1—B1—C6	107.42 (11)	C6A—B2—C11A	110.38 (11)
C5—N1—C1	124.52 (12)	C1A—N1A—C5A	125.39 (13)
C5—N1—H1	117.7	C1A—N1A—H1A	117.3
C1—N1—H1	117.7	C5A—N1A—H1A	117.3
C10—N2—C6	118.82 (13)	C10A—N2A—C6A	119.14 (13)
C15—N3—C11	120.12 (12)	C15A—N3A—C11A	120.19 (13)
N1—C1—C2	115.77 (12)	N1A—C1A—C2A	115.51 (13)
N1—C1—B1	120.77 (11)	N1A—C1A—B2	120.56 (12)
C2—C1—B1	123.45 (12)	C2A—C1A—B2	123.91 (13)
C3—C2—C1	121.49 (13)	C3A—C2A—C1A	121.16 (15)
C3—C2—H2	119.3	C3A—C2A—H2A	119.4
C1—C2—H2	119.3	C1A—C2A—H2A	119.4
C2—C3—C4	119.67 (13)	C2A—C3A—C4A	119.85 (15)
C2—C3—H3	120.2	C2A—C3A—H3A	120.1
C4—C3—H3	120.2	C4A—C3A—H3A	120.1
C5—C4—C3	118.36 (13)	C5A—C4A—C3A	118.70 (14)
C5—C4—H4	120.8	C5A—C4A—H4A	120.7
C3—C4—H4	120.8	C3A—C4A—H4A	120.7
N1—C5—C4	120.17 (13)	N1A—C5A—C4A	119.34 (15)
N1—C5—H5	119.9	N1A—C5A—H5A	120.3
C4—C5—H5	119.9	C4A—C5A—H5A	120.3
N2—C6—C7	119.57 (13)	N2A—C6A—C7A	118.62 (13)
N2—C6—B1	119.34 (12)	N2A—C6A—B2	115.44 (12)

C7—C6—B1	121.01 (13)	C7A—C6A—B2	125.91 (13)
C8—C7—C6	120.76 (15)	C8A—C7A—C6A	121.24 (15)
C8—C7—H7	119.6	C8A—C7A—H7A	119.4
C6—C7—H7	119.6	C6A—C7A—H7A	119.4
C7—C8—C9	118.89 (14)	C9A—C8A—C7A	118.98 (16)
C7—C8—H8	120.6	C9A—C8A—H8A	120.5
C9—C8—H8	120.6	C7A—C8A—H8A	120.5
C10—C9—C8	117.70 (14)	C10A—C9A—C8A	117.49 (15)
C10—C9—H9	121.1	C10A—C9A—H9A	121.3
C8—C9—H9	121.1	C8A—C9A—H9A	121.3
N2—C10—C9	124.24 (15)	N2A—C10A—C9A	124.52 (14)
N2—C10—H10	117.9	N2A—C10A—H10A	117.7
C9—C10—H10	117.9	C9A—C10A—H10A	117.7
N3—C11—C12	118.87 (12)	N3A—C11A—C12A	118.46 (13)
N3—C11—B1	117.86 (12)	N3A—C11A—B2	119.10 (12)
C12—C11—B1	122.89 (12)	C12A—C11A—B2	122.27 (13)
C13—C12—C11	120.71 (13)	C13A—C12A—C11A	120.98 (15)
C13—C12—H12	119.6	C13A—C12A—H12A	119.5
C11—C12—H12	119.6	C11A—C12A—H12A	119.5
C12—C13—C14	119.15 (14)	C14A—C13A—C12A	119.09 (14)
C12—C13—H13	120.4	C14A—C13A—H13A	120.5
C14—C13—H13	120.4	C12A—C13A—H13A	120.5
C15—C14—C13	118.04 (13)	C15A—C14A—C13A	118.02 (14)
C15—C14—H14	121.0	C15A—C14A—H14A	121.0
C13—C14—H14	121.0	C13A—C14A—H14A	121.0
N3—C15—C14	123.09 (13)	N3A—C15A—C14A	123.23 (15)
N3—C15—H15	118.5	N3A—C15A—H15A	118.4
C14—C15—H15	118.5	C14A—C15A—H15A	118.4
C21—C16—C17	114.96 (12)	C21A—C16A—C17A	114.93 (12)
C21—C16—B1	121.66 (12)	C21A—C16A—B2	124.18 (12)
C17—C16—B1	123.21 (11)	C17A—C16A—B2	120.80 (12)
C18—C17—C16	122.49 (12)	C18A—C17A—C16A	122.79 (13)
C18—C17—H17	118.8	C18A—C17A—H17A	118.6
C16—C17—H17	118.8	C16A—C17A—H17A	118.6
C17—C18—C19	121.70 (13)	C17A—C18A—C19A	121.48 (13)
C17—C18—H18	119.1	C17A—C18A—H18A	119.3
C19—C18—H18	119.1	C19A—C18A—H18A	119.3
C20—C19—C18	116.43 (12)	C20A—C19A—C18A	116.75 (13)
C20—C19—C22	122.38 (12)	C20A—C19A—C22A	122.49 (13)
C18—C19—C22	121.19 (12)	C18A—C19A—C22A	120.64 (13)
C21—C20—C19	121.51 (12)	C19A—C20A—C21A	121.26 (13)
C21—C20—H20	119.2	C19A—C20A—H20A	119.4
C19—C20—H20	119.2	C21A—C20A—H20A	119.4
C20—C21—C16	122.90 (13)	C20A—C21A—C16A	122.77 (13)
C20—C21—H21	118.6	C20A—C21A—H21A	118.6
C16—C21—H21	118.6	C16A—C21A—H21A	118.6
C24—C22—C23	109.25 (13)	C25A—C22A—C24A	108.94 (17)
C24—C22—C19	111.59 (12)	C25A—C22A—C19A	111.81 (12)
C23—C22—C19	109.97 (12)	C24A—C22A—C19A	111.06 (13)
C24—C22—C25	107.52 (13)	C25A—C22A—C23A	109.03 (17)
C23—C22—C25	109.37 (14)	C24A—C22A—C23A	108.69 (13)
C19—C22—C25	109.09 (11)	C19A—C22A—C23A	107.23 (13)
C22—C23—H23A	109.5	C22A—C23A—H23E	109.5
C22—C23—H23B	109.5	C22A—C23A—H23D	109.5

H23A—C23—H23B	109.5	H23E—C23A—H23D	109.5
C22—C23—H23C	109.5	C22A—C23A—H23F	109.5
H23A—C23—H23C	109.5	H23E—C23A—H23F	109.5
H23B—C23—H23C	109.5	H23D—C23A—H23F	109.5
C22—C24—H24A	109.5	C22A—C24A—H24D	109.5
C22—C24—H24B	109.5	C22A—C24A—H24E	109.5
H24A—C24—H24B	109.5	H24D—C24A—H24E	109.5
C22—C24—H24C	109.5	C22A—C24A—H24F	109.5
H24A—C24—H24C	109.5	H24D—C24A—H24F	109.5
H24B—C24—H24C	109.5	H24E—C24A—H24F	109.5
C22—C25—H25A	109.5	C22A—C25A—H25E	109.5
C22—C25—H25B	109.5	C22A—C25A—H25D	109.5
H25A—C25—H25B	109.5	H25E—C25A—H25D	109.5
C22—C25—H25C	109.5	C22A—C25A—H25F	109.5
H25A—C25—H25C	109.5	H25E—C25A—H25F	109.5
H25B—C25—H25C	109.5	H25D—C25A—H25F	109.5

C5—N1—C1—C2	0.86 (19)	C5A—N1A—C1A—C2A	−1.94 (19)
C5—N1—C1—B1	179.57 (12)	C5A—N1A—C1A—B2	179.76 (12)
C16—B1—C1—N1	145.83 (11)	C16A—B2—C1A—N1A	102.96 (13)
C11—B1—C1—N1	19.60 (16)	C11A—B2—C1A—N1A	−14.10 (16)
C6—B1—C1—N1	−94.35 (13)	C6A—B2—C1A—N1A	−135.00 (12)
C16—B1—C1—C2	−35.57 (16)	C16A—B2—C1A—C2A	−75.20 (15)
C11—B1—C1—C2	−161.80 (12)	C11A—B2—C1A—C2A	167.74 (12)
C6—B1—C1—C2	84.25 (15)	C6A—B2—C1A—C2A	46.85 (16)
N1—C1—C2—C3	−1.4 (2)	N1A—C1A—C2A—C3A	−0.23 (19)
B1—C1—C2—C3	179.98 (12)	B2—C1A—C2A—C3A	178.01 (12)
C1—C2—C3—C4	1.0 (2)	C1A—C2A—C3A—C4A	2.0 (2)
C2—C3—C4—C5	−0.1 (2)	C2A—C3A—C4A—C5A	−1.7 (2)
C1—N1—C5—C4	0.0 (2)	C1A—N1A—C5A—C4A	2.2 (2)
C3—C4—C5—N1	−0.4 (2)	C3A—C4A—C5A—N1A	−0.3 (2)
C10—N2—C6—C7	−0.61 (17)	C10A—N2A—C6A—C7A	0.96 (19)
C10—N2—C6—B1	176.18 (11)	C10A—N2A—C6A—B2	−177.32 (12)
C16—B1—C6—N2	134.30 (11)	C1A—B2—C6A—N2A	54.93 (14)
C11—B1—C6—N2	−103.29 (12)	C16A—B2—C6A—N2A	173.48 (11)
C1—B1—C6—N2	16.62 (14)	C11A—B2—C6A—N2A	−67.02 (14)
C16—B1—C6—C7	−48.95 (14)	C1A—B2—C6A—C7A	−123.20 (14)
C11—B1—C6—C7	73.46 (14)	C16A—B2—C6A—C7A	−4.65 (18)
C1—B1—C6—C7	−166.63 (11)	C11A—B2—C6A—C7A	114.84 (15)
N2—C6—C7—C8	0.79 (19)	N2A—C6A—C7A—C8A	−0.5 (2)
B1—C6—C7—C8	−175.95 (12)	B2—C6A—C7A—C8A	177.55 (14)
C6—C7—C8—C9	−0.1 (2)	C6A—C7A—C8A—C9A	−0.3 (3)
C7—C8—C9—C10	−0.8 (2)	C7A—C8A—C9A—C10A	0.7 (2)
C6—N2—C10—C9	−0.3 (2)	C6A—N2A—C10A—C9A	−0.6 (2)
C8—C9—C10—N2	1.0 (2)	C8A—C9A—C10A—N2A	−0.3 (2)
C15—N3—C11—C12	1.63 (18)	C15A—N3A—C11A—C12A	−0.58 (18)
C15—N3—C11—B1	−171.49 (11)	C15A—N3A—C11A—B2	174.82 (11)
C16—B1—C11—N3	−150.68 (11)	C1A—B2—C11A—N3A	27.39 (15)
C1—B1—C11—N3	−27.57 (15)	C16A—B2—C11A—N3A	−90.62 (13)
C6—B1—C11—N3	88.49 (13)	C6A—B2—C11A—N3A	145.77 (11)
C16—B1—C11—C12	36.48 (16)	C1A—B2—C11A—C12A	−157.38 (12)
C1—B1—C11—C12	159.59 (12)	C16A—B2—C11A—C12A	84.61 (14)
C6—B1—C11—C12	−84.35 (14)	C6A—B2—C11A—C12A	−39.01 (16)
N3—C11—C12—C13	−1.50 (19)	N3A—C11A—C12A—C13A	1.5 (2)

B1—C11—C12—C13	171.26 (12)	B2—C11A—C12A—C13A	−173.80 (12)
C11—C12—C13—C14	0.1 (2)	C11A—C12A—C13A—C14A	−1.0 (2)
C12—C13—C14—C15	1.2 (2)	C12A—C13A—C14A—C15A	−0.3 (2)
C11—N3—C15—C14	−0.3 (2)	C11A—N3A—C15A—C14A	−0.8 (2)
C13—C14—C15—N3	−1.1 (2)	C13A—C14A—C15A—N3A	1.2 (2)
C11—B1—C16—C21	−145.27 (11)	C1A—B2—C16A—C21A	−8.22 (17)
C1—B1—C16—C21	88.82 (13)	C11A—B2—C16A—C21A	112.48 (13)
C6—B1—C16—C21	−28.61 (15)	C6A—B2—C16A—C21A	−125.72 (13)
C11—B1—C16—C17	39.69 (16)	C1A—B2—C16A—C17A	175.23 (12)
C1—B1—C16—C17	−86.21 (13)	C11A—B2—C16A—C17A	−64.07 (16)
C6—B1—C16—C17	156.35 (11)	C6A—B2—C16A—C17A	57.73 (16)
C21—C16—C17—C18	0.75 (17)	C21A—C16A—C17A—C18A	1.3 (2)
B1—C16—C17—C18	176.10 (11)	B2—C16A—C17A—C18A	178.13 (13)
C16—C17—C18—C19	−0.45 (19)	C16A—C17A—C18A—C19A	−0.2 (2)
C17—C18—C19—C20	−0.49 (18)	C17A—C18A—C19A—C20A	−1.2 (2)
C17—C18—C19—C22	178.70 (11)	C17A—C18A—C19A—C22A	−177.10 (14)
C18—C19—C20—C21	1.09 (17)	C18A—C19A—C20A—C21A	1.5 (2)
C22—C19—C20—C21	−178.08 (11)	C22A—C19A—C20A—C21A	177.28 (14)
C19—C20—C21—C16	−0.80 (18)	C17A—C16A—C21A—C20A	−1.0 (2)
C17—C16—C21—C20	−0.14 (17)	B2—C16A—C21A—C20A	−177.74 (13)
B1—C16—C21—C20	−175.56 (11)	C19A—C20A—C21A—C16A	−0.4 (2)
C20—C19—C22—C24	2.44 (17)	C20A—C19A—C22A—C25A	26.1 (2)
C18—C19—C22—C24	−176.69 (12)	C18A—C19A—C22A—C25A	−158.28 (18)
C20—C19—C22—C23	−118.95 (14)	C20A—C19A—C22A—C24A	147.86 (14)
C18—C19—C22—C23	61.92 (16)	C18A—C19A—C22A—C24A	−36.48 (19)
C20—C19—C22—C25	121.06 (13)	C20A—C19A—C22A—C23A	−93.50 (16)
C18—C19—C22—C25	−58.07 (16)	C18A—C19A—C22A—C23A	82.17 (17)

Experimental

Crystal data

$C_{50}H_{50}B_2FeN_6 \cdot C_7H_8$
$M_r = 904.56$
Monoclinic, $C2/c$
$a = 18.0553$ (2) Å
$b = 10.0207$ (1) Å
$c = 26.1009$ (4) Å
$\beta = 105.384$ (1)°
$V = 4553.1$ (1) Å^3
$Z = 4$
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
$\mu = 3.01$ mm^{-1}
$T = 100$ K
0.25 × 0.21 × 0.14 mm

Data collection

Bruker SMART CCD Apex-II area-detector diffractometer
Absorption correction: Numerical *SADABS* (Sheldrick, 2008a)
$T_{min} = 0.520$, $T_{max} = 0.678$
17098 measured reflections
3964 independent reflections
3630 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.090$
$S = 1.05$
3964 reflections
305 parameters
0 restraints
H-atom parameters constrained
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ e Å^{-3}

Data collection: *APEX* 2 (Bruker, 2006); cell refinement: *APEX* 2; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008b); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

References

Bruker (2005). *SAINT* Version 7.23a. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (2006). *APEX 2* Version 2.0-2. Bruker AXS Inc., Madison, Wisconsin, USA.

Sheldrick, G. M. (2008*a*). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (2008*b*). *Acta Cryst.*A**64**, 112—122.

Refinement

All H atoms for (I) were found in electron density difference maps. The methyl H atoms were put in ideally staggered positions with C—H distances of 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C). The aromatic Hs were placed in geometrically idealized positions and constrained to ride on their parent C atoms with distances of 0.95 Å, and U_{iso}(H) = 1.2U_{eq}(C). The toluene methyl group Hs were disordered and were set at 0.50.

(complex2)

Crystal data

$C_{50}H_{50}B_2FeN_6{\cdot}C_7H_8$	F(000) = 1912
M_r = 904.56	D_x = 1.320 Mg m^{-3}
Monoclinic, $C2/c$	Cu $K\alpha$ radiation, λ = 1.54178 Å
Hall symbol: -C 2yc	Cell parameters from 9961 reflections
a = 18.0553 (2) Å	θ = 3.5–66.7°
b = 10.0207 (1) Å	μ = 3.01 mm^{-1}
c = 26.1009 (4) Å	T = 100 K
β = 105.384 (1)°	Parallelepiped, Orange
V = 4553.1 (1) Å^3	0.25 × 0.21 × 0.14 mm
Z = 4	

Data collection

Bruker SMART CCD Apex-II area-detector diffractometer	3964 independent reflections
Radiation source: fine-focus sealed tube	3630 reflections with $I > 2\sigma(I)$
Graphite monochromator	R_{int} = 0.027
φ and ω scans	θ_{max} = 67.3°, θ_{min} = 3.5°
Absorption correction: Numerical *SADABS* (Sheldrick, 2008a)	h = −21→20
T_{min} = 0.520, T_{max} = 0.678	k = 0→11
17098 measured reflections	l = 0→30

Refinement

Refinement on F^2	Primary atom site location: Structure-invariant direct methods
Least-squares matrix: Full	Secondary atom site location: Difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.033	Hydrogen site location: Inferred from neighbouring sites
$wR(F^2)$ = 0.090	H-atom parameters constrained
S = 1.05	$w = 1/[\sigma^2(F_o^2) + (0.0561P)^2 + 3.0717P]$ where $P = (F_o^2 + 2F_c^2)/3$
3964 reflections	$(\Delta/\sigma)_{max} < 0.001$
305 parameters	$\Delta\rho_{max}$ = 0.34 e Å^{-3}
0 restraints	$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Special details

Experimental. 'crystal mounted on a Cryoloop using Paratone-N'

Geometry. 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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR 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 $F^2 > 2\text{sigma}(F^2)$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Fe1	0.2500	0.2500	0.0000	0.01230 (11)	
B1	0.29574 (11)	0.25467 (17)	0.12453 (7)	0.0156 (4)	
N1	0.32916 (7)	0.13486 (13)	0.04708 (5)	0.0147 (3)	
N2	0.29132 (7)	0.40699 (13)	0.04529 (5)	0.0148 (3)	
N3	0.17893 (7)	0.21340 (13)	0.04391 (5)	0.0146 (3)	
C1	0.34755 (9)	0.14898 (15)	0.10092 (6)	0.0155 (3)	
C2	0.41202 (9)	0.08005 (17)	0.13131 (6)	0.0195 (4)	
H2	0.4278	0.0941	0.1686	0.023*	
C3	0.45325 (9)	−0.00744 (17)	0.10872 (7)	0.0215 (4)	
H3	0.4958	−0.0550	0.1301	0.026*	
C4	0.43113 (9)	−0.02437 (16)	0.05399 (7)	0.0199 (4)	
H4	0.4573	−0.0852	0.0370	0.024*	
C5	0.37003 (9)	0.04969 (15)	0.02501 (6)	0.0176 (3)	
H5	0.3558	0.0405	−0.0126	0.021*	
C6	0.31524 (9)	0.39632 (16)	0.09933 (6)	0.0157 (3)	
C7	0.35661 (9)	0.50250 (16)	0.12821 (7)	0.0192 (3)	
H7	0.3768	0.4933	0.1655	0.023*	
C8	0.36899 (9)	0.61990 (17)	0.10427 (7)	0.0209 (4)	
H8	0.3969	0.6911	0.1246	0.025*	
C9	0.33971 (9)	0.63163 (16)	0.04963 (7)	0.0200 (4)	
H9	0.3451	0.7122	0.0318	0.024*	
C10	0.30261 (9)	0.52299 (16)	0.02202 (6)	0.0178 (3)	
H10	0.2839	0.5300	−0.0155	0.021*	
C11	0.20426 (9)	0.22457 (15)	0.09770 (6)	0.0149 (3)	
C12	0.15070 (9)	0.21056 (16)	0.12780 (6)	0.0177 (3)	
H12	0.1675	0.2201	0.1653	0.021*	
C13	0.07428 (9)	0.18328 (16)	0.10419 (7)	0.0191 (4)	
H13	0.0386	0.1756	0.1250	0.023*	
C14	0.05060 (9)	0.16730 (16)	0.04947 (7)	0.0195 (4)	
H14	−0.0012	0.1457	0.0321	0.023*	
C15	0.10411 (9)	0.18362 (15)	0.02102 (6)	0.0169 (3)	
H15	0.0879	0.1736	−0.0165	0.020*	
C16	0.31047 (9)	0.25381 (15)	0.18905 (7)	0.0156 (3)	
C17	0.33116 (9)	0.13966 (16)	0.22066 (6)	0.0175 (3)	
H17	0.3389	0.0586	0.2039	0.021*	
C18	0.34100 (9)	0.13930 (16)	0.27554 (6)	0.0178 (3)	
H18	0.3565	0.0593	0.2949	0.021*	
C19	0.32867 (10)	0.25327 (15)	0.30252 (7)	0.0166 (4)	
C20	0.30269 (9)	0.36549 (16)	0.27123 (6)	0.0182 (3)	
H20	0.2909	0.4443	0.2877	0.022*	
C21	0.29365 (9)	0.36518 (16)	0.21676 (6)	0.0180 (3)	
H21	0.2752	0.4439	0.1973	0.022*	
C22	0.34554 (11)	0.26061 (15)	0.36325 (7)	0.0203 (4)	
C23	0.42465 (11)	0.32689 (19)	0.38481 (7)	0.0308 (4)	
H23A	0.4248	0.4141	0.3678	0.046*	

H23C	0.4644	0.2701	0.3770	0.046*	
H23B	0.4350	0.3387	0.4233	0.046*	
C24	0.28377 (12)	0.34388 (19)	0.37933 (7)	0.0306 (4)	
H24A	0.2327	0.3098	0.3610	0.046*	
H24B	0.2880	0.4373	0.3694	0.046*	
H24C	0.2912	0.3375	0.4178	0.046*	
C25	0.34763 (11)	0.12260 (17)	0.38902 (7)	0.0246 (4)	
H25C	0.3591	0.1326	0.4277	0.037*	
H25B	0.3875	0.0680	0.3801	0.037*	
H25A	0.2976	0.0790	0.3757	0.037*	
C26	0.0000	0.3551 (3)	0.2500	0.0283 (6)	
H26	0.0000	0.4499	0.2500	0.034*	
C27	0.06368 (11)	0.28538 (19)	0.24457 (7)	0.0271 (4)	
H27	0.1078	0.3324	0.2412	0.033*	
C28	0.06313 (10)	0.14713 (18)	0.24408 (7)	0.0237 (4)	
H28	0.1068	0.1005	0.2396	0.028*	
C29	0.0000	0.0749 (2)	0.2500	0.0211 (5)	
C30	0.0000	−0.0759 (3)	0.2500	0.0295 (6)	
H30A	0.0346	−0.1085	0.2295	0.044*	0.50
H30B	−0.0522	−0.1085	0.2339	0.044*	0.50
H30C	0.0175	−0.1085	0.2866	0.044*	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.01448 (19)	0.01202 (19)	0.01032 (19)	−0.00022 (13)	0.00316 (14)	0.00028 (12)
B1	0.0173 (10)	0.0161 (9)	0.0128 (10)	−0.0009 (6)	0.0033 (8)	0.0003 (6)
N1	0.0164 (7)	0.0130 (6)	0.0147 (7)	−0.0004 (5)	0.0040 (5)	0.0004 (5)
N2	0.0156 (6)	0.0148 (7)	0.0143 (7)	−0.0002 (5)	0.0045 (5)	−0.0001 (5)
N3	0.0165 (7)	0.0131 (6)	0.0143 (7)	0.0006 (5)	0.0043 (5)	0.0008 (5)
C1	0.0166 (8)	0.0145 (8)	0.0155 (8)	−0.0038 (6)	0.0043 (6)	0.0011 (6)
C2	0.0192 (8)	0.0240 (9)	0.0154 (8)	0.0000 (7)	0.0046 (7)	0.0022 (6)
C3	0.0187 (8)	0.0218 (9)	0.0233 (9)	0.0042 (7)	0.0046 (7)	0.0065 (7)
C4	0.0216 (8)	0.0154 (8)	0.0247 (9)	0.0015 (6)	0.0096 (7)	−0.0003 (6)
C5	0.0206 (8)	0.0152 (8)	0.0180 (8)	−0.0015 (6)	0.0068 (7)	−0.0010 (6)
C6	0.0142 (8)	0.0182 (8)	0.0154 (8)	0.0016 (6)	0.0053 (6)	0.0001 (6)
C7	0.0187 (8)	0.0231 (9)	0.0159 (8)	−0.0020 (7)	0.0048 (6)	−0.0027 (6)
C8	0.0187 (8)	0.0207 (9)	0.0246 (9)	−0.0047 (7)	0.0080 (7)	−0.0068 (7)
C9	0.0209 (8)	0.0158 (8)	0.0253 (9)	−0.0017 (6)	0.0098 (7)	0.0006 (6)
C10	0.0195 (8)	0.0173 (8)	0.0170 (8)	0.0002 (6)	0.0057 (6)	0.0014 (6)
C11	0.0188 (8)	0.0105 (7)	0.0156 (8)	0.0015 (6)	0.0047 (6)	0.0013 (6)
C12	0.0215 (9)	0.0175 (8)	0.0149 (8)	0.0018 (7)	0.0061 (7)	0.0011 (6)
C13	0.0200 (8)	0.0177 (8)	0.0218 (9)	0.0022 (6)	0.0096 (7)	0.0022 (6)
C14	0.0160 (8)	0.0186 (8)	0.0228 (9)	−0.0001 (6)	0.0033 (7)	0.0010 (6)
C15	0.0181 (8)	0.0160 (8)	0.0153 (8)	−0.0002 (6)	0.0023 (6)	0.0004 (6)
C16	0.0132 (8)	0.0182 (8)	0.0150 (9)	−0.0016 (6)	0.0032 (7)	−0.0007 (6)
C17	0.0202 (8)	0.0155 (8)	0.0174 (8)	−0.0013 (6)	0.0063 (7)	−0.0027 (6)
C18	0.0222 (8)	0.0148 (8)	0.0161 (8)	0.0004 (6)	0.0046 (7)	0.0021 (6)
C19	0.0158 (8)	0.0186 (9)	0.0151 (9)	−0.0029 (6)	0.0037 (7)	−0.0003 (6)
C20	0.0208 (8)	0.0163 (8)	0.0188 (9)	0.0008 (6)	0.0076 (7)	−0.0015 (6)
C21	0.0183 (8)	0.0183 (8)	0.0170 (8)	0.0020 (6)	0.0041 (6)	0.0033 (6)
C22	0.0293 (10)	0.0173 (9)	0.0140 (9)	−0.0008 (6)	0.0051 (7)	−0.0010 (6)
C23	0.0412 (11)	0.0261 (10)	0.0190 (9)	−0.0060 (8)	−0.0025 (8)	−0.0003 (7)
C24	0.0515 (12)	0.0250 (9)	0.0191 (9)	0.0057 (9)	0.0159 (9)	0.0002 (7)
C25	0.0374 (10)	0.0214 (9)	0.0153 (9)	0.0003 (7)	0.0076 (7)	0.0013 (7)

C26	0.0445 (16)	0.0194 (13)	0.0188 (13)	0.000	0.0045 (11)	0.000
C27	0.0324 (11)	0.0269 (9)	0.0212 (9)	−0.0044 (8)	0.0057 (8)	0.0046 (7)
C28	0.0256 (9)	0.0257 (9)	0.0192 (9)	0.0030 (7)	0.0049 (7)	0.0047 (7)
C29	0.0248 (12)	0.0223 (12)	0.0130 (11)	0.000	−0.0007 (9)	0.000
C30	0.0242 (13)	0.0235 (13)	0.0379 (16)	0.000	0.0033 (11)	0.000

Geometric parameters (Å, º)

Fe1—N3^{i}	1.9685 (13)	C14—H14	0.9500
Fe1—N3	1.9685 (13)	C15—H15	0.9500
Fe1—N1	1.9880 (13)	C16—C17	1.402 (2)
Fe1—N1^{i}	1.9881 (13)	C16—C21	1.406 (2)
Fe1—N2	1.9902 (13)	C17—C18	1.396 (2)
Fe1—N2^{i}	1.9903 (13)	C17—H17	0.9500
B1—C16	1.634 (2)	C18—C19	1.390 (2)
B1—C1	1.638 (2)	C18—H18	0.9500
B1—C6	1.641 (2)	C19—C20	1.396 (2)
B1—C11	1.642 (2)	C19—C22	1.534 (2)
N1—C5	1.353 (2)	C20—C21	1.387 (2)
N1—C1	1.363 (2)	C20—H20	0.9500
N2—C10	1.352 (2)	C21—H21	0.9500
N2—C6	1.365 (2)	C22—C25	1.534 (2)
N3—C15	1.357 (2)	C22—C24	1.538 (3)
N3—C11	1.361 (2)	C22—C23	1.540 (3)
C1—C2	1.404 (2)	C23—H23A	0.9800
C2—C3	1.379 (2)	C23—H23C	0.9800
C2—H2	0.9500	C23—H23B	0.9800
C3—C4	1.388 (2)	C24—H24A	0.9800
C3—H3	0.9500	C24—H24B	0.9800
C4—C5	1.377 (2)	C24—H24C	0.9800
C4—H4	0.9500	C25—H25C	0.9800
C5—H5	0.9500	C25—H25B	0.9800
C6—C7	1.400 (2)	C25—H25A	0.9800
C7—C8	1.378 (2)	C26—C27^{ii}	1.384 (2)
C7—H7	0.9500	C26—C27	1.384 (2)
C8—C9	1.388 (2)	C26—H26	0.9500
C8—H8	0.9500	C27—C28	1.385 (3)
C9—C10	1.377 (2)	C27—H27	0.9500
C9—H9	0.9500	C28—C29	1.393 (2)
C10—H10	0.9500	C28—H28	0.9500
C11—C12	1.405 (2)	C29—C28^{ii}	1.393 (2)
C12—C13	1.381 (2)	C29—C30	1.511 (3)
C12—H12	0.9500	C30—H30A	0.9800
C13—C14	1.387 (2)	C30—H30B	0.9800
C13—H13	0.9500	C30—H30C	0.9800
C14—C15	1.376 (2)		

N3^{i}—Fe1—N3	180.0	C14—C13—H13	120.6
N3^{i}—Fe1—N1	89.73 (5)	C15—C14—C13	118.25 (15)
N3—Fe1—N1	90.27 (5)	C15—C14—H14	120.9
N3^{i}—Fe1—N1^{i}	90.27 (5)	C13—C14—H14	120.9
N3—Fe1—N1^{i}	89.73 (5)	N3—C15—C14	123.23 (15)
N1—Fe1—N1^{i}	180.0	N3—C15—H15	118.4
N3^{i}—Fe1—N2	89.94 (5)	C14—C15—H15	118.4
N3—Fe1—N2	90.06 (5)	C17—C16—C21	113.89 (15)

N1—Fe1—N2	89.82 (5)	C17—C16—B1	123.78 (13)
N1^{i}—Fe1—N2	90.18 (5)	C21—C16—B1	121.86 (14)
N3^{i}—Fe1—N2^{i}	90.06 (5)	C18—C17—C16	123.20 (15)
N3—Fe1—N2^{i}	89.94 (5)	C18—C17—H17	118.4
N1—Fe1—N2^{i}	90.18 (5)	C16—C17—H17	118.4
N1^{i}—Fe1—N2^{i}	89.82 (5)	C19—C18—C17	121.59 (15)
N2—Fe1—N2^{i}	180.0	C19—C18—H18	119.2
C16—B1—C1	115.56 (13)	C17—C18—H18	119.2
C16—B1—C6	115.09 (13)	C18—C19—C20	116.06 (15)
C1—B1—C6	101.76 (13)	C18—C19—C22	123.24 (14)
C16—B1—C11	107.99 (13)	C20—C19—C22	120.64 (14)
C1—B1—C11	109.33 (13)	C21—C20—C19	121.85 (15)
C6—B1—C11	106.64 (13)	C21—C20—H20	119.1
C5—N1—C1	119.56 (13)	C19—C20—H20	119.1
C5—N1—Fe1	119.13 (11)	C20—C21—C16	123.11 (15)
C1—N1—Fe1	121.04 (10)	C20—C21—H21	118.4
C10—N2—C6	119.17 (13)	C16—C21—H21	118.4
C10—N2—Fe1	119.35 (11)	C25—C22—C19	112.64 (13)
C6—N2—Fe1	121.18 (10)	C25—C22—C24	107.74 (15)
C15—N3—C11	119.67 (14)	C19—C22—C24	110.39 (14)
C15—N3—Fe1	120.74 (11)	C25—C22—C23	108.42 (15)
C11—N3—Fe1	119.52 (10)	C19—C22—C23	107.99 (14)
N1—C1—C2	118.04 (14)	C24—C22—C23	109.62 (15)
N1—C1—B1	116.61 (13)	C22—C23—H23A	109.5
C2—C1—B1	125.19 (14)	C22—C23—H23C	109.5
C3—C2—C1	122.13 (15)	H23A—C23—H23C	109.5
C3—C2—H2	118.9	C22—C23—H23B	109.5
C1—C2—H2	118.9	H23A—C23—H23B	109.5
C2—C3—C4	118.49 (15)	H23C—C23—H23B	109.5
C2—C3—H3	120.8	C22—C24—H24A	109.5
C4—C3—H3	120.8	C22—C24—H24B	109.5
C5—C4—C3	117.98 (15)	H24A—C24—H24B	109.5
C5—C4—H4	121.0	C22—C24—H24C	109.5
C3—C4—H4	121.0	H24A—C24—H24C	109.5
N1—C5—C4	123.64 (15)	H24B—C24—H24C	109.5
N1—C5—H5	118.2	C22—C25—H25C	109.5
C4—C5—H5	118.2	C22—C25—H25B	109.5
N2—C6—C7	118.30 (14)	H25C—C25—H25B	109.5
N2—C6—B1	116.04 (13)	C22—C25—H25A	109.5
C7—C6—B1	125.59 (14)	H25C—C25—H25A	109.5
C8—C7—C6	122.16 (15)	H25B—C25—H25A	109.5
C8—C7—H7	118.9	C27^{ii}—C26—C27	119.4 (2)
C6—C7—H7	118.9	C27^{ii}—C26—H26	120.3
C7—C8—C9	118.35 (15)	C27—C26—H26	120.3
C7—C8—H8	120.8	C26—C27—C28	120.10 (18)
C9—C8—H8	120.8	C26—C27—H27	119.9
C10—C9—C8	118.06 (15)	C28—C27—H27	119.9
C10—C9—H9	121.0	C27—C28—C29	121.50 (17)
C8—C9—H9	121.0	C27—C28—H28	119.3
N2—C10—C9	123.71 (15)	C29—C28—H28	119.3
N2—C10—H10	118.1	C28^{ii}—C29—C28	117.4 (2)
C9—C10—H10	118.1	C28^{ii}—C29—C30	121.29 (11)
N3—C11—C12	118.41 (14)	C28—C29—C30	121.29 (11)
N3—C11—B1	118.67 (14)	C29—C30—H30A	109.5

C12—C11—B1	122.92 (14)	C29—C30—H30B	109.5
C13—C12—C11	121.63 (15)	H30A—C30—H30B	109.5
C13—C12—H12	119.2	C29—C30—H30C	109.5
C11—C12—H12	119.2	H30A—C30—H30C	109.5
C12—C13—C14	118.75 (15)	H30B—C30—H30C	109.5
C12—C13—H13	120.6		

N3^{i}—Fe1—N1—C5	−42.74 (12)	C16—B1—C6—C7	13.7 (2)
N3—Fe1—N1—C5	137.26 (12)	C1—B1—C6—C7	−112.07 (17)
N1^{i}—Fe1—N1—C5	21 (6)	C11—B1—C6—C7	133.39 (16)
N2—Fe1—N1—C5	−132.69 (12)	N2—C6—C7—C8	4.7 (2)
N2^{i}—Fe1—N1—C5	47.31 (12)	B1—C6—C7—C8	−178.33 (15)
N3^{i}—Fe1—N1—C1	131.28 (12)	C6—C7—C8—C9	−0.5 (2)
N3—Fe1—N1—C1	−48.72 (12)	C7—C8—C9—C10	−2.7 (2)
N1^{i}—Fe1—N1—C1	−165 (6)	C6—N2—C10—C9	2.4 (2)
N2—Fe1—N1—C1	41.34 (12)	Fe1—N2—C10—C9	−171.51 (12)
N2^{i}—Fe1—N1—C1	−138.66 (12)	C8—C9—C10—N2	1.8 (2)
N3^{i}—Fe1—N2—C10	44.60 (12)	C15—N3—C11—C12	−2.8 (2)
N3—Fe1—N2—C10	−135.40 (12)	Fe1—N3—C11—C12	173.96 (11)
N1—Fe1—N2—C10	134.33 (12)	C15—N3—C11—B1	177.56 (13)
N1^{i}—Fe1—N2—C10	−45.67 (12)	Fe1—N3—C11—B1	−5.67 (18)
N2^{i}—Fe1—N2—C10	−32 (10)	C16—B1—C11—N3	−176.59 (13)
N3^{i}—Fe1—N2—C6	−129.14 (12)	C1—B1—C11—N3	−50.10 (18)
N3—Fe1—N2—C6	50.86 (12)	C6—B1—C11—N3	59.19 (17)
N1—Fe1—N2—C6	−39.42 (12)	C16—B1—C11—C12	3.8 (2)
N1^{i}—Fe1—N2—C6	140.59 (12)	C1—B1—C11—C12	130.29 (16)
N2^{i}—Fe1—N2—C6	154 (10)	C6—B1—C11—C12	−120.43 (16)
N3^{i}—Fe1—N3—C15	−150 (12)	N3—C11—C12—C13	1.4 (2)
N1—Fe1—N3—C15	−135.24 (12)	B1—C11—C12—C13	−179.02 (14)
N1^{i}—Fe1—N3—C15	44.76 (12)	C11—C12—C13—C14	1.1 (2)
N2—Fe1—N3—C15	134.94 (12)	C12—C13—C14—C15	−2.0 (2)
N2^{i}—Fe1—N3—C15	−45.06 (12)	C11—N3—C15—C14	1.9 (2)
N3^{i}—Fe1—N3—C11	34 (12)	Fe1—N3—C15—C14	−174.83 (12)
N1—Fe1—N3—C11	48.02 (12)	C13—C14—C15—N3	0.6 (2)
N1^{i}—Fe1—N3—C11	−131.98 (12)	C1—B1—C16—C17	−32.0 (2)
N2—Fe1—N3—C11	−41.80 (12)	C6—B1—C16—C17	−150.28 (15)
N2^{i}—Fe1—N3—C11	138.20 (12)	C11—B1—C16—C17	90.74 (18)
C5—N1—C1—C2	4.0 (2)	C1—B1—C16—C21	156.35 (15)
Fe1—N1—C1—C2	−169.96 (11)	C6—B1—C16—C21	38.1 (2)
C5—N1—C1—B1	179.61 (13)	C11—B1—C16—C21	−80.89 (17)
Fe1—N1—C1—B1	5.62 (18)	C21—C16—C17—C18	−5.5 (2)
C16—B1—C1—N1	171.41 (13)	B1—C16—C17—C18	−177.73 (15)
C6—B1—C1—N1	−63.16 (16)	C16—C17—C18—C19	1.8 (2)
C11—B1—C1—N1	49.36 (18)	C17—C18—C19—C20	2.8 (2)
C16—B1—C1—C2	−13.4 (2)	C17—C18—C19—C22	−174.49 (15)
C6—B1—C1—C2	112.06 (17)	C18—C19—C20—C21	−3.3 (2)
C11—B1—C1—C2	−135.42 (16)	C22—C19—C20—C21	174.04 (15)
N1—C1—C2—C3	−4.6 (2)	C19—C20—C21—C16	−0.7 (3)
B1—C1—C2—C3	−179.78 (15)	C17—C16—C21—C20	5.0 (2)
C1—C2—C3—C4	1.8 (3)	B1—C16—C21—C20	177.36 (15)
C2—C3—C4—C5	1.4 (2)	C18—C19—C22—C25	−21.6 (2)
C1—N1—C5—C4	−0.8 (2)	C20—C19—C22—C25	161.28 (16)
Fe1—N1—C5—C4	173.26 (12)	C18—C19—C22—C24	−142.05 (17)
C3—C4—C5—N1	−2.0 (2)	C20—C19—C22—C24	40.8 (2)

C10—N2—C6—C7	−5.5 (2)	C18—C19—C22—C23	98.12 (18)
Fe1—N2—C6—C7	168.29 (11)	C20—C19—C22—C23	−79.02 (19)
C10—N2—C6—B1	177.25 (14)	C27^{ii}—C26—C27—C28	0.62 (12)
Fe1—N2—C6—B1	−9.00 (18)	C26—C27—C28—C29	−1.3 (2)
C16—B1—C6—N2	−169.26 (13)	C27—C28—C29—C28^{ii}	0.64 (12)
C1—B1—C6—N2	65.00 (16)	C27—C28—C29—C30	−179.36 (12)
C11—B1—C6—N2	−49.53 (17)		

Symmetry codes: (i) −*x*+1/2, −*y*+1/2, −*z*; (ii) −*x*, *y*, −*z*+1/2.

Experimental

Crystal data

$C_{50}H_{50}B_2FeN_6{\cdot}Cl_4Fe$
$M_r = 1010.08$
Orthorhombic, $Pna2_1$
$a = 27.5963$ (5) Å
$b = 12.7473$ (2) Å
$c = 13.6801$ (2) Å
$V = 4812.36$ (14) Å^3
$Z = 4$
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
$\mu = 7.20$ mm^{-1}
$T = 100$ K
0.24 × 0.16 × 0.13 mm

Data collection

Bruker SMART CCD Apex-II area-detector diffractometer
Absorption correction: Numerical *SADABS* (Sheldrick, 2008a)
$T_{min} = 0.277$, $T_{max} = 0.455$
41913 measured reflections
8157 independent reflections
7259 reflections with $I > 2\sigma(I)$
$R_{int} = 0.061$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.084$
$S = 1.02$
8157 reflections
584 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max} = 0.51$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}
Absolute structure: Flack (1983), 3788 Friedel pairs
Flack parameter: 0.685 (3)

Data collection: *APEX* 2 (Bruker, 2006); cell refinement: *APEX* 2; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008b); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

References

Bruker (2005). *SAINT* Version 7.23a. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (2006). *APEX 2* Version 2.0-2. Bruker AXS Inc., Madison, Wisconsin, USA.

Sheldrick, G. M. (2008*a*). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (2008*b*). *Acta Cryst.*A**64**, 112—122.

Refinement

All H atoms for (I) were found in electron density difference maps. The methyl H atoms were put in ideally staggered positions with C—H distances of 0.98 Å and $U_{iso}(H) = 1.5U_{eq}(C)$. The pyridinium and aromatic Hs were placed in geometrically idealized positions and constrained to ride on their parent C or N atoms with distances of 0.88 and 0.95 Å, respectively, and $U_{iso}(H) = 1.2U_{eq}(C)$. This crystal is non-merohedrally twinned. The final refinement resulted in a ratio of 0.685 (3): 0.315 (3) for the two domains, with a final wR2 = 0.084 and R1 = 0.037.

(Complex2+)

Crystal data

$C_{50}H_{50}B_2FeN_6{\cdot}Cl_4Fe$	$F(000) = 2088$
$M_r = 1010.08$	$D_x = 1.394$ Mg m^{-3}
Orthorhombic, $Pna2_1$	Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Hall symbol: P 2c -2n	Cell parameters from 9958 reflections
$a = 27.5963$ (5) Å	$\theta = 3.5–66.8°$
$b = 12.7473$ (2) Å	$\mu = 7.20$ mm^{-1}
$c = 13.6801$ (2) Å	$T = 100$ K
$V = 4812.36$ (14) Å^3	Block, Red purple
$Z = 4$	0.24 × 0.16 × 0.13 mm

Data collection

Bruker SMART CCD Apex-II area-detector diffractometer	8157 independent reflections
Radiation source: fine-focus sealed tube	7259 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.061$
φ and ω scans	$\theta_{max} = 67.5°$, $\theta_{min} = 3.2°$
Absorption correction: Numerical *SADABS* (Sheldrick, 2008a)	$h = -31\rightarrow32$
$T_{min} = 0.277$, $T_{max} = 0.455$	$k = -12\rightarrow14$
41913 measured reflections	$l = -16\rightarrow16$

Refinement

Refinement on F^2	Secondary atom site location: Difference Fourier map
Least-squares matrix: Full	Hydrogen site location: Inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.084$	$w = 1/[\sigma^2(F_o^2) + (0.0459P)^2 + 0.0721P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$
8157 reflections	$\Delta\rho_{max} = 0.51$ e Å^{-3}
584 parameters	$\Delta\rho_{min} = -0.27$ e Å^{-3}
1 restraint	Absolute structure: Flack (1983), 3788 Friedel pairs
Primary atom site location: Structure-invariant direct methods	Flack parameter: 0.685 (3)

Special details

Experimental. 'crystal mounted on a Cryoloop using Paratone-N'

Geometry. 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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR 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 $F^2 > 2\text{sigma}(F^2)$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.879853 (16)	0.73064 (3)	0.61770 (4)	0.01476 (11)
B1	0.92696 (13)	0.6916 (3)	0.4131 (3)	0.0173 (8)
B2	0.83225 (14)	0.7751 (3)	0.8213 (3)	0.0175 (8)
N1	0.85696 (10)	0.6265 (2)	0.5190 (2)	0.0163 (6)
N2	0.88627 (10)	0.8382 (2)	0.5155 (2)	0.0173 (6)
N3	0.94748 (9)	0.6820 (2)	0.59535 (18)	0.0166 (6)
N4	0.90361 (10)	0.8348 (2)	0.7172 (2)	0.0179 (6)
N5	0.87252 (9)	0.6238 (2)	0.7228 (2)	0.0157 (6)
N6	0.81195 (9)	0.7778 (2)	0.63918 (18)	0.0162 (6)
C1	0.88296 (11)	0.6092 (3)	0.4360 (2)	0.0169 (7)
C2	0.87279 (12)	0.5179 (3)	0.3825 (3)	0.0194 (8)
H2A	0.8917	0.5016	0.3265	0.023*
C3	0.83586 (12)	0.4516 (3)	0.4096 (2)	0.0195 (7)
H3A	0.8301	0.3890	0.3739	0.023*
C4	0.80717 (12)	0.4763 (3)	0.4890 (2)	0.0203 (8)
H4A	0.7801	0.4342	0.5062	0.024*
C5	0.81914 (11)	0.5640 (3)	0.5423 (2)	0.0184 (7)
H5A	0.8001	0.5814	0.5978	0.022*
C6	0.90530 (11)	0.8098 (3)	0.4282 (2)	0.0175 (7)
C7	0.90425 (13)	0.8847 (3)	0.3531 (3)	0.0249 (8)
H7A	0.9169	0.8668	0.2907	0.030*
C8	0.88546 (14)	0.9829 (3)	0.3673 (3)	0.0301 (9)
H8A	0.8848	1.0322	0.3153	0.036*
C9	0.86736 (12)	1.0098 (3)	0.4592 (3)	0.0265 (8)
H9A	0.8544	1.0776	0.4714	0.032*
C10	0.86893 (11)	0.9360 (3)	0.5304 (3)	0.0218 (8)
H10A	0.8573	0.9539	0.5936	0.026*
C11	0.96329 (11)	0.6623 (2)	0.5032 (2)	0.0152 (7)
C12	1.00771 (12)	0.6097 (3)	0.4922 (2)	0.0201 (8)
H12A	1.0193	0.5943	0.4283	0.024*
C13	1.03465 (13)	0.5802 (3)	0.5717 (3)	0.0245 (8)
H13A	1.0641	0.5426	0.5632	0.029*
C14	1.01851 (12)	0.6058 (3)	0.6648 (3)	0.0235 (8)
H14A	1.0372	0.5890	0.7209	0.028*
C15	0.97513 (12)	0.6556 (3)	0.6732 (3)	0.0196 (7)
H15A	0.9637	0.6727	0.7368	0.024*
C16	0.95140 (12)	0.6869 (3)	0.3061 (2)	0.0187 (7)
C17	0.92612 (12)	0.6665 (3)	0.2203 (3)	0.0210 (8)
H17A	0.8939	0.6405	0.2252	0.025*
C18	0.94563 (11)	0.6822 (2)	0.1276 (3)	0.0210 (7)
H18A	0.9267	0.6655	0.0717	0.025*

C19	0.99226 (11)	0.7218 (2)	0.1150 (3)	0.0200 (6)
C20	1.01781 (13)	0.7457 (3)	0.2002 (3)	0.0194 (8)
H20A	1.0496	0.7737	0.1951	0.023*
C21	0.99775 (12)	0.7296 (3)	0.2923 (3)	0.0214 (8)
H21A	1.0162	0.7483	0.3483	0.026*
C22	1.01508 (13)	0.7436 (3)	0.0154 (3)	0.0229 (8)
C23	0.98264 (16)	0.7079 (3)	−0.0690 (3)	0.0390 (11)
H23A	0.9510	0.7423	−0.0637	0.058*
H23B	0.9784	0.6316	−0.0659	0.058*
H23C	0.9978	0.7269	−0.1313	0.058*
C24	1.02401 (16)	0.8608 (3)	0.0043 (3)	0.0353 (10)
H24A	1.0464	0.8845	0.0554	0.053*
H24B	0.9932	0.8986	0.0105	0.053*
H24C	1.0381	0.8748	−0.0601	0.053*
C25	1.06326 (14)	0.6849 (3)	0.0076 (3)	0.0381 (10)
H25A	1.0574	0.6092	0.0119	0.057*
H25B	1.0847	0.7066	0.0611	0.057*
H25C	1.0786	0.7013	−0.0552	0.057*
C1A	0.87789 (12)	0.8539 (3)	0.7997 (2)	0.0168 (7)
C2A	0.88940 (13)	0.9421 (3)	0.8555 (3)	0.0216 (8)
H2B	0.8695	0.9605	0.9096	0.026*
C3A	0.92941 (13)	1.0032 (3)	0.8333 (3)	0.0246 (8)
H3B	0.9374	1.0624	0.8723	0.030*
C4A	0.95759 (12)	0.9766 (3)	0.7533 (2)	0.0211 (8)
H4B	0.9862	1.0149	0.7382	0.025*
C5A	0.94326 (11)	0.8934 (3)	0.6964 (2)	0.0189 (7)
H5B	0.9619	0.8763	0.6403	0.023*
C6A	0.85286 (12)	0.6556 (3)	0.8090 (2)	0.0174 (7)
C7A	0.85246 (12)	0.5814 (3)	0.8854 (2)	0.0208 (8)
H7B	0.8390	0.6007	0.9467	0.025*
C8A	0.87079 (12)	0.4830 (3)	0.8741 (3)	0.0228 (8)
H8B	0.8706	0.4349	0.9272	0.027*
C9A	0.88981 (12)	0.4534 (3)	0.7841 (3)	0.0230 (8)
H9B	0.9027	0.3851	0.7740	0.028*
C10A	0.88933 (11)	0.5264 (3)	0.7101 (3)	0.0192 (7)
H10B	0.9014	0.5068	0.6476	0.023*
C11A	0.79689 (12)	0.8034 (2)	0.7304 (2)	0.0170 (7)
C12A	0.75406 (12)	0.8609 (2)	0.7402 (3)	0.0211 (7)
H12B	0.7441	0.8835	0.8033	0.025*
C13A	0.72595 (12)	0.8853 (3)	0.6598 (3)	0.0233 (8)
H13B	0.6970	0.9246	0.6675	0.028*
C14A	0.74041 (12)	0.8519 (3)	0.5680 (3)	0.0224 (8)
H14B	0.7209	0.8648	0.5120	0.027*
C15A	0.78390 (12)	0.7996 (3)	0.5604 (2)	0.0189 (7)
H15B	0.7947	0.7780	0.4975	0.023*
C16A	0.80600 (11)	0.7799 (3)	0.9273 (2)	0.0186 (7)
C17A	0.75996 (12)	0.7346 (3)	0.9394 (3)	0.0196 (8)
H17B	0.7427	0.7131	0.8827	0.023*
C18A	0.73855 (13)	0.7198 (3)	1.0302 (3)	0.0221 (8)
H18B	0.7073	0.6887	1.0339	0.027*
C19A	0.76189 (11)	0.7496 (2)	1.1156 (3)	0.0209 (7)
C20A	0.80753 (11)	0.7934 (2)	1.1056 (3)	0.0210 (7)
H20B	0.8246	0.8147	1.1625	0.025*
C21A	0.82900 (12)	0.8070 (3)	1.0152 (2)	0.0214 (8)

H21B	0.8607	0.8359	1.0125	0.026*
C22A	0.73864 (13)	0.7364 (3)	1.2178 (3)	0.0230 (8)
C23A	0.68974 (15)	0.6810 (4)	1.2128 (3)	0.0445 (11)
H23D	0.6766	0.6735	1.2790	0.067*
H23E	0.6939	0.6115	1.1834	0.067*
H23F	0.6673	0.7225	1.1729	0.067*
C24A	0.77215 (15)	0.6721 (3)	1.2838 (3)	0.0336 (9)
H24D	0.7760	0.6015	1.2565	0.050*
H24E	0.7580	0.6672	1.3493	0.050*
H24F	0.8039	0.7064	1.2878	0.050*
C25A	0.73205 (15)	0.8460 (3)	1.2634 (3)	0.0352 (10)
H25D	0.7637	0.8804	1.2693	0.053*
H25E	0.7174	0.8390	1.3283	0.053*
H25F	0.7109	0.8883	1.2215	0.053*
Fe2	0.631028 (17)	0.64613 (4)	0.61657 (5)	0.02128 (12)
Cl1	0.61674 (3)	0.75420 (7)	0.73878 (7)	0.0323 (2)
Cl2	0.70196 (3)	0.57666 (7)	0.64372 (9)	0.0459 (3)
Cl3	0.62864 (4)	0.72542 (8)	0.47430 (7)	0.0376 (3)
Cl4	0.57539 (3)	0.52317 (7)	0.61511 (8)	0.0327 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0165 (2)	0.0161 (3)	0.0117 (2)	−0.00003 (17)	0.0011 (3)	−0.0006 (3)
B1	0.019 (2)	0.020 (2)	0.013 (2)	−0.0011 (15)	0.0004 (16)	−0.0005 (15)
B2	0.020 (2)	0.020 (2)	0.013 (2)	0.0027 (15)	−0.0005 (16)	−0.0014 (15)
N1	0.0172 (15)	0.0167 (16)	0.0151 (16)	0.0036 (11)	0.0002 (12)	−0.0047 (11)
N2	0.0195 (16)	0.0163 (17)	0.0160 (16)	0.0001 (11)	−0.0003 (12)	0.0000 (11)
N3	0.0168 (14)	0.0214 (16)	0.0116 (16)	−0.0007 (10)	0.0000 (11)	0.0000 (10)
N4	0.0168 (16)	0.0237 (17)	0.0132 (15)	0.0011 (11)	−0.0009 (12)	−0.0063 (11)
N5	0.0134 (15)	0.0171 (16)	0.0167 (16)	−0.0006 (10)	−0.0007 (12)	0.0019 (11)
N6	0.0173 (14)	0.0173 (15)	0.0141 (16)	−0.0014 (10)	0.0011 (11)	0.0005 (11)
C1	0.0140 (17)	0.022 (2)	0.0150 (18)	0.0032 (13)	−0.0025 (14)	−0.0012 (14)
C2	0.0183 (19)	0.026 (2)	0.0143 (19)	0.0049 (14)	0.0005 (14)	−0.0014 (14)
C3	0.023 (2)	0.0162 (19)	0.0192 (19)	0.0001 (13)	−0.0074 (15)	−0.0018 (14)
C4	0.0196 (19)	0.024 (2)	0.0172 (19)	−0.0015 (13)	−0.0013 (14)	−0.0011 (14)
C5	0.0144 (17)	0.026 (2)	0.0147 (17)	−0.0005 (14)	0.0018 (14)	0.0018 (13)
C6	0.0152 (18)	0.0208 (19)	0.0165 (19)	−0.0015 (13)	−0.0012 (14)	0.0016 (13)
C7	0.029 (2)	0.033 (2)	0.0135 (19)	0.0052 (16)	0.0039 (16)	0.0012 (15)
C8	0.039 (2)	0.022 (2)	0.029 (2)	0.0060 (17)	0.0022 (18)	0.0066 (17)
C9	0.028 (2)	0.022 (2)	0.029 (2)	0.0040 (15)	0.0013 (17)	0.0005 (15)
C10	0.0187 (19)	0.024 (2)	0.023 (2)	0.0019 (14)	0.0035 (15)	−0.0041 (14)
C11	0.0156 (18)	0.0174 (19)	0.0127 (18)	−0.0035 (13)	0.0010 (14)	0.0012 (13)
C12	0.0229 (19)	0.022 (2)	0.0152 (19)	−0.0003 (14)	0.0057 (14)	−0.0013 (14)
C13	0.023 (2)	0.025 (2)	0.026 (2)	0.0023 (14)	0.0024 (17)	0.0034 (16)
C14	0.023 (2)	0.030 (2)	0.017 (2)	−0.0007 (15)	−0.0051 (16)	0.0035 (15)
C15	0.026 (2)	0.021 (2)	0.0116 (18)	−0.0008 (14)	−0.0007 (15)	−0.0014 (13)
C16	0.0180 (18)	0.020 (2)	0.0178 (19)	0.0030 (14)	0.0022 (14)	−0.0030 (13)
C17	0.0190 (18)	0.022 (2)	0.022 (2)	0.0007 (13)	−0.0010 (15)	−0.0032 (14)
C18	0.0225 (17)	0.0241 (18)	0.0163 (19)	0.0008 (12)	−0.0003 (16)	−0.0012 (16)
C19	0.0252 (17)	0.0183 (17)	0.0166 (17)	0.0056 (12)	0.0003 (18)	−0.0007 (16)
C20	0.0208 (19)	0.017 (2)	0.021 (2)	−0.0004 (14)	0.0031 (15)	0.0008 (14)
C21	0.026 (2)	0.022 (2)	0.017 (2)	0.0005 (14)	−0.0034 (16)	−0.0034 (14)
C22	0.027 (2)	0.024 (2)	0.017 (2)	0.0001 (15)	0.0058 (16)	0.0000 (15)
C23	0.055 (3)	0.052 (3)	0.011 (2)	−0.011 (2)	0.0019 (19)	0.0029 (17)

C24	0.052 (3)	0.034 (2)	0.020 (2)	−0.0010 (18)	0.0102 (19)	0.0060 (16)
C25	0.042 (3)	0.049 (3)	0.023 (2)	0.0176 (19)	0.0135 (18)	0.0100 (18)
C1A	0.0180 (19)	0.0174 (19)	0.0150 (19)	0.0011 (13)	−0.0008 (14)	0.0021 (13)
C2A	0.025 (2)	0.023 (2)	0.016 (2)	−0.0012 (15)	0.0046 (15)	0.0001 (15)
C3A	0.034 (2)	0.022 (2)	0.0183 (19)	−0.0035 (15)	−0.0010 (16)	−0.0065 (14)
C4A	0.0200 (19)	0.022 (2)	0.021 (2)	−0.0048 (14)	0.0005 (15)	0.0021 (14)
C5A	0.0176 (18)	0.023 (2)	0.0161 (18)	−0.0017 (13)	0.0056 (14)	0.0012 (13)
C6A	0.0156 (18)	0.023 (2)	0.0139 (18)	−0.0053 (13)	−0.0023 (14)	−0.0027 (13)
C7A	0.0222 (19)	0.024 (2)	0.016 (2)	−0.0010 (14)	0.0006 (15)	0.0013 (14)
C8A	0.029 (2)	0.022 (2)	0.017 (2)	−0.0011 (15)	−0.0046 (16)	0.0079 (15)
C9A	0.0222 (19)	0.019 (2)	0.028 (2)	0.0000 (13)	−0.0034 (16)	0.0013 (15)
C10A	0.0202 (18)	0.018 (2)	0.019 (2)	−0.0002 (13)	−0.0005 (15)	−0.0045 (13)
C11A	0.0194 (18)	0.0176 (19)	0.0141 (18)	−0.0017 (12)	0.0040 (15)	0.0009 (13)
C12A	0.0227 (19)	0.0203 (19)	0.0201 (19)	−0.0013 (13)	0.0016 (15)	−0.0048 (15)
C13A	0.0200 (19)	0.020 (2)	0.030 (2)	0.0043 (14)	0.0042 (16)	−0.0003 (15)
C14A	0.0171 (19)	0.029 (2)	0.021 (2)	0.0021 (14)	−0.0040 (15)	0.0055 (15)
C15A	0.026 (2)	0.019 (2)	0.0120 (19)	−0.0009 (14)	0.0003 (15)	0.0005 (14)
C16A	0.0174 (18)	0.023 (2)	0.0154 (19)	0.0029 (13)	0.0028 (14)	−0.0009 (14)
C17A	0.0229 (19)	0.018 (2)	0.018 (2)	−0.0001 (13)	−0.0016 (15)	−0.0030 (13)
C18A	0.022 (2)	0.025 (2)	0.019 (2)	−0.0009 (14)	0.0021 (15)	0.0020 (14)
C19A	0.0244 (17)	0.0209 (18)	0.0173 (18)	0.0035 (11)	0.0044 (18)	−0.0019 (17)
C20A	0.0256 (18)	0.0222 (19)	0.0152 (18)	0.0027 (12)	−0.0001 (16)	−0.0016 (14)
C21A	0.024 (2)	0.021 (2)	0.0194 (19)	−0.0031 (14)	0.0039 (15)	−0.0018 (14)
C22A	0.024 (2)	0.031 (2)	0.014 (2)	0.0003 (15)	0.0031 (16)	0.0019 (15)
C23A	0.039 (3)	0.070 (3)	0.024 (2)	−0.015 (2)	0.0089 (19)	0.006 (2)
C24A	0.047 (3)	0.031 (2)	0.022 (2)	0.0045 (18)	0.0012 (19)	0.0050 (16)
C25A	0.046 (3)	0.041 (3)	0.018 (2)	0.0126 (18)	0.0126 (18)	0.0025 (16)
Fe2	0.0253 (3)	0.0178 (3)	0.0208 (3)	−0.00041 (18)	0.0044 (3)	−0.0009 (3)
Cl1	0.0375 (6)	0.0324 (6)	0.0270 (5)	0.0032 (4)	−0.0005 (4)	−0.0117 (4)
Cl2	0.0274 (5)	0.0316 (6)	0.0788 (9)	0.0073 (4)	0.0131 (5)	0.0114 (5)
Cl3	0.0619 (7)	0.0281 (6)	0.0227 (5)	−0.0110 (4)	0.0036 (5)	0.0042 (4)
Cl4	0.0384 (5)	0.0363 (5)	0.0235 (4)	−0.0159 (3)	0.0030 (5)	−0.0013 (4)

Geometric parameters (Å, º)

Fe1—N2	1.966 (3)	C22—C25	1.530 (5)
Fe1—N6	1.990 (2)	C22—C23	1.530 (5)
Fe1—N3	1.990 (3)	C23—H23A	0.9800
Fe1—N5	1.991 (3)	C23—H23B	0.9800
Fe1—N1	1.996 (3)	C23—H23C	0.9800
Fe1—N4	2.011 (3)	C24—H24A	0.9800
B1—C16	1.613 (5)	C24—H24B	0.9800
B1—C11	1.632 (5)	C24—H24C	0.9800
B1—C6	1.633 (5)	C25—H25A	0.9800
B1—C1	1.636 (5)	C25—H25B	0.9800
B2—C16A	1.621 (5)	C25—H25C	0.9800
B2—C11A	1.622 (5)	C1A—C2A	1.396 (5)
B2—C6A	1.635 (5)	C2A—C3A	1.385 (5)
B2—C1A	1.637 (5)	C2A—H2B	0.9500
N1—C5	1.351 (4)	C3A—C4A	1.385 (5)
N1—C1	1.361 (4)	C3A—H3B	0.9500
N2—C10	1.351 (4)	C4A—C5A	1.373 (5)
N2—C6	1.354 (4)	C4A—H4B	0.9500
N3—C15	1.353 (4)	C5A—H5B	0.9500
N3—C11	1.357 (4)	C6A—C7A	1.410 (5)

N4—C5A	1.355 (4)	C7A—C8A	1.361 (5)
N4—C1A	1.356 (4)	C7A—H7B	0.9500
N5—C10A	1.337 (4)	C8A—C9A	1.391 (5)
N5—C6A	1.360 (4)	C8A—H8B	0.9500
N6—C11A	1.355 (4)	C9A—C10A	1.375 (5)
N6—C15A	1.356 (4)	C9A—H9B	0.9500
C1—C2	1.404 (5)	C10A—H10B	0.9500
C2—C3	1.375 (5)	C11A—C12A	1.397 (4)
C2—H2A	0.9500	C12A—C13A	1.381 (5)
C3—C4	1.381 (5)	C12A—H12B	0.9500
C3—H3A	0.9500	C13A—C14A	1.385 (5)
C4—C5	1.375 (5)	C13A—H13B	0.9500
C4—H4A	0.9500	C14A—C15A	1.377 (5)
C5—H5A	0.9500	C14A—H14B	0.9500
C6—C7	1.404 (5)	C15A—H15B	0.9500
C7—C8	1.369 (5)	C16A—C21A	1.404 (5)
C7—H7A	0.9500	C16A—C17A	1.405 (4)
C8—C9	1.395 (5)	C17A—C18A	1.389 (5)
C8—H8A	0.9500	C17A—H17B	0.9500
C9—C10	1.354 (5)	C18A—C19A	1.388 (5)
C9—H9A	0.9500	C18A—H18B	0.9500
C10—H10A	0.9500	C19A—C20A	1.384 (4)
C11—C12	1.406 (5)	C19A—C22A	1.547 (5)
C12—C13	1.370 (5)	C20A—C21A	1.381 (5)
C12—H12A	0.9500	C20A—H20B	0.9500
C13—C14	1.388 (5)	C21A—H21B	0.9500
C13—H13A	0.9500	C22A—C23A	1.524 (5)
C14—C15	1.360 (5)	C22A—C24A	1.531 (5)
C14—H14A	0.9500	C22A—C25A	1.541 (5)
C15—H15A	0.9500	C23A—H23D	0.9800
C16—C17	1.390 (5)	C23A—H23E	0.9800
C16—C21	1.403 (5)	C23A—H23F	0.9800
C17—C18	1.393 (5)	C24A—H24D	0.9800
C17—H17A	0.9500	C24A—H24E	0.9800
C18—C19	1.393 (4)	C24A—H24F	0.9800
C18—H18A	0.9500	C25A—H25D	0.9800
C19—C20	1.395 (5)	C25A—H25E	0.9800
C19—C22	1.527 (5)	C25A—H25F	0.9800
C20—C21	1.392 (5)	Fe2—Cl2	2.1804 (10)
C20—H20A	0.9500	Fe2—Cl3	2.1941 (12)
C21—H21A	0.9500	Fe2—Cl4	2.1943 (9)
C22—C24	1.521 (5)	Fe2—Cl1	2.2018 (11)

N2—Fe1—N6	88.80 (11)	C25—C22—C23	108.1 (3)
N2—Fe1—N3	91.35 (11)	C22—C23—H23A	109.5
N6—Fe1—N3	179.32 (11)	C22—C23—H23B	109.5
N2—Fe1—N5	178.81 (13)	H23A—C23—H23B	109.5
N6—Fe1—N5	90.25 (10)	C22—C23—H23C	109.5
N3—Fe1—N5	89.60 (11)	H23A—C23—H23C	109.5
N2—Fe1—N1	90.65 (12)	H23B—C23—H23C	109.5
N6—Fe1—N1	90.16 (11)	C22—C24—H24A	109.5
N3—Fe1—N1	89.18 (11)	C22—C24—H24B	109.5
N5—Fe1—N1	90.07 (11)	H24A—C24—H24B	109.5
N2—Fe1—N4	89.49 (11)	C22—C24—H24C	109.5

N6—Fe1—N4	90.44 (11)	H24A—C24—H24C	109.5
N3—Fe1—N4	90.23 (11)	H24B—C24—H24C	109.5
N5—Fe1—N4	89.81 (12)	C22—C25—H25A	109.5
N1—Fe1—N4	179.39 (12)	C22—C25—H25B	109.5
C16—B1—C11	114.8 (3)	H25A—C25—H25B	109.5
C16—B1—C6	107.6 (3)	C22—C25—H25C	109.5
C11—B1—C6	109.9 (3)	H25A—C25—H25C	109.5
C16—B1—C1	117.4 (3)	H25B—C25—H25C	109.5
C11—B1—C1	99.4 (3)	N4—C1A—C2A	118.7 (3)
C6—B1—C1	107.3 (3)	N4—C1A—B2	116.3 (3)
C16A—B2—C11A	114.1 (3)	C2A—C1A—B2	124.8 (3)
C16A—B2—C6A	106.4 (3)	C3A—C2A—C1A	121.0 (3)
C11A—B2—C6A	109.7 (3)	C3A—C2A—H2B	119.5
C16A—B2—C1A	118.8 (3)	C1A—C2A—H2B	119.5
C11A—B2—C1A	100.8 (3)	C4A—C3A—C2A	118.9 (3)
C6A—B2—C1A	106.6 (3)	C4A—C3A—H3B	120.5
C5—N1—C1	120.6 (3)	C2A—C3A—H3B	120.5
C5—N1—Fe1	118.5 (2)	C5A—C4A—C3A	118.4 (3)
C1—N1—Fe1	120.3 (2)	C5A—C4A—H4B	120.8
C10—N2—C6	121.1 (3)	C3A—C4A—H4B	120.8
C10—N2—Fe1	120.4 (2)	N4—C5A—C4A	122.7 (3)
C6—N2—Fe1	118.4 (2)	N4—C5A—H5B	118.7
C15—N3—C11	120.3 (3)	C4A—C5A—H5B	118.7
C15—N3—Fe1	119.0 (2)	N5—C6A—C7A	116.5 (3)
C11—N3—Fe1	120.1 (2)	N5—C6A—B2	120.4 (3)
C5A—N4—C1A	119.9 (3)	C7A—C6A—B2	123.1 (3)
C5A—N4—Fe1	119.1 (2)	C8A—C7A—C6A	122.1 (3)
C1A—N4—Fe1	120.7 (2)	C8A—C7A—H7B	118.9
C10A—N5—C6A	121.9 (3)	C6A—C7A—H7B	118.9
C10A—N5—Fe1	120.4 (2)	C7A—C8A—C9A	119.3 (3)
C6A—N5—Fe1	117.5 (2)	C7A—C8A—H8B	120.3
C11A—N6—C15A	120.5 (3)	C9A—C8A—H8B	120.3
C11A—N6—Fe1	119.9 (2)	C10A—C9A—C8A	117.7 (3)
C15A—N6—Fe1	118.8 (2)	C10A—C9A—H9B	121.1
N1—C1—C2	117.7 (3)	C8A—C9A—H9B	121.1
N1—C1—B1	116.5 (3)	N5—C10A—C9A	122.4 (3)
C2—C1—B1	125.5 (3)	N5—C10A—H10B	118.8
C3—C2—C1	121.1 (3)	C9A—C10A—H10B	118.8
C3—C2—H2A	119.5	N6—C11A—C12A	118.3 (3)
C1—C2—H2A	119.5	N6—C11A—B2	117.9 (3)
C2—C3—C4	119.8 (3)	C12A—C11A—B2	123.5 (3)
C2—C3—H3A	120.1	C13A—C12A—C11A	121.1 (3)
C4—C3—H3A	120.1	C13A—C12A—H12B	119.4
C5—C4—C3	117.7 (3)	C11A—C12A—H12B	119.4
C5—C4—H4A	121.1	C12A—C13A—C14A	119.4 (3)
C3—C4—H4A	121.1	C12A—C13A—H13B	120.3
N1—C5—C4	122.7 (3)	C14A—C13A—H13B	120.3
N1—C5—H5A	118.7	C15A—C14A—C13A	117.9 (3)
C4—C5—H5A	118.7	C15A—C14A—H14B	121.0
N2—C6—C7	117.1 (3)	C13A—C14A—H14B	121.0
N2—C6—B1	120.0 (3)	N6—C15A—C14A	122.4 (3)
C7—C6—B1	122.8 (3)	N6—C15A—H15B	118.8
C8—C7—C6	121.7 (3)	C14A—C15A—H15B	118.8
C8—C7—H7A	119.1	C21A—C16A—C17A	114.1 (3)

C6—C7—H7A	119.1	C21A—C16A—B2	125.0 (3)
C7—C8—C9	119.2 (3)	C17A—C16A—B2	119.6 (3)
C7—C8—H8A	120.4	C18A—C17A—C16A	123.1 (3)
C9—C8—H8A	120.4	C18A—C17A—H17B	118.5
C10—C9—C8	117.7 (3)	C16A—C17A—H17B	118.5
C10—C9—H9A	121.1	C19A—C18A—C17A	121.3 (3)
C8—C9—H9A	121.1	C19A—C18A—H18B	119.4
N2—C10—C9	123.0 (3)	C17A—C18A—H18B	119.4
N2—C10—H10A	118.5	C20A—C19A—C18A	116.7 (4)
C9—C10—H10A	118.5	C20A—C19A—C22A	120.7 (3)
N3—C11—C12	117.9 (3)	C18A—C19A—C22A	122.6 (3)
N3—C11—B1	117.5 (3)	C21A—C20A—C19A	122.0 (3)
C12—C11—B1	124.3 (3)	C21A—C20A—H20B	119.0
C13—C12—C11	121.2 (3)	C19A—C20A—H20B	119.0
C13—C12—H12A	119.4	C20A—C21A—C16A	122.8 (3)
C11—C12—H12A	119.4	C20A—C21A—H21B	118.6
C12—C13—C14	119.3 (3)	C16A—C21A—H21B	118.6
C12—C13—H13A	120.3	C23A—C22A—C24A	108.3 (3)
C14—C13—H13A	120.3	C23A—C22A—C25A	109.5 (3)
C15—C14—C13	118.1 (3)	C24A—C22A—C25A	108.5 (3)
C15—C14—H14A	121.0	C23A—C22A—C19A	112.2 (3)
C13—C14—H14A	121.0	C24A—C22A—C19A	109.9 (3)
N3—C15—C14	123.1 (3)	C25A—C22A—C19A	108.4 (3)
N3—C15—H15A	118.5	C22A—C23A—H23D	109.5
C14—C15—H15A	118.5	C22A—C23A—H23E	109.5
C17—C16—C21	114.6 (3)	H23D—C23A—H23E	109.5
C17—C16—B1	124.3 (3)	C22A—C23A—H23F	109.5
C21—C16—B1	119.3 (3)	H23D—C23A—H23F	109.5
C16—C17—C18	123.2 (3)	H23E—C23A—H23F	109.5
C16—C17—H17A	118.4	C22A—C24A—H24D	109.5
C18—C17—H17A	118.4	C22A—C24A—H24E	109.5
C19—C18—C17	121.4 (3)	H24D—C24A—H24E	109.5
C19—C18—H18A	119.3	C22A—C24A—H24F	109.5
C17—C18—H18A	119.3	H24D—C24A—H24F	109.5
C18—C19—C20	116.3 (4)	H24E—C24A—H24F	109.5
C18—C19—C22	123.9 (3)	C22A—C25A—H25D	109.5
C20—C19—C22	119.8 (3)	C22A—C25A—H25E	109.5
C21—C20—C19	121.5 (3)	H25D—C25A—H25E	109.5
C21—C20—H20A	119.2	C22A—C25A—H25F	109.5
C19—C20—H20A	119.2	H25D—C25A—H25F	109.5
C20—C21—C16	122.8 (3)	H25E—C25A—H25F	109.5
C20—C21—H21A	118.6	Cl2—Fe2—Cl3	111.42 (5)
C16—C21—H21A	118.6	Cl2—Fe2—Cl4	109.86 (4)
C24—C22—C19	109.6 (3)	Cl3—Fe2—Cl4	107.46 (5)
C24—C22—C25	109.4 (3)	Cl2—Fe2—Cl1	106.59 (5)
C19—C22—C25	109.4 (3)	Cl3—Fe2—Cl1	112.33 (5)
C24—C22—C23	108.2 (3)	Cl4—Fe2—Cl1	109.18 (4)
C19—C22—C23	112.2 (3)		

N2—Fe1—N1—C5	−137.0 (3)	C1—B1—C11—C12	109.3 (3)
N6—Fe1—N1—C5	−48.2 (2)	N3—C11—C12—C13	−0.8 (5)
N3—Fe1—N1—C5	131.6 (2)	B1—C11—C12—C13	−174.8 (3)
N5—Fe1—N1—C5	42.0 (2)	C11—C12—C13—C14	−2.1 (5)
N4—Fe1—N1—C5	120 (12)	C12—C13—C14—C15	2.8 (5)

N2—Fe1—N1—C1	51.8 (3)	C11—N3—C15—C14	−2.3 (5)
N6—Fe1—N1—C1	140.7 (3)	Fe1—N3—C15—C14	168.9 (3)
N3—Fe1—N1—C1	−39.5 (3)	C13—C14—C15—N3	−0.7 (5)
N5—Fe1—N1—C1	−129.1 (3)	C11—B1—C16—C17	152.7 (3)
N4—Fe1—N1—C1	−51 (13)	C6—B1—C16—C17	−84.6 (4)
N6—Fe1—N2—C10	43.7 (3)	C1—B1—C16—C17	36.4 (5)
N3—Fe1—N2—C10	−137.0 (3)	C11—B1—C16—C21	−43.5 (4)
N5—Fe1—N2—C10	7 (6)	C6—B1—C16—C21	79.3 (4)
N1—Fe1—N2—C10	133.8 (3)	C1—B1—C16—C21	−159.7 (3)
N4—Fe1—N2—C10	−46.8 (3)	C21—C16—C17—C18	2.9 (5)
N6—Fe1—N2—C6	−131.8 (2)	B1—C16—C17—C18	167.3 (3)
N3—Fe1—N2—C6	47.5 (3)	C16—C17—C18—C19	−1.1 (5)
N5—Fe1—N2—C6	−169 (23)	C17—C18—C19—C20	−0.7 (4)
N1—Fe1—N2—C6	−41.7 (2)	C17—C18—C19—C22	−178.2 (3)
N4—Fe1—N2—C6	137.7 (2)	C18—C19—C20—C21	0.7 (5)
N2—Fe1—N3—C15	140.2 (2)	C22—C19—C20—C21	178.3 (3)
N6—Fe1—N3—C15	−117 (10)	C19—C20—C21—C16	1.2 (5)
N5—Fe1—N3—C15	−39.1 (2)	C17—C16—C21—C20	−2.9 (5)
N1—Fe1—N3—C15	−129.2 (2)	B1—C16—C21—C20	−168.2 (3)
N4—Fe1—N3—C15	50.7 (2)	C18—C19—C22—C24	115.0 (4)
N2—Fe1—N3—C11	−48.6 (2)	C20—C19—C22—C24	−62.3 (4)
N6—Fe1—N3—C11	55 (10)	C18—C19—C22—C25	−125.0 (3)
N5—Fe1—N3—C11	132.1 (2)	C20—C19—C22—C25	57.6 (4)
N1—Fe1—N3—C11	42.1 (2)	C18—C19—C22—C23	−5.1 (5)
N4—Fe1—N3—C11	−138.1 (2)	C20—C19—C22—C23	177.5 (3)
N2—Fe1—N4—C5A	−46.5 (3)	C5A—N4—C1A—C2A	7.8 (5)
N6—Fe1—N4—C5A	−135.3 (3)	Fe1—N4—C1A—C2A	−165.8 (2)
N3—Fe1—N4—C5A	44.9 (3)	C5A—N4—C1A—B2	−176.9 (3)
N5—Fe1—N4—C5A	134.5 (3)	Fe1—N4—C1A—B2	9.5 (4)
N1—Fe1—N4—C5A	56 (13)	C16A—B2—C1A—N4	169.2 (3)
N2—Fe1—N4—C1A	127.1 (3)	C11A—B2—C1A—N4	−65.3 (3)
N6—Fe1—N4—C1A	38.3 (3)	C6A—B2—C1A—N4	49.2 (4)
N3—Fe1—N4—C1A	−141.5 (3)	C16A—B2—C1A—C2A	−15.9 (5)
N5—Fe1—N4—C1A	−51.9 (3)	C11A—B2—C1A—C2A	109.6 (4)
N1—Fe1—N4—C1A	−130 (12)	C6A—B2—C1A—C2A	−135.9 (3)
N2—Fe1—N5—C10A	173 (100)	N4—C1A—C2A—C3A	−6.7 (5)
N6—Fe1—N5—C10A	136.4 (2)	B2—C1A—C2A—C3A	178.5 (3)
N3—Fe1—N5—C10A	−42.9 (2)	C1A—C2A—C3A—C4A	1.1 (5)
N1—Fe1—N5—C10A	46.2 (2)	C2A—C3A—C4A—C5A	3.2 (5)
N4—Fe1—N5—C10A	−133.2 (2)	C1A—N4—C5A—C4A	−3.6 (5)
N2—Fe1—N5—C6A	−11 (6)	Fe1—N4—C5A—C4A	170.1 (3)
N6—Fe1—N5—C6A	−47.8 (2)	C3A—C4A—C5A—N4	−2.0 (5)
N3—Fe1—N5—C6A	132.9 (2)	C10A—N5—C6A—C7A	1.9 (5)
N1—Fe1—N5—C6A	−137.9 (2)	Fe1—N5—C6A—C7A	−173.9 (2)
N4—Fe1—N5—C6A	42.7 (2)	C10A—N5—C6A—B2	−179.5 (3)
N2—Fe1—N6—C11A	−127.2 (2)	Fe1—N5—C6A—B2	4.8 (4)
N3—Fe1—N6—C11A	130 (10)	C16A—B2—C6A—N5	173.2 (3)
N5—Fe1—N6—C11A	52.1 (2)	C11A—B2—C6A—N5	49.3 (4)
N1—Fe1—N6—C11A	142.2 (2)	C1A—B2—C6A—N5	−59.1 (4)
N4—Fe1—N6—C11A	−37.7 (2)	C16A—B2—C6A—C7A	−8.2 (4)
N2—Fe1—N6—C15A	42.4 (2)	C11A—B2—C6A—C7A	−132.1 (3)
N3—Fe1—N6—C15A	−61 (10)	C1A—B2—C6A—C7A	119.5 (3)
N5—Fe1—N6—C15A	−138.3 (2)	N5—C6A—C7A—C8A	0.1 (5)
N1—Fe1—N6—C15A	−48.3 (2)	B2—C6A—C7A—C8A	−178.5 (3)

N4—Fe1—N6—C15A	131.9 (2)	C6A—C7A—C8A—C9A	−1.2 (5)
C5—N1—C1—C2	−7.3 (5)	C7A—C8A—C9A—C10A	0.3 (5)
Fe1—N1—C1—C2	163.6 (2)	C6A—N5—C10A—C9A	−2.8 (5)
C5—N1—C1—B1	178.2 (3)	Fe1—N5—C10A—C9A	172.8 (3)
Fe1—N1—C1—B1	−10.9 (4)	C8A—C9A—C10A—N5	1.6 (5)
C16—B1—C1—N1	−168.4 (3)	C15A—N6—C11A—C12A	−5.6 (4)
C11—B1—C1—N1	67.2 (3)	Fe1—N6—C11A—C12A	163.8 (2)
C6—B1—C1—N1	−47.2 (4)	C15A—N6—C11A—B2	−180.0 (3)
C16—B1—C1—C2	17.7 (5)	Fe1—N6—C11A—B2	−10.5 (4)
C11—B1—C1—C2	−106.8 (3)	C16A—B2—C11A—N6	−164.7 (3)
C6—B1—C1—C2	138.8 (3)	C6A—B2—C11A—N6	−45.4 (4)
N1—C1—C2—C3	3.9 (5)	C1A—B2—C11A—N6	66.8 (3)
B1—C1—C2—C3	177.8 (3)	C16A—B2—C11A—C12A	21.3 (5)
C1—C2—C3—C4	2.0 (5)	C6A—B2—C11A—C12A	140.6 (3)
C2—C3—C4—C5	−4.4 (5)	C1A—B2—C11A—C12A	−107.3 (3)
C1—N1—C5—C4	5.1 (5)	N6—C11A—C12A—C13A	4.1 (5)
Fe1—N1—C5—C4	−166.0 (3)	B2—C11A—C12A—C13A	178.2 (3)
C3—C4—C5—N1	1.0 (5)	C11A—C12A—C13A—C14A	0.2 (5)
C10—N2—C6—C7	−2.7 (5)	C12A—C13A—C14A—C15A	−3.1 (5)
Fe1—N2—C6—C7	172.8 (2)	C11A—N6—C15A—C14A	2.8 (5)
C10—N2—C6—B1	178.8 (3)	Fe1—N6—C15A—C14A	−166.7 (3)
Fe1—N2—C6—B1	−5.7 (4)	C13A—C14A—C15A—N6	1.7 (5)
C16—B1—C6—N2	−174.5 (3)	C11A—B2—C16A—C21A	−149.0 (3)
C11—B1—C6—N2	−48.8 (4)	C6A—B2—C16A—C21A	89.9 (4)
C1—B1—C6—N2	58.4 (4)	C1A—B2—C16A—C21A	−30.2 (5)
C16—B1—C6—C7	7.1 (4)	C11A—B2—C16A—C17A	44.7 (4)
C11—B1—C6—C7	132.8 (3)	C6A—B2—C16A—C17A	−76.4 (4)
C1—B1—C6—C7	−120.0 (3)	C1A—B2—C16A—C17A	163.5 (3)
N2—C6—C7—C8	0.9 (5)	C21A—C16A—C17A—C18A	1.3 (5)
B1—C6—C7—C8	179.3 (3)	B2—C16A—C17A—C18A	169.0 (3)
C6—C7—C8—C9	0.7 (6)	C16A—C17A—C18A—C19A	0.1 (5)
C7—C8—C9—C10	−0.6 (6)	C17A—C18A—C19A—C20A	−0.7 (5)
C6—N2—C10—C9	3.0 (5)	C17A—C18A—C19A—C22A	178.7 (3)
Fe1—N2—C10—C9	−172.4 (3)	C18A—C19A—C20A—C21A	0.0 (5)
C8—C9—C10—N2	−1.3 (5)	C22A—C19A—C20A—C21A	−179.4 (3)
C15—N3—C11—C12	3.0 (4)	C19A—C20A—C21A—C16A	1.5 (5)
Fe1—N3—C11—C12	−168.2 (2)	C17A—C16A—C21A—C20A	−2.0 (5)
C15—N3—C11—B1	177.4 (3)	B2—C16A—C21A—C20A	−168.9 (3)
Fe1—N3—C11—B1	6.2 (4)	C20A—C19A—C22A—C23A	−176.7 (3)
C16—B1—C11—N3	169.0 (3)	C18A—C19A—C22A—C23A	3.9 (4)
C6—B1—C11—N3	47.6 (4)	C20A—C19A—C22A—C24A	−56.2 (4)
C1—B1—C11—N3	−64.8 (3)	C18A—C19A—C22A—C24A	124.4 (4)
C16—B1—C11—C12	−16.9 (5)	C20A—C19A—C22A—C25A	62.3 (4)
C6—B1—C11—C12	−138.4 (3)	C18A—C19A—C22A—C25A	−117.1 (4)