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Crystal structure of bis(1-ethyl-1*H*-imidazole-κN^3)-(*meso*-tetramesitylporphyrinato-$\kappa^4 N,N',N'',N'''$)-iron(III) perchlorate chlorobenzene sesquisolvate

Nana Zhan, Haimang Wang and Jianfeng Li*

College of Materials Science and Opto-electronic Technology, CAS Center for Excellence in Topological Quantum Computation & Center of Materials Science and Optoelectronics Engineering, University of Chinese Academy of Sciences, Yanqi Lake, Huairou District, Beijing 101408, People's Republic of China. *Correspondence e-mail: jfli@ucas.ac.cn

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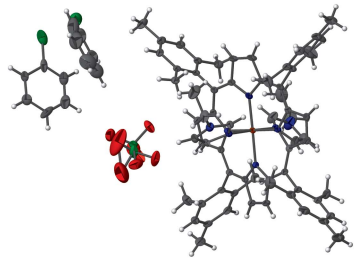
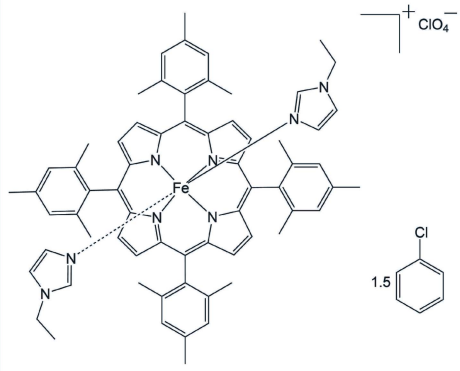
In the complex cation of title compound, $[Fe(C_{56}H_{52}N_4)(C_5H_8N_2)_2]ClO_4\cdot 1.5C_6H_5Cl$, the iron^{III} atom is coordinated in a distorted octahedral manner by four pyrrole N atoms of the porphyrin ring system in the equatorial plane, and by two N atoms of the 1-ethylimidazole ligands in the axial sites. A disordered perchlorate anion and one and a half chlorobenzene solvent molecules are also present. The cationic complex exhibits a highly ruffled porphyrin core. The average Fe—N_p (N_p is a porphyrin N atom) bond length is 1.988 (5), and the axial Fe—N_{Im} (N_{Im} is an imidazole N atom) bond lengths are 1.962 (3) and 1.976 (3) Å. The two 1-ethylimidazole ligands are inclined to each other by a dihedral angle of 68.62 (16)°. The dihedral angles between the 1-ethylimidazole planes and the planes of the closest Fe—N_p vector are 28.52 (18) and 43.57 (13)°. Intermolecular C—H···Cl interactions are observed.

3D view



Chemical scheme



Structure description

For several decades, porphyrin-based model systems of the heme active site have been used in an attempt to understand structure–function relationships in myoglobin (Mb) or hemoglobin (Hb) (Jameson & Ibers, 1983). Complexes of iron^{III} porphyrins with additional imidazole or pyridine ligands provide useful models for bis-histidine-coordinated heme centers, which are involved in a number of cytochrome-containing systems (Walker, 2004). Crystal structures of iron^{III} porphyrinates, *e.g.* $[Fe(TMP)(1,2\text{-}Me_2Im)_2]ClO_4$ (TMP = tetramesitylporphyrin; 1,2-Me_2Im = 1,2-dimethylimidazole; Munro *et al.*, 1995), $[Fe(TPP)(2\text{-}MeHIm)_2]ClO_4$ (TPP = *meso*-tetraphenylporphyrin; 2-MeHIm = 2-methylimidazole; Scheidt *et al.*, 1987) and $[Fe(OETPP)(1\text{-}MeIm)_2]Cl$ (OETPP =

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C(B4—H(B4···Cl1S^{i}	0.95	2.91	3.713 (4)	143

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.

octaethyltetraphenylporphyrin; l-MeIm = 1-methylimidazole; Yatsunyk *et al.*, 2003) have been determined. Herein, the crystal structure of a new iron^{III} porphyrin complex, [Fe(TMP)(1-EtIm)$_2$]ClO$_4$·1.5PhCl is reported.

In the title compound, the counter-ion to the positively charged bis(1-ethylimidazole)[*meso*-tetramesitylporphyrinato]iron(III) complex is a negatively charged perchlorate ion (Fig. 1). In addition, one and a half chlorobenzene solvent molecules are present per complex molecule in the crystal structure. The perchlorate anion is disordered over two sets of sites, and one chlorobenzene solvate molecule is disordered about an inversion center.

Additional quantitative information on the structure is given in Fig. 2, which displays the detailed displacement of each porphyrin core atom (in units of 0.01 Å) from the 24-atom mean plane. Averaged values of the chemically unique bond length (Å) and angles (°) are also shown. The 1-ethylimidazole ligand containing the N7 atom makes a dihedral angle of 28.52 (18)° with the closest Fe—N$_p$ vector, the other 1-ethylimidazole ligand containing N5 making an angle of 43.57 (13)°. The two 1-ethylimidazole planes are inclined to each other at an dihedral angle of 68.62 (16)°. Fig. 2 also shows that the cationic complex has a ruffled porphyrin core conformation, and the iron(III) atom is slightly displaced from the 24-atom plane. The mean absolute core-atom displacements of C_a, C_b, C_m and C_{av} are 0.13 (6), 0.12 (9), 0.23 (4) and 0.15 (8) Å, respectively, where C_a represents the α-C position relative to the N atom in the pyrrole ring, C_b the β-C position relative to the N atom in the pyrrole ring, C_m the *meso*-C atoms in the bridging position between the two pyrroles of the porphyrin core, and C_{av} all C atoms in the 24-atom plane of the porphyrin core. The structural parameters of [Fe(TMP)(1-EtIm)$_2$]ClO$_4$·1.5PhCl are consistent with those of reported iron(III) analogues. The average Fe—N$_p$ (N$_p$ is a porphyrin nitrogen atom) bond length is 1.988 (5), almost equivalent to 1.99 (2) Å in [Fe(TMP)(1-MeIm)$_2$]ClO$_4$ (A) and 1.987 (1) Å in [Fe(TMP)(1-MeIm)$_2$]ClO$_4$ (*B*) (Safo *et al.*, 1991), all of which are in the narrow range of 1.937 (12)-2.041 (9) Å (Hu *et al.*, 2006). The axial Fe—N$_{Im}$ (N$_{Im}$ is an imidazole nitrogen atom) bond lengths are 1.962 (3) and 1.976 (3) Å, in accordance with the narrow range of 1.957 (6)-2.032 (5) Å typical for low-spin iron(III) bis-imidazole ligated porphyrinates (Wang *et al.*, 2018). The average N$_p$—Fe—N$_p$ angle is nearly ideal at 90.4 (3)°.

A C—H···Cl hydrogen bond between a pyrrol C—H group and the Cl atom of one of the solvent molecules is observed in the crystal structure of the title compound (Table 1, Fig. 3). The distance of 2.91 Å between H(B4) and Cl1S is in the range 2.0 < H···Cl(d/Å) < 3.3, and the C(B4)—H(B4)···Cl1S angle

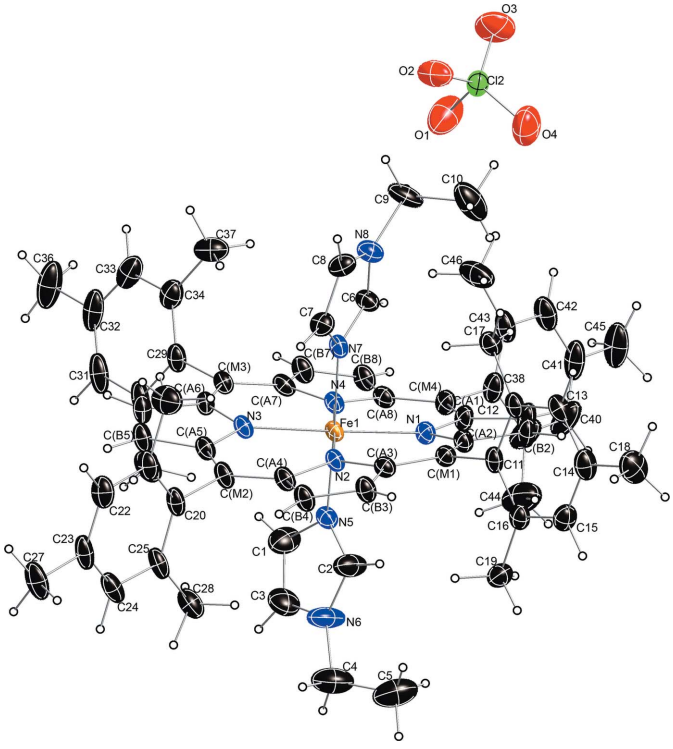


Figure 1
The molecular entities in the title compound, with displacement ellipsoids drawn at the 50% probability level. Only the major part of the disordered perchlorate anion is displayed; the chlorobenzene solvent molecules were omitted for clarity.

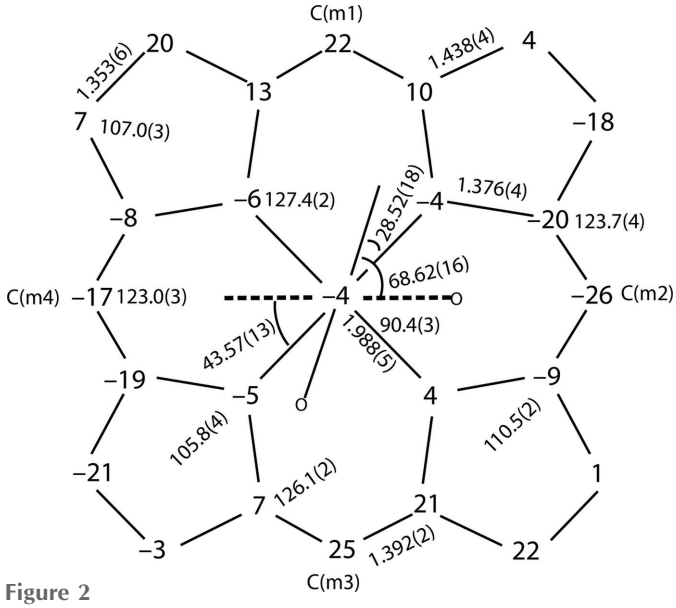


Figure 2
A formal diagram of the porphinato core of the title compound. Averaged values of the chemically unique bond length (Å) and angles (°) are shown. The numbers in parentheses are the standard uncertainties calculated on the assumption that the averaged values were all drawn from the same population. The perpendicular displacements (in units of 0.01 Å) of the porphyrin core atoms from the 24-atom mean plane are also displayed. Negative values indicate a displacement toward the N7 1-ethylimidazole nitrogen atom. The solid line in this perspective indicates the 1-ethylimidazole ligand containing atom N7, and the dashed line indicates the 1-ethylimidazole ligand containing atom N5. The circle represents the position of the ethyl group on the axial ligand.

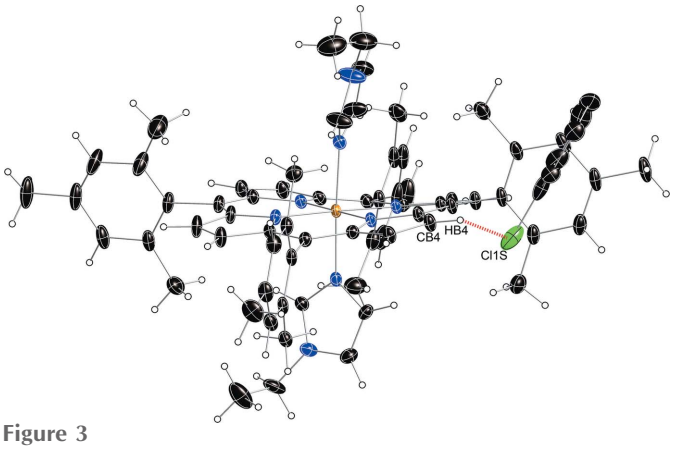


Figure 3
C—H···Cl interactions in the title compound, indicated by dashed lines.

of 143.2° is in the range (90 < C–H···Cl(θ/°) <180), both corresponding to a typical C—H···Cl interaction (Thallapally & Nangia *et al.*, 2001). The molecular packing is shown in Fig. 4.

Synthesis and crystallization

General Information. All reactions were done using standard Schlenk techniques unless otherwise specified. 1-Ethylimidazole (1-EtIm) was distilled under an argon atmosphere. Hexanes were distilled from sodium and potassium alloy; chlorobenzene was first washed with concentrated sulfuric acid and then with water until the aqueous layer was neutral, dried with anhydrous $MgSO_4$, and distilled twice over P_2O_5 under argon. H_2TMP, [Fe(TMP)]Cl, [Fe(TMP)]OH were prepared according to previously reported methods (Lindsey & Wagner, 1989; Reed *et al.*,1979).

Synthesis of [*meso*-tetramesitylporphyrinato]iron(III) perchlorate

Solid [Fe(TMP)]OH (500 mg, 0.59 mmol) was dissolved in benzene which was shaken with 2 *M* aqueous perchloric acid three times in a separatory funnel. The aqueous phase was discarded and the benzene solution was gradually replaced by methanol. The organic phase was brought to dryness using a rotary evaporator at 303 K. A purple solid was obtained by filtration and washed with deionized water.

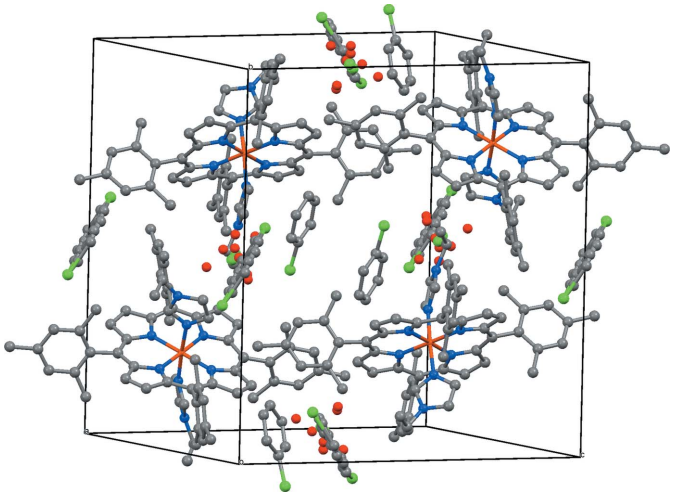


Figure 4
A view of the molecular packing of the title compound. Hydrogen atoms have been omitted for clarity.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Fe(C_{56}H_{52}N_4)(C_5H_8N_2)_2]ClO_4\cdot 1.5C_6H_5Cl$
M_r	2594.81
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
a, b, c (Å)	16.0479 (8), 21.0653 (11), 19.5828 (9)
β (°)	98.599 (2)
V (Å^3)	6545.6 (6)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.39
Crystal size (mm)	0.38 × 0.37 × 0.23
Data collection	
Diffractometer	Brucker D8 QUEST System
Absorption correction	Multi-scan (*SADABS*; Bruker, 2013)
T_{min}, T_{max}	0.862, 0.914
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	163914, 13956, 11781
R_{int}	0.046
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.634
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.076, 0.235, 1.03
No. of reflections	13956
No. of parameters	906
No. of restraints	19
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.56, −2.30

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *CrystalMaker* (Palmer, 2014), *Mercury* (Macrae *et al.*, 2008) and *enCIFer* (Allen *et al.*, 2004).

Synthesis of bis(1-ethyl-1*H*-imidazole-κN^3)(*meso*-tetra-*mesityl*porphyrinato-$\kappa^4 N$)iron(III) perchlorate chlorobenzene sesquisolvate

[Fe(TMP)]ClO_4 (10 mg, 0.01 mmol) and excess 1-EtIm (0.1 ml, 1.25 mmol) were dissolved in 6 ml chlorobenzene. After 20 min of stirring, the solution was transferred into glass tubes which were layered with hexanes as non-solvent. Several days later, black block-shaped crystals suitable for the single-crystal X-ray diffraction study were collected.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. One chlorobenzene molecule is equally disordered about an inversion center; the perchlorate anion is disordered over two sets of sites in a ratio of 0.68:0.32. The three atoms (O2*S*, O3*S*, O4*S*) of the anion exhibited unusual thermal motions, and thus were restrained by ISOR commands. Anisotropic displacement parameters (ADP) of

C48 and C49 were restrained using the DELU instruction. Sixteen outliers were omitted in the last cycles of refinement.

Funding information

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full crystallographic data

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Crystal structure of bis(1-ethyl-1*H*-imidazole-κN^3)(*meso*-tetramesitylporphyrinato-$\kappa^4 N,N',N'',N'''$)iron(III) perchlorate chlorobenzene sesquisolvate

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Bis(1-ethyl-1*H*-imidazole-κN^3)(*meso*-tetramesitylporphyrinato-$\kappa^4 N,N',N'',N'''$)iron(III) perchlorate chlorobenzene sesquisolvate

Crystal data

$[Fe(C_{56}H_{52}N_4)(C_5H_8N_2)_2]ClO_4 \cdot 1.5C_6H_5Cl$
$M_r = 2594.81$
Monoclinic, $P2_1/n$
$a = 16.0479$ (8) Å
$b = 21.0653$ (11) Å
$c = 19.5828$ (9) Å
$\beta = 98.599$ (2)°
$V = 6545.6$ (6) Å^3
$Z = 2$
$F(000) = 2728$
$D_x = 1.317$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9614 reflections
$\theta = 2.3$–$26.8°$
$\mu = 0.39$ mm^{-1}
$T = 100$ K
Block, black
0.38 × 0.37 × 0.23 mm

Data collection

Bruker D8 QUEST System diffractometer
Radiation source: fine-focus sealed tube
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
$T_{min} = 0.862$, $T_{max} = 0.914$
163914 measured reflections
13956 independent reflections
11781 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 26.8°$, $\theta_{min} = 1.4°$
$h = -20 \rightarrow 20$
$k = -26 \rightarrow 26$
$l = -24 \rightarrow 24$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.076$
$wR(F^2) = 0.235$
$S = 1.03$
13956 reflections
906 parameters
19 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1369P)^2 + 19.8909P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 1.56$ e Å^{-3}
$\Delta\rho_{min} = -2.30$ e Å^{-3}

Special details

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	0.73934 (3)	0.22192 (2)	0.15982 (2)	0.01290 (14)	
N1	0.68202 (16)	0.18692 (12)	0.07074 (12)	0.0164 (5)	
N2	0.64998 (16)	0.18425 (12)	0.20782 (12)	0.0152 (5)	
N3	0.79468 (15)	0.25918 (12)	0.24797 (12)	0.0149 (5)	
N4	0.82832 (16)	0.25876 (12)	0.11139 (13)	0.0154 (5)	
N5	0.80718 (16)	0.14445 (13)	0.18287 (13)	0.0185 (5)	
N6	0.8393 (2)	0.04804 (16)	0.2185 (2)	0.0442 (9)	
N7	0.67024 (16)	0.29861 (12)	0.14172 (13)	0.0162 (5)	
N8	0.60495 (18)	0.37762 (13)	0.08369 (15)	0.0236 (6)	
C1	0.8889 (2)	0.1423 (2)	0.2138 (2)	0.0387 (9)	
H1	0.926295	0.177563	0.219145	0.046*	
C(A1	0.7072 (2)	0.19237 (15)	0.00657 (15)	0.0193 (6)	
C2	0.7786 (3)	0.08691 (19)	0.1883 (3)	0.0405 (10)	
H2	0.722049	0.074259	0.172958	0.049*	
C(A2	0.60352 (19)	0.15989 (14)	0.05862 (15)	0.0173 (6)	
C3	0.9090 (3)	0.0830 (2)	0.2355 (2)	0.0393 (9)	
H3	0.962041	0.068735	0.258411	0.047*	
C(A3	0.57684 (19)	0.15543 (14)	0.17822 (15)	0.0162 (6)	
C4	0.8305 (4)	−0.0177 (2)	0.2437 (3)	0.0559 (13)	
H4A	0.813401	−0.016074	0.290206	0.067*	
H4B	0.885885	−0.039238	0.247992	0.067*	
C(A4	0.65051 (19)	0.18111 (15)	0.27821 (15)	0.0175 (6)	
C5	0.7675 (4)	−0.0550 (2)	0.1968 (3)	0.0609 (14)	
H5A	0.711093	−0.037476	0.197820	0.091*	
H5B	0.768887	−0.099372	0.212127	0.091*	
H5C	0.780785	−0.052895	0.149663	0.091*	
C(A5	0.77460 (19)	0.24760 (15)	0.31294 (15)	0.0170 (6)	
C6	0.6667 (2)	0.33518 (15)	0.08609 (16)	0.0201 (6)	
H6	0.703362	0.331494	0.052455	0.024*	
C(A6	0.86173 (19)	0.30066 (14)	0.25733 (15)	0.0163 (6)	
C7	0.6068 (2)	0.31988 (15)	0.17641 (17)	0.0216 (6)	
H7	0.593784	0.303138	0.218612	0.026*	
C(A7	0.89334 (19)	0.29776 (15)	0.13927 (15)	0.0172 (6)	
C8	0.5659 (2)	0.36879 (16)	0.14024 (19)	0.0256 (7)	
H8	0.519362	0.392099	0.152022	0.031*	

C(A8	0.83856 (19)	0.25021 (14)	0.04337 (15)	0.0171 (6)
C9	0.5775 (2)	0.42021 (19)	0.0247 (2)	0.0346 (9)
H9A	0.626380	0.431307	0.001619	0.042*
H9B	0.554500	0.459926	0.041449	0.042*
C(B1	0.6437 (2)	0.16685 (17)	−0.04556 (16)	0.0262 (7)
H(B1	0.646383	0.164413	−0.093625	0.031*
C10	0.5108 (3)	0.3879 (3)	−0.0262 (3)	0.0538 (13)
H10A	0.533342	0.348134	−0.041911	0.081*
H10B	0.494307	0.415861	−0.065934	0.081*
H10C	0.461448	0.378746	−0.003812	0.081*
C(B2	0.5796 (2)	0.14701 (16)	−0.01381 (16)	0.0236 (7)
H(B2	0.528497	0.128143	−0.035097	0.028*
C11	0.46654 (19)	0.11880 (15)	0.08355 (15)	0.0177 (6)
C(B3	0.5296 (2)	0.13442 (16)	0.23078 (16)	0.0199 (6)
H(B3	0.476061	0.114237	0.223653	0.024*
C12	0.4007 (2)	0.16062 (15)	0.05844 (15)	0.0190 (6)
C(B4	0.5759 (2)	0.14887 (16)	0.29242 (16)	0.0203 (6)
H(B4	0.561775	0.139496	0.336737	0.024*
C13	0.3204 (2)	0.13602 (17)	0.03628 (17)	0.0241 (7)
H13	0.275417	0.164203	0.020353	0.029*
C(B5	0.8297 (2)	0.28283 (16)	0.36358 (16)	0.0215 (7)
H(B5	0.829306	0.282662	0.412036	0.026*
C14	0.3048 (2)	0.07087 (18)	0.03706 (18)	0.0275 (7)
C(B6	0.8828 (2)	0.31653 (16)	0.32934 (16)	0.0217 (6)
H(B6	0.925583	0.345047	0.349140	0.026*
C15	0.3711 (2)	0.03044 (17)	0.06116 (17)	0.0250 (7)
H15	0.361084	−0.013995	0.061492	0.030*
C(B7	0.9465 (2)	0.31258 (16)	0.08802 (16)	0.0213 (6)
H(B7	0.995555	0.338455	0.094351	0.026*
C16	0.4519 (2)	0.05302 (16)	0.08486 (16)	0.0210 (6)
C(B8	0.9129 (2)	0.28246 (16)	0.02927 (16)	0.0203 (6)
H(B8	0.934478	0.282638	−0.013332	0.024*
C17	0.4159 (2)	0.23094 (15)	0.05315 (17)	0.0224 (6)
H17A	0.443825	0.239449	0.012883	0.034*
H17B	0.451883	0.245598	0.095061	0.034*
H17C	0.361924	0.253497	0.048081	0.034*
C(M1	0.55204 (19)	0.14549 (14)	0.10794 (15)	0.0166 (6)
C18	0.2171 (2)	0.0455 (2)	0.0135 (2)	0.0397 (9)
H18A	0.220709	0.006277	−0.012820	0.060*
H18B	0.184289	0.077108	−0.015851	0.060*
H18C	0.189511	0.036685	0.053851	0.060*
C(M2	0.7093 (2)	0.20893 (16)	0.32820 (15)	0.0185 (6)
C19	0.5221 (2)	0.00706 (16)	0.10905 (19)	0.0270 (7)
H19A	0.498508	−0.035486	0.112914	0.040*
H19B	0.551370	0.020511	0.154252	0.040*
H19C	0.561944	0.006253	0.075737	0.040*
C(M3	0.90830 (19)	0.32021 (15)	0.20681 (15)	0.0173 (6)
C20	0.7026 (2)	0.19671 (16)	0.40282 (15)	0.0198 (6)

C(M4	0.7813 (2)	0.22055 (15)	−0.00750 (16)	0.0193 (6)
C21	0.6547 (2)	0.23688 (18)	0.43862 (17)	0.0249 (7)
C22	0.6517 (2)	0.22390 (18)	0.50837 (18)	0.0278 (7)
H22	0.619297	0.250823	0.533120	0.033*
C23	0.6942 (2)	0.17333 (19)	0.54246 (16)	0.0267 (7)
C24	0.7413 (2)	0.13389 (18)	0.50592 (17)	0.0253 (7)
H24	0.771278	0.099191	0.528869	0.030*
C25	0.7454 (2)	0.14447 (17)	0.43595 (16)	0.0227 (7)
C26	0.6069 (3)	0.2918 (2)	0.4036 (2)	0.0376 (9)
H26A	0.646122	0.320796	0.385622	0.056*
H26B	0.577678	0.314332	0.436854	0.056*
H26C	0.565491	0.276189	0.365380	0.056*
C27	0.6882 (3)	0.1590 (2)	0.61708 (18)	0.0366 (9)
H27A	0.677748	0.198366	0.641007	0.055*
H27B	0.741240	0.140014	0.639212	0.055*
H27C	0.641852	0.129180	0.619475	0.055*
C28	0.7923 (2)	0.09910 (19)	0.39693 (19)	0.0305 (8)
H28A	0.816761	0.065276	0.427984	0.046*
H28B	0.837373	0.121748	0.378460	0.046*
H28C	0.753438	0.080544	0.358776	0.046*
C29	0.9796 (2)	0.36588 (16)	0.22490 (15)	0.0202 (6)
C30	1.0590 (2)	0.34443 (18)	0.25727 (16)	0.0250 (7)
C31	1.1250 (2)	0.3879 (2)	0.27061 (17)	0.0321 (9)
H31	1.178448	0.373795	0.292896	0.039*
C32	1.1145 (3)	0.4518 (2)	0.25198 (19)	0.0362 (9)
C33	1.0370 (3)	0.47137 (19)	0.2198 (2)	0.0350 (9)
H33	1.029629	0.514611	0.206468	0.042*
C34	0.9684 (2)	0.42991 (18)	0.20584 (18)	0.0275 (7)
C35	1.0735 (2)	0.2753 (2)	0.2745 (2)	0.0326 (8)
H35A	1.133518	0.268095	0.290705	0.049*
H35B	1.055606	0.249546	0.233255	0.049*
H35C	1.040729	0.263171	0.310919	0.049*
C36	1.1877 (3)	0.4975 (3)	0.2650 (2)	0.0522 (13)
H36A	1.203113	0.511302	0.220768	0.078*
H36B	1.235979	0.476262	0.292238	0.078*
H36C	1.171526	0.534422	0.290415	0.078*
C37	0.8857 (3)	0.4546 (2)	0.1681 (2)	0.0405 (9)
H37A	0.880365	0.499850	0.178040	0.061*
H37B	0.838991	0.431263	0.183514	0.061*
H37C	0.884006	0.448534	0.118298	0.061*
C38	0.7995 (2)	0.22252 (16)	−0.08044 (17)	0.0240 (7)
C39	0.8303 (3)	0.16967 (19)	−0.1103 (2)	0.0396 (10)
C40	0.8530 (3)	0.1745 (2)	−0.1763 (2)	0.0421 (10)
H40	0.873576	0.137811	−0.196597	0.050*
C41	0.8468 (3)	0.2295 (2)	−0.21241 (19)	0.0347 (9)
C42	0.8101 (2)	0.2812 (2)	−0.18399 (18)	0.0317 (8)
H42	0.801453	0.319361	−0.209874	0.038*
C43	0.7856 (2)	0.27848 (18)	−0.11871 (17)	0.0258 (7)

C44	0.8311 (4)	0.1070 (2)	−0.0761 (3)	0.0595 (14)	
H44A	0.863163	0.109890	−0.029480	0.089*	
H44B	0.857534	0.075608	−0.102955	0.089*	
H44C	0.773144	0.093896	−0.073100	0.089*	
C45	0.8757 (3)	0.2344 (3)	−0.2822 (2)	0.0465 (12)	
H45A	0.933943	0.249909	−0.276369	0.070*	
H45B	0.839166	0.264039	−0.311430	0.070*	
H45C	0.872824	0.192486	−0.304110	0.070*	
C46	0.7437 (3)	0.3350 (2)	−0.0915 (2)	0.0411 (10)	
H46A	0.690908	0.321683	−0.076293	0.062*	
H46B	0.731623	0.366891	−0.128095	0.062*	
H46C	0.781223	0.353316	−0.052376	0.062*	
Cl1	−0.02637 (10)	−0.05596 (8)	0.12432 (9)	0.0705 (4)	
C47	0.0196 (3)	0.0185 (3)	0.1236 (3)	0.0636 (15)	
C48	−0.0142 (4)	0.0591 (4)	0.0725 (4)	0.084 (2)	
H48	−0.056871	0.046198	0.036221	0.101*	
C49	0.0185 (5)	0.1220 (4)	0.0768 (4)	0.0809 (19)	
H49	−0.006766	0.152869	0.044937	0.097*	
C50	0.0864 (6)	0.1399 (4)	0.1261 (4)	0.087 (2)	
H50	0.109362	0.181445	0.125585	0.104*	
C51	0.1207 (5)	0.0954 (3)	0.1771 (4)	0.0720 (17)	
H51	0.165819	0.106197	0.212364	0.086*	
C52	0.0846 (3)	0.0346 (3)	0.1728 (3)	0.0548 (12)	
H52	0.106669	0.003552	0.205701	0.066*	
Cl1S	−0.07214 (17)	0.40934 (11)	−0.09293 (15)	0.0505 (6)	0.5
C1S	−0.0270 (7)	0.4654 (6)	−0.0374 (6)	0.037 (2)	0.5
C2S	−0.0744 (8)	0.5192 (6)	−0.0201 (7)	0.028 (3)	0.5
H2S	−0.132164	0.523418	−0.038961	0.034*	0.5
C3S	−0.0347 (9)	0.5658 (6)	0.0252 (7)	0.037 (3)	0.5
H3S	−0.066030	0.601838	0.035828	0.045*	0.5
C4S	0.0486 (8)	0.5603 (9)	0.0543 (7)	0.054 (4)	0.5
H4S	0.074754	0.592068	0.084668	0.065*	0.5
C5S	0.0936 (9)	0.5073 (8)	0.0384 (8)	0.051 (3)	0.5
H5S	0.151042	0.503111	0.058419	0.061*	0.5
C6S	0.0558 (8)	0.4591 (8)	−0.0070 (8)	0.042 (3)	0.5
H6S	0.087466	0.422812	−0.016307	0.051*	0.5
Cl2	0.3751 (3)	0.48593 (18)	0.13585 (15)	0.0230 (6)	0.6752
O1	0.2866 (4)	0.4991 (3)	0.1158 (4)	0.0592 (17)	0.6752
O2	0.4062 (3)	0.4660 (2)	0.0759 (2)	0.0390 (10)	0.6752
O3	0.3750 (8)	0.4349 (6)	0.1837 (8)	0.054 (3)	0.6752
O4	0.4132 (4)	0.5464 (3)	0.1611 (3)	0.0567 (14)	0.6752
Cl3	0.3864 (6)	0.4981 (4)	0.1516 (5)	0.0404 (19)	0.3248
O1S	0.4694 (6)	0.5043 (4)	0.1524 (7)	0.058 (3)	0.3248
O2S	0.3746 (14)	0.5443 (12)	0.2022 (13)	0.132 (8)	0.3248
O3S	0.3241 (12)	0.5193 (11)	0.1203 (15)	0.138 (8)	0.3248
O4S	0.3989 (18)	0.4455 (14)	0.1927 (17)	0.070 (8)	0.3248

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0148 (2)	0.0158 (2)	0.0083 (2)	0.00082 (15)	0.00250 (15)	0.00107 (14)
N1	0.0203 (13)	0.0187 (12)	0.0109 (11)	−0.0006 (10)	0.0050 (9)	0.0000 (9)
N2	0.0175 (12)	0.0187 (12)	0.0092 (11)	0.0002 (9)	0.0018 (9)	0.0014 (9)
N3	0.0145 (12)	0.0205 (12)	0.0098 (11)	0.0007 (9)	0.0021 (9)	0.0016 (9)
N4	0.0164 (12)	0.0186 (12)	0.0112 (11)	0.0011 (10)	0.0017 (9)	0.0010 (9)
N5	0.0194 (13)	0.0211 (13)	0.0149 (12)	0.0020 (10)	0.0021 (10)	0.0015 (10)
N6	0.0354 (18)	0.0246 (16)	0.069 (3)	0.0046 (14)	−0.0045 (17)	0.0138 (16)
N7	0.0166 (12)	0.0201 (12)	0.0115 (11)	0.0009 (10)	0.0012 (9)	−0.0005 (9)
N8	0.0226 (14)	0.0212 (13)	0.0264 (14)	0.0039 (11)	0.0012 (11)	0.0049 (11)
C1	0.0226 (18)	0.032 (2)	0.059 (3)	0.0049 (15)	−0.0017 (17)	−0.0029 (18)
C(A1	0.0274 (16)	0.0218 (15)	0.0097 (13)	−0.0032 (12)	0.0060 (12)	−0.0028 (11)
C2	0.031 (2)	0.0239 (18)	0.061 (3)	0.0011 (15)	−0.0094 (19)	0.0074 (18)
C(A2	0.0204 (14)	0.0188 (14)	0.0125 (14)	−0.0020 (11)	0.0018 (11)	0.0006 (11)
C3	0.031 (2)	0.041 (2)	0.044 (2)	0.0129 (17)	−0.0012 (17)	0.0034 (18)
C(A3	0.0167 (14)	0.0176 (14)	0.0148 (14)	0.0008 (11)	0.0037 (11)	0.0016 (11)
C4	0.061 (3)	0.035 (2)	0.072 (3)	0.009 (2)	0.011 (3)	0.015 (2)
C(A4	0.0179 (14)	0.0239 (15)	0.0112 (13)	0.0002 (12)	0.0043 (11)	0.0030 (11)
C5	0.062 (3)	0.033 (2)	0.090 (4)	0.000 (2)	0.022 (3)	0.006 (2)
C(A5	0.0190 (14)	0.0224 (15)	0.0100 (13)	0.0008 (12)	0.0029 (11)	0.0013 (11)
C6	0.0214 (15)	0.0226 (15)	0.0164 (14)	0.0036 (12)	0.0033 (12)	0.0038 (12)
C(A6	0.0167 (14)	0.0193 (14)	0.0125 (13)	0.0003 (11)	0.0006 (11)	−0.0021 (11)
C7	0.0239 (16)	0.0220 (15)	0.0207 (15)	0.0038 (12)	0.0089 (12)	−0.0027 (12)
C(A7	0.0163 (14)	0.0215 (14)	0.0140 (14)	0.0008 (11)	0.0026 (11)	0.0044 (11)
C8	0.0254 (17)	0.0223 (16)	0.0302 (18)	0.0037 (13)	0.0080 (14)	−0.0024 (13)
C(A8	0.0192 (14)	0.0200 (15)	0.0126 (13)	0.0011 (11)	0.0046 (11)	0.0026 (11)
C9	0.0318 (19)	0.0320 (19)	0.040 (2)	0.0105 (15)	0.0038 (16)	0.0197 (16)
C(B1	0.0359 (19)	0.0311 (18)	0.0127 (14)	−0.0106 (15)	0.0072 (13)	−0.0056 (13)
C10	0.039 (2)	0.073 (3)	0.045 (3)	0.002 (2)	−0.008 (2)	0.029 (2)
C(B2	0.0289 (17)	0.0286 (17)	0.0133 (14)	−0.0089 (13)	0.0033 (12)	−0.0046 (12)
C11	0.0194 (14)	0.0239 (15)	0.0101 (13)	−0.0032 (12)	0.0027 (11)	−0.0016 (11)
C(B3	0.0174 (14)	0.0271 (16)	0.0150 (14)	−0.0037 (12)	0.0019 (11)	0.0022 (12)
C12	0.0225 (15)	0.0249 (16)	0.0098 (13)	−0.0012 (12)	0.0028 (11)	0.0004 (11)
C(B4	0.0199 (15)	0.0287 (16)	0.0125 (14)	−0.0032 (12)	0.0033 (11)	0.0029 (12)
C13	0.0203 (15)	0.0343 (18)	0.0174 (15)	−0.0002 (13)	0.0018 (12)	0.0026 (13)
C(B5	0.0199 (15)	0.0329 (17)	0.0116 (14)	−0.0037 (13)	0.0022 (12)	−0.0004 (12)
C14	0.0232 (17)	0.0372 (19)	0.0219 (16)	−0.0091 (14)	0.0029 (13)	−0.0003 (14)
C(B6	0.0208 (15)	0.0303 (17)	0.0138 (14)	−0.0063 (13)	0.0018 (12)	−0.0024 (12)
C15	0.0289 (17)	0.0242 (16)	0.0224 (16)	−0.0074 (13)	0.0055 (13)	−0.0009 (13)
C(B7	0.0179 (14)	0.0315 (17)	0.0152 (14)	−0.0017 (12)	0.0045 (12)	0.0034 (12)
C16	0.0247 (16)	0.0245 (16)	0.0144 (14)	−0.0039 (12)	0.0048 (12)	−0.0008 (12)
C(B8	0.0190 (15)	0.0288 (17)	0.0144 (14)	−0.0008 (12)	0.0061 (12)	0.0028 (12)
C17	0.0264 (16)	0.0243 (16)	0.0160 (14)	0.0007 (13)	0.0018 (12)	0.0021 (12)
C(M1	0.0199 (14)	0.0166 (14)	0.0135 (13)	−0.0013 (11)	0.0034 (11)	0.0006 (11)
C18	0.0269 (19)	0.046 (2)	0.043 (2)	−0.0137 (17)	−0.0033 (16)	0.0044 (19)
C(M2	0.0187 (14)	0.0280 (16)	0.0091 (13)	−0.0012 (12)	0.0030 (11)	0.0023 (11)

C19	0.0323 (18)	0.0207 (16)	0.0278 (17)	−0.0014 (13)	0.0045 (14)	−0.0017 (13)
C(M3	0.0165 (14)	0.0207 (14)	0.0141 (14)	0.0001 (11)	0.0001 (11)	0.0008 (11)
C20	0.0198 (15)	0.0301 (17)	0.0099 (13)	−0.0065 (13)	0.0031 (11)	0.0011 (12)
C(M4	0.0254 (16)	0.0223 (15)	0.0116 (14)	−0.0019 (12)	0.0073 (12)	−0.0009 (11)
C21	0.0254 (16)	0.0352 (18)	0.0150 (15)	−0.0051 (14)	0.0061 (12)	−0.0007 (13)
C22	0.0266 (17)	0.040 (2)	0.0185 (16)	−0.0066 (14)	0.0093 (13)	−0.0034 (14)
C23	0.0243 (16)	0.043 (2)	0.0122 (14)	−0.0139 (14)	0.0020 (12)	0.0007 (13)
C24	0.0197 (15)	0.0381 (19)	0.0170 (15)	−0.0080 (13)	−0.0010 (12)	0.0088 (13)
C25	0.0163 (14)	0.0375 (18)	0.0135 (14)	−0.0066 (13)	−0.0007 (11)	0.0037 (13)
C26	0.048 (2)	0.040 (2)	0.0275 (19)	0.0091 (18)	0.0164 (17)	0.0018 (16)
C27	0.036 (2)	0.062 (3)	0.0132 (16)	−0.0088 (18)	0.0054 (14)	0.0053 (16)
C28	0.0261 (17)	0.041 (2)	0.0236 (17)	0.0060 (15)	0.0009 (14)	0.0074 (15)
C29	0.0201 (15)	0.0291 (17)	0.0120 (13)	−0.0062 (12)	0.0038 (11)	−0.0009 (12)
C30	0.0194 (15)	0.044 (2)	0.0116 (14)	−0.0061 (14)	0.0032 (12)	−0.0034 (13)
C31	0.0209 (16)	0.062 (3)	0.0144 (15)	−0.0110 (16)	0.0056 (12)	−0.0083 (16)
C32	0.039 (2)	0.053 (2)	0.0203 (17)	−0.0248 (19)	0.0165 (15)	−0.0151 (16)
C33	0.047 (2)	0.0333 (19)	0.0280 (18)	−0.0164 (17)	0.0165 (17)	−0.0071 (15)
C34	0.0331 (18)	0.0299 (18)	0.0211 (16)	−0.0064 (14)	0.0091 (14)	−0.0031 (13)
C35	0.0210 (17)	0.047 (2)	0.0286 (19)	0.0036 (15)	−0.0005 (14)	0.0055 (16)
C36	0.048 (3)	0.074 (3)	0.039 (2)	−0.037 (2)	0.018 (2)	−0.021 (2)
C37	0.046 (2)	0.0275 (19)	0.048 (2)	0.0026 (17)	0.0080 (19)	0.0073 (17)
C38	0.0295 (17)	0.0300 (18)	0.0142 (15)	−0.0083 (13)	0.0088 (13)	−0.0049 (12)
C39	0.067 (3)	0.0282 (19)	0.029 (2)	−0.0063 (18)	0.0272 (19)	−0.0062 (15)
C40	0.064 (3)	0.036 (2)	0.032 (2)	−0.013 (2)	0.028 (2)	−0.0148 (17)
C41	0.038 (2)	0.051 (2)	0.0176 (17)	−0.0219 (18)	0.0124 (15)	−0.0099 (15)
C42	0.0323 (19)	0.048 (2)	0.0148 (16)	−0.0110 (16)	0.0050 (14)	0.0049 (14)
C43	0.0246 (17)	0.039 (2)	0.0136 (15)	−0.0070 (14)	0.0029 (12)	0.0003 (13)
C44	0.099 (4)	0.041 (3)	0.045 (3)	0.011 (3)	0.032 (3)	0.001 (2)
C45	0.053 (3)	0.068 (3)	0.0224 (19)	−0.031 (2)	0.0210 (18)	−0.0121 (19)
C46	0.048 (2)	0.050 (2)	0.0278 (19)	0.017 (2)	0.0127 (17)	0.0148 (18)
Cl1	0.0559 (8)	0.0756 (10)	0.0798 (10)	−0.0070 (7)	0.0095 (7)	−0.0022 (8)
C47	0.045 (3)	0.092 (4)	0.057 (3)	0.017 (3)	0.019 (2)	0.008 (3)
C48	0.060 (4)	0.124 (6)	0.071 (4)	0.031 (4)	0.022 (3)	0.031 (4)
C49	0.072 (4)	0.091 (5)	0.079 (4)	0.026 (4)	0.007 (4)	0.022 (4)
C50	0.111 (6)	0.070 (4)	0.083 (5)	−0.012 (4)	0.029 (4)	0.004 (4)
C51	0.083 (4)	0.062 (4)	0.076 (4)	−0.002 (3)	0.026 (3)	0.004 (3)
C52	0.054 (3)	0.064 (3)	0.050 (3)	0.008 (2)	0.017 (2)	−0.003 (2)
Cl1S	0.0578 (15)	0.0395 (11)	0.0622 (16)	0.0086 (11)	0.0356 (13)	0.0165 (11)
C1S	0.027 (6)	0.049 (6)	0.038 (6)	0.013 (4)	0.019 (5)	0.023 (5)
C2S	0.026 (7)	0.021 (7)	0.038 (9)	0.008 (5)	0.007 (6)	0.003 (5)
C3S	0.039 (7)	0.031 (7)	0.042 (6)	0.005 (5)	0.006 (5)	0.005 (5)
C4S	0.032 (6)	0.082 (11)	0.042 (7)	−0.022 (6)	−0.013 (5)	0.016 (7)
C5S	0.038 (7)	0.067 (10)	0.047 (7)	0.019 (7)	0.005 (5)	0.019 (7)
C6S	0.035 (10)	0.038 (11)	0.056 (13)	0.009 (7)	0.013 (9)	0.010 (7)
Cl2	0.0256 (11)	0.0238 (15)	0.0195 (9)	−0.0042 (9)	0.0035 (7)	−0.0016 (8)
O1	0.034 (3)	0.056 (4)	0.087 (4)	0.003 (2)	0.006 (3)	−0.025 (3)
O2	0.056 (3)	0.036 (2)	0.031 (2)	0.0142 (19)	0.0244 (19)	0.0079 (17)
O3	0.069 (5)	0.041 (4)	0.056 (6)	−0.003 (3)	0.019 (4)	0.023 (4)

O4	0.058 (3)	0.061 (4)	0.048 (3)	−0.020 (3)	−0.003 (2)	−0.007 (3)
Cl3	0.029 (3)	0.022 (3)	0.072 (6)	−0.002 (2)	0.014 (3)	−0.005 (3)
O1S	0.025 (5)	0.028 (5)	0.120 (10)	−0.001 (4)	0.011 (5)	−0.009 (5)
O2S	0.110 (12)	0.140 (14)	0.159 (15)	0.019 (11)	0.062 (12)	−0.034 (12)
O3S	0.063 (10)	0.117 (13)	0.223 (18)	0.017 (10)	−0.015 (11)	0.097 (13)
O4S	0.109 (17)	0.060 (13)	0.049 (9)	0.040 (12)	0.038 (12)	0.013 (8)

Geometric parameters (Å, º)

Fe1—N7	1.962 (3)	C21—C26	1.497 (5)
Fe1—N5	1.976 (3)	C22—C23	1.382 (5)
Fe1—N3	1.982 (2)	C22—H22	0.9500
Fe1—N4	1.987 (3)	C23—C24	1.392 (5)
Fe1—N1	1.988 (3)	C23—C27	1.509 (4)
Fe1—N2	1.993 (2)	C24—C25	1.399 (4)
N1—C(A2	1.370 (4)	C24—H24	0.9500
N1—C(A1	1.381 (4)	C25—C28	1.495 (5)
N2—C(A3	1.371 (4)	C26—H26A	0.9800
N2—C(A4	1.379 (4)	C26—H26B	0.9800
N3—C(A6	1.377 (4)	C26—H26C	0.9800
N3—C(A5	1.380 (4)	C27—H27A	0.9800
N4—C(A7	1.375 (4)	C27—H27B	0.9800
N4—C(A8	1.378 (4)	C27—H27C	0.9800
N5—C2	1.306 (5)	C28—H28A	0.9800
N5—C1	1.361 (5)	C28—H28B	0.9800
N6—C3	1.340 (6)	C28—H28C	0.9800
N6—C2	1.340 (5)	C29—C34	1.404 (5)
N6—C4	1.483 (6)	C29—C30	1.409 (5)
N7—C6	1.328 (4)	C30—C31	1.396 (5)
N7—C7	1.381 (4)	C30—C35	1.506 (5)
N8—C6	1.330 (4)	C31—C32	1.397 (6)
N8—C8	1.365 (5)	C31—H31	0.9500
N8—C9	1.477 (4)	C32—C33	1.371 (6)
C1—C3	1.343 (6)	C32—C36	1.511 (5)
C1—H1	0.9500	C33—C34	1.400 (5)
C(A1—C(M4	1.393 (4)	C33—H33	0.9500
C(A1—C(B1	1.435 (5)	C34—C37	1.512 (6)
C2—H2	0.9500	C35—H35A	0.9800
C(A2—C(M1	1.395 (4)	C35—H35B	0.9800
C(A2—C(B2	1.439 (4)	C35—H35C	0.9800
C3—H3	0.9500	C36—H36A	0.9800
C(A3—C(M1	1.390 (4)	C36—H36B	0.9800
C(A3—C(B3	1.436 (4)	C36—H36C	0.9800
C4—C5	1.487 (8)	C37—H37A	0.9800
C4—H4A	0.9900	C37—H37B	0.9800
C4—H4B	0.9900	C37—H37C	0.9800
C(A4—C(M2	1.384 (4)	C38—C39	1.383 (5)
C(A4—C(B4	1.439 (4)	C38—C43	1.397 (5)

C5—H5A	0.9800	C39—C40	1.399 (5)
C5—H5B	0.9800	C39—C44	1.480 (6)
C5—H5C	0.9800	C40—C41	1.354 (6)
C(A5—C(M2	1.394 (4)	C40—H40	0.9500
C(A5—C(B5	1.433 (4)	C41—C42	1.392 (6)
C6—H6	0.9500	C41—C45	1.511 (5)
C(A6—C(M3	1.389 (4)	C42—C43	1.394 (5)
C(A6—C(B6	1.440 (4)	C42—H42	0.9500
C7—C8	1.362 (5)	C43—C46	1.504 (6)
C7—H7	0.9500	C44—H44A	0.9800
C(A7—C(M3	1.391 (4)	C44—H44B	0.9800
C(A7—C(B7	1.445 (4)	C44—H44C	0.9800
C8—H8	0.9500	C45—H45A	0.9800
C(A8—C(M4	1.398 (4)	C45—H45B	0.9800
C(A8—C(B8	1.435 (4)	C45—H45C	0.9800
C9—C10	1.512 (7)	C46—H46A	0.9800
C9—H9A	0.9900	C46—H46B	0.9800
C9—H9B	0.9900	C46—H46C	0.9800
C(B1—C(B2	1.345 (5)	Cl1—C47	1.733 (7)
C(B1—H(B1	0.9500	C47—C52	1.353 (8)
C10—H10A	0.9800	C47—C48	1.367 (9)
C10—H10B	0.9800	C48—C49	1.421 (11)
C10—H10C	0.9800	C48—H48	0.9500
C(B2—H(B2	0.9500	C49—C50	1.396 (11)
C11—C16	1.406 (5)	C49—H49	0.9500
C11—C12	1.407 (4)	C50—C51	1.420 (10)
C11—C(M1	1.494 (4)	C50—H50	0.9500
C(B3—C(B4	1.354 (4)	C51—C52	1.402 (9)
C(B3—H(B3	0.9500	C51—H51	0.9500
C12—C13	1.397 (5)	C52—H52	0.9500
C12—C17	1.508 (4)	Cl1S—C4S^{i}	1.019 (15)
C(B4—H(B4	0.9500	Cl1S—C1S	1.693 (14)
C13—C14	1.395 (5)	Cl1S—C3S^{i}	2.072 (14)
C13—H13	0.9500	Cl1S—C5S^{i}	2.110 (17)
C(B5—C(B6	1.360 (5)	C1S—C4S^{i}	0.699 (14)
C(B5—H(B5	0.9500	C1S—C3S^{i}	1.183 (16)
C14—C15	1.389 (5)	C1S—C5S^{i}	1.212 (17)
C14—C18	1.512 (5)	C1S—C6S	1.379 (18)
C(B6—H(B6	0.9500	C1S—C2S	1.434 (15)
C15—C16	1.394 (5)	C1S—C2S^{i}	1.86 (2)
C15—H15	0.9500	C1S—C6S^{i}	1.90 (2)
C(B7—C(B8	1.353 (5)	C2S—C3S	1.410 (16)
C(B7—H(B7	0.9500	C2S—C4S^{i}	1.87 (2)
C16—C19	1.506 (5)	C2S—H2S	0.9500
C(B8—H(B8	0.9500	C3S—C4S	1.377 (19)
C17—H17A	0.9800	C3S—H3S	0.9500
C17—H17B	0.9800	C4S—C5S	1.39 (2)
C17—H17C	0.9800	C4S—C6S^{i}	1.84 (2)

C18—H18A	0.9800	C4S—H4S	0.9500
C18—H18B	0.9800	C5S—C6S	1.42 (2)
C18—H18C	0.9800	C5S—H5S	0.9500
C(M2—C20	1.504 (4)	C6S—H6S	0.9500
C19—H19A	0.9800	Cl2—O2	1.407 (5)
C19—H19B	0.9800	Cl2—O3	1.425 (14)
C19—H19C	0.9800	Cl2—O1	1.443 (7)
C(M3—C29	1.497 (4)	Cl2—O4	1.467 (5)
C20—C21	1.400 (5)	Cl3—O3S	1.18 (2)
C20—C25	1.404 (5)	Cl3—O1S	1.336 (13)
C(M4—C38	1.501 (4)	Cl3—O4S	1.36 (3)
C21—C22	1.401 (5)	Cl3—O2S	1.42 (2)

N7—Fe1—N5	177.03 (10)	C(A1—C(M4—C38	119.6 (3)
N7—Fe1—N3	89.93 (10)	C(A8—C(M4—C38	117.7 (3)
N5—Fe1—N3	88.18 (11)	C20—C21—C22	118.2 (3)
N7—Fe1—N4	91.10 (10)	C20—C21—C26	121.3 (3)
N5—Fe1—N4	91.19 (11)	C22—C21—C26	120.5 (3)
N3—Fe1—N4	90.03 (10)	C23—C22—C21	122.4 (3)
N7—Fe1—N1	88.40 (10)	C23—C22—H22	118.8
N5—Fe1—N1	93.50 (11)	C21—C22—H22	118.8
N3—Fe1—N1	178.32 (11)	C22—C23—C24	118.6 (3)
N4—Fe1—N1	89.84 (10)	C22—C23—C27	121.6 (4)
N7—Fe1—N2	89.20 (10)	C24—C23—C27	119.7 (3)
N5—Fe1—N2	88.52 (11)	C23—C24—C25	121.1 (3)
N3—Fe1—N2	90.41 (10)	C23—C24—H24	119.4
N4—Fe1—N2	179.47 (11)	C25—C24—H24	119.4
N1—Fe1—N2	89.72 (10)	C24—C25—C20	119.1 (3)
C(A2—N1—C(A1	105.3 (2)	C24—C25—C28	120.0 (3)
C(A2—N1—Fe1	126.8 (2)	C20—C25—C28	120.9 (3)
C(A1—N1—Fe1	127.4 (2)	C21—C26—H26A	109.5
C(A3—N2—C(A4	106.2 (2)	C21—C26—H26B	109.5
C(A3—N2—Fe1	127.43 (19)	H26A—C26—H26B	109.5
C(A4—N2—Fe1	126.4 (2)	C21—C26—H26C	109.5
C(A6—N3—C(A5	106.0 (2)	H26A—C26—H26C	109.5
C(A6—N3—Fe1	127.36 (19)	H26B—C26—H26C	109.5
C(A5—N3—Fe1	126.7 (2)	C23—C27—H27A	109.5
C(A7—N4—C(A8	105.6 (2)	C23—C27—H27B	109.5
C(A7—N4—Fe1	126.9 (2)	H27A—C27—H27B	109.5
C(A8—N4—Fe1	127.5 (2)	C23—C27—H27C	109.5
C2—N5—C1	105.1 (3)	H27A—C27—H27C	109.5
C2—N5—Fe1	126.6 (2)	H27B—C27—H27C	109.5
C1—N5—Fe1	126.2 (2)	C25—C28—H28A	109.5
C3—N6—C2	107.4 (3)	C25—C28—H28B	109.5
C3—N6—C4	123.2 (4)	H28A—C28—H28B	109.5
C2—N6—C4	128.2 (4)	C25—C28—H28C	109.5
C6—N7—C7	105.7 (3)	H28A—C28—H28C	109.5
C6—N7—Fe1	125.4 (2)	H28B—C28—H28C	109.5

C7—N7—Fe1	128.1 (2)	C34—C29—C30	119.9 (3)
C6—N8—C8	108.1 (3)	C34—C29—C(M3	119.4 (3)
C6—N8—C9	124.7 (3)	C30—C29—C(M3	120.5 (3)
C8—N8—C9	126.7 (3)	C31—C30—C29	118.9 (4)
C3—C1—N5	109.9 (4)	C31—C30—C35	120.4 (3)
C3—C1—H1	125.0	C29—C30—C35	120.7 (3)
N5—C1—H1	125.0	C30—C31—C32	121.6 (4)
N1—C(A1—C(M4	126.2 (3)	C30—C31—H31	119.2
N1—C(A1—C(B1	110.1 (3)	C32—C31—H31	119.2
C(M4—C(A1—C(B1	123.7 (3)	C33—C32—C31	118.5 (3)
N5—C2—N6	111.2 (4)	C33—C32—C36	121.0 (4)
N5—C2—H2	124.4	C31—C32—C36	120.5 (4)
N6—C2—H2	124.4	C32—C33—C34	122.3 (4)
N1—C(A2—C(M1	126.5 (3)	C32—C33—H33	118.9
N1—C(A2—C(B2	110.6 (3)	C34—C33—H33	118.9
C(M1—C(A2—C(B2	122.9 (3)	C33—C34—C29	118.8 (4)
N6—C3—C1	106.3 (3)	C33—C34—C37	119.3 (4)
N6—C3—H3	126.8	C29—C34—C37	121.9 (3)
C1—C3—H3	126.8	C30—C35—H35A	109.5
N2—C(A3—C(M1	125.9 (3)	C30—C35—H35B	109.5
N2—C(A3—C(B3	110.1 (3)	H35A—C35—H35B	109.5
C(M1—C(A3—C(B3	124.0 (3)	C30—C35—H35C	109.5
N6—C4—C5	112.2 (4)	H35A—C35—H35C	109.5
N6—C4—H4A	109.2	H35B—C35—H35C	109.5
C5—C4—H4A	109.2	C32—C36—H36A	109.5
N6—C4—H4B	109.2	C32—C36—H36B	109.5
C5—C4—H4B	109.2	H36A—C36—H36B	109.5
H4A—C4—H4B	107.9	C32—C36—H36C	109.5
N2—C(A4—C(M2	126.0 (3)	H36A—C36—H36C	109.5
N2—C(A4—C(B4	109.6 (3)	H36B—C36—H36C	109.5
C(M2—C(A4—C(B4	124.2 (3)	C34—C37—H37A	109.5
C4—C5—H5A	109.5	C34—C37—H37B	109.5
C4—C5—H5B	109.5	H37A—C37—H37B	109.5
H5A—C5—H5B	109.5	C34—C37—H37C	109.5
C4—C5—H5C	109.5	H37A—C37—H37C	109.5
H5A—C5—H5C	109.5	H37B—C37—H37C	109.5
H5B—C5—H5C	109.5	C39—C38—C43	119.4 (3)
N3—C(A5—C(M2	126.0 (3)	C39—C38—C(M4	120.9 (3)
N3—C(A5—C(B5	109.9 (3)	C43—C38—C(M4	119.7 (3)
C(M2—C(A5—C(B5	124.1 (3)	C38—C39—C40	119.5 (4)
N7—C6—N8	111.1 (3)	C38—C39—C44	120.4 (3)
N7—C6—H6	124.5	C40—C39—C44	119.8 (4)
N8—C6—H6	124.5	C41—C40—C39	122.4 (4)
N3—C(A6—C(M3	125.9 (3)	C41—C40—H40	118.8
N3—C(A6—C(B6	110.0 (3)	C39—C40—H40	118.8
C(M3—C(A6—C(B6	123.8 (3)	C40—C41—C42	117.6 (3)
C8—C7—N7	108.9 (3)	C40—C41—C45	121.4 (4)
C8—C7—H7	125.6	C42—C41—C45	120.9 (4)

N7—C7—H7	125.6	C41—C42—C43	122.0 (4)
N4—C(A7—C(M3	126.4 (3)	C41—C42—H42	119.0
N4—C(A7—C(B7	110.2 (3)	C43—C42—H42	119.0
C(M3—C(A7—C(B7	123.4 (3)	C42—C43—C38	118.8 (3)
C7—C8—N8	106.3 (3)	C42—C43—C46	119.7 (3)
C7—C8—H8	126.9	C38—C43—C46	121.5 (3)
N8—C8—H8	126.9	C39—C44—H44A	109.5
N4—C(A8—C(M4	125.9 (3)	C39—C44—H44B	109.5
N4—C(A8—C(B8	110.3 (3)	H44A—C44—H44B	109.5
C(M4—C(A8—C(B8	123.5 (3)	C39—C44—H44C	109.5
N8—C9—C10	110.0 (3)	H44A—C44—H44C	109.5
N8—C9—H9A	109.7	H44B—C44—H44C	109.5
C10—C9—H9A	109.7	C41—C45—H45A	109.5
N8—C9—H9B	109.7	C41—C45—H45B	109.5
C10—C9—H9B	109.7	H45A—C45—H45B	109.5
H9A—C9—H9B	108.2	C41—C45—H45C	109.5
C(B2—C(B1—C(A1	107.3 (3)	H45A—C45—H45C	109.5
C(B2—C(B1—H(B1	126.3	H45B—C45—H45C	109.5
C(A1—C(B1—H(B1	126.3	C43—C46—H46A	109.5
C9—C10—H10A	109.5	C43—C46—H46B	109.5
C9—C10—H10B	109.5	H46A—C46—H46B	109.5
H10A—C10—H10B	109.5	C43—C46—H46C	109.5
C9—C10—H10C	109.5	H46A—C46—H46C	109.5
H10A—C10—H10C	109.5	H46B—C46—H46C	109.5
H10B—C10—H10C	109.5	C52—C47—C48	122.8 (7)
C(B1—C(B2—C(A2	106.7 (3)	C52—C47—Cl1	120.4 (5)
C(B1—C(B2—H(B2	126.6	C48—C47—Cl1	116.8 (6)
C(A2—C(B2—H(B2	126.6	C47—C48—C49	116.0 (7)
C16—C11—C12	120.3 (3)	C47—C48—H48	122.0
C16—C11—C(M1	120.9 (3)	C49—C48—H48	122.0
C12—C11—C(M1	118.8 (3)	C50—C49—C48	122.4 (6)
C(B4—C(B3—C(A3	106.9 (3)	C50—C49—H49	118.8
C(B4—C(B3—H(B3	126.5	C48—C49—H49	118.8
C(A3—C(B3—H(B3	126.5	C49—C50—C51	119.2 (7)
C13—C12—C11	119.1 (3)	C49—C50—H50	120.4
C13—C12—C17	119.7 (3)	C51—C50—H50	120.4
C11—C12—C17	121.2 (3)	C52—C51—C50	116.5 (7)
C(B3—C(B4—C(A4	107.2 (3)	C52—C51—H51	121.7
C(B3—C(B4—H(B4	126.4	C50—C51—H51	121.7
C(A4—C(B4—H(B4	126.4	C47—C52—C51	122.8 (6)
C14—C13—C12	121.3 (3)	C47—C52—H52	118.6
C14—C13—H13	119.4	C51—C52—H52	118.6
C12—C13—H13	119.4	C4S^{i}—Cl1S—C1S	8.1 (9)
C(B6—C(B5—C(A5	107.3 (3)	C4S^{i}—C1S—C6S	120 (2)
C(B6—C(B5—H(B5	126.4	C3S^{i}—C1S—C6S	30.2 (7)
C(A5—C(B5—H(B5	126.4	C5S^{i}—C1S—C6S	147.6 (14)
C15—C14—C13	118.6 (3)	C4S^{i}—C1S—C2S	119 (2)
C15—C14—C18	121.2 (3)	C3S^{i}—C1S—C2S	148.1 (14)

C13—C14—C18	120.3 (3)	C5S^{i}—C1S—C2S	29.6 (7)
C(B5—C(B6—C(A6	106.8 (3)	C6S—C1S—C2S	119.0 (11)
C(B5—C(B6—H(B6	126.6	C4S^{i}—C1S—Cl1S	11.9 (14)
C(A6—C(B6—H(B6	126.6	C3S^{i}—C1S—Cl1S	90.4 (10)
C14—C15—C16	122.1 (3)	C5S^{i}—C1S—Cl1S	91.6 (12)
C14—C15—H15	119.0	C6S—C1S—Cl1S	120.1 (10)
C16—C15—H15	119.0	C2S—C1S—Cl1S	120.8 (9)
C(B8—C(B7—C(A7	106.7 (3)	C3S—C2S—C1S	119.6 (13)
C(B8—C(B7—H(B7	126.7	C3S—C2S—C4S^{i}	138.2 (12)
C(A7—C(B7—H(B7	126.7	C1S—C2S—C4S^{i}	19.1 (6)
C15—C16—C11	118.7 (3)	C1S^{i}—C2S—C4S^{i}	98.8 (8)
C15—C16—C19	120.0 (3)	C3S—C2S—H2S	120.2
C11—C16—C19	121.3 (3)	C1S—C2S—H2S	120.2
C(B7—C(B8—C(A8	107.2 (3)	C1S^{i}—C2S—H2S	158.8
C(B7—C(B8—H(B8	126.4	C4S^{i}—C2S—H2S	101.5
C(A8—C(B8—H(B8	126.4	C4S—C3S—C2S	121.4 (15)
C12—C17—H17A	109.5	C4S—C3S—H3S	119.3
C12—C17—H17B	109.5	C2S—C3S—H3S	119.3
H17A—C17—H17B	109.5	Cl1S^{i}—C3S—H3S	94.2
C12—C17—H17C	109.5	C3S—C4S—C5S	118.7 (14)
H17A—C17—H17C	109.5	C3S—C4S—H4S	120.7
H17B—C17—H17C	109.5	C5S—C4S—H4S	120.7
C(A3—C(M1—C(A2	122.8 (3)	C6S^{i}—C4S—H4S	139.2
C(A3—C(M1—C11	119.1 (3)	C2S^{i}—C4S—H4S	138.9
C(A2—C(M1—C11	118.1 (3)	C4S—C5S—C6S	121.7 (14)
C14—C18—H18A	109.5	C4S—C5S—H5S	119.2
C14—C18—H18B	109.5	C6S—C5S—H5S	119.2
H18A—C18—H18B	109.5	Cl1S^{i}—C5S—H5S	95.2
C14—C18—H18C	109.5	C1S—C6S—C5S	119.6 (13)
H18A—C18—H18C	109.5	C1S—C6S—C4S^{i}	19.2 (8)
H18B—C18—H18C	109.5	C5S—C6S—C4S^{i}	138.2 (13)
C(A4—C(M2—C(A5	123.4 (3)	C1S—C6S—H6S	120.2
C(A4—C(M2—C20	118.3 (3)	C5S—C6S—H6S	120.2
C(A5—C(M2—C20	118.3 (3)	C4S^{i}—C6S—H6S	101.4
C16—C19—H19A	109.5	C1S^{i}—C6S—H6S	159.0
C16—C19—H19B	109.5	O2—Cl2—O3	111.1 (7)
H19A—C19—H19B	109.5	O2—Cl2—O1	106.7 (4)
C16—C19—H19C	109.5	O3—Cl2—O1	103.0 (6)
H19A—C19—H19C	109.5	O2—Cl2—O4	111.0 (4)
H19B—C19—H19C	109.5	O3—Cl2—O4	118.4 (6)
C(A6—C(M3—C(A7	122.8 (3)	O1—Cl2—O4	105.6 (4)
C(A6—C(M3—C29	119.7 (3)	O3S—Cl3—O1S	137.3 (15)
C(A7—C(M3—C29	117.4 (3)	O3S—Cl3—O4S	130.7 (18)
C21—C20—C25	120.7 (3)	O1S—Cl3—O4S	90.8 (14)
C21—C20—C(M2	120.5 (3)	O3S—Cl3—O2S	84.9 (18)
C25—C20—C(M2	118.8 (3)	O1S—Cl3—O2S	99.3 (11)
C(A1—C(M4—C(A8	122.6 (3)	O4S—Cl3—O2S	99.7 (18)

C2—N5—C1—C3	1.9 (5)	C22—C23—C24—C25	−0.6 (5)
Fe1—N5—C1—C3	166.2 (3)	C27—C23—C24—C25	177.4 (3)
C(A2—N1—C(A1—C(M4	176.2 (3)	C23—C24—C25—C20	1.5 (5)
Fe1—N1—C(A1—C(M4	4.2 (5)	C23—C24—C25—C28	−176.3 (3)
C(A2—N1—C(A1—C(B1	−1.3 (4)	C21—C20—C25—C24	−1.6 (5)
Fe1—N1—C(A1—C(B1	−173.3 (2)	C(M2—C20—C25—C24	178.2 (3)
C1—N5—C2—N6	−2.7 (5)	C21—C20—C25—C28	176.2 (3)
Fe1—N5—C2—N6	−166.9 (3)	C(M2—C20—C25—C28	−4.0 (5)
C3—N6—C2—N5	2.6 (6)	C(A6—C(M3—C29—C34	−102.9 (4)
C4—N6—C2—N5	169.8 (5)	C(A7—C(M3—C29—C34	78.9 (4)
C(A1—N1—C(A2—C(M1	−179.4 (3)	C(A6—C(M3—C29—C30	80.7 (4)
Fe1—N1—C(A2—C(M1	−7.3 (5)	C(A7—C(M3—C29—C30	−97.5 (4)
C(A1—N1—C(A2—C(B2	1.2 (3)	C34—C29—C30—C31	0.8 (5)
Fe1—N1—C(A2—C(B2	173.2 (2)	C(M3—C29—C30—C31	177.2 (3)
C2—N6—C3—C1	−1.3 (6)	C34—C29—C30—C35	−176.6 (3)
C4—N6—C3—C1	−169.4 (5)	C(M3—C29—C30—C35	−0.2 (5)
N5—C1—C3—N6	−0.3 (5)	C29—C30—C31—C32	−0.7 (5)
C(A4—N2—C(A3—C(M1	−177.1 (3)	C35—C30—C31—C32	176.8 (3)
Fe1—N2—C(A3—C(M1	1.8 (4)	C30—C31—C32—C33	−0.1 (5)
C(A4—N2—C(A3—C(B3	0.8 (3)	C30—C31—C32—C36	−178.1 (3)
Fe1—N2—C(A3—C(B3	179.8 (2)	C31—C32—C33—C34	0.8 (5)
C3—N6—C4—C5	−155.4 (5)	C36—C32—C33—C34	178.8 (3)
C2—N6—C4—C5	39.1 (8)	C32—C33—C34—C29	−0.7 (5)
C(A3—N2—C(A4—C(M2	−174.4 (3)	C32—C33—C34—C37	−178.1 (4)
Fe1—N2—C(A4—C(M2	6.6 (5)	C30—C29—C34—C33	−0.2 (5)
C(A3—N2—C(A4—C(B4	0.6 (3)	C(M3—C29—C34—C33	−176.6 (3)
Fe1—N2—C(A4—C(B4	−178.4 (2)	C30—C29—C34—C37	177.2 (3)
C(A6—N3—C(A5—C(M2	178.8 (3)	C(M3—C29—C34—C37	0.7 (5)
Fe1—N3—C(A5—C(M2	−2.3 (5)	C(A1—C(M4—C38—C39	−79.0 (5)
C(A6—N3—C(A5—C(B5	0.4 (3)	C(A8—C(M4—C38—C39	104.0 (4)
Fe1—N3—C(A5—C(B5	179.2 (2)	C(A1—C(M4—C38—C43	101.4 (4)
C7—N7—C6—N8	−0.3 (4)	C(A8—C(M4—C38—C43	−75.7 (4)
Fe1—N7—C6—N8	170.4 (2)	C43—C38—C39—C40	4.8 (6)
C8—N8—C6—N7	0.0 (4)	C(M4—C38—C39—C40	−174.9 (4)
C9—N8—C6—N7	−172.3 (3)	C43—C38—C39—C44	−168.9 (5)
C(A5—N3—C(A6—C(M3	172.9 (3)	C(M4—C38—C39—C44	11.4 (7)
Fe1—N3—C(A6—C(M3	−5.9 (4)	C38—C39—C40—C41	0.6 (7)
C(A5—N3—C(A6—C(B6	−1.3 (3)	C44—C39—C40—C41	174.4 (5)
Fe1—N3—C(A6—C(B6	179.8 (2)	C39—C40—C41—C42	−5.2 (7)
C6—N7—C7—C8	0.5 (4)	C39—C40—C41—C45	177.0 (4)
Fe1—N7—C7—C8	−169.8 (2)	C40—C41—C42—C43	4.4 (6)
C(A8—N4—C(A7—C(M3	179.1 (3)	C45—C41—C42—C43	−177.7 (4)
Fe1—N4—C(A7—C(M3	−1.6 (5)	C41—C42—C43—C38	0.9 (5)
C(A8—N4—C(A7—C(B7	−1.4 (3)	C41—C42—C43—C46	−178.1 (4)
Fe1—N4—C(A7—C(B7	177.9 (2)	C39—C38—C43—C42	−5.5 (5)
N7—C7—C8—N8	−0.5 (4)	C(M4—C38—C43—C42	174.2 (3)
C6—N8—C8—C7	0.3 (4)	C39—C38—C43—C46	173.4 (4)
C9—N8—C8—C7	172.4 (3)	C(M4—C38—C43—C46	−6.9 (5)

C(A7—N4—C(A8—C(M4	−171.4 (3)	C52—C47—C48—C49	−4.9 (9)
Fe1—N4—C(A8—C(M4	9.2 (4)	Cl1—C47—C48—C49	173.8 (5)
C(A7—N4—C(A8—C(B8	2.2 (3)	C47—C48—C49—C50	5.9 (10)
Fe1—N4—C(A8—C(B8	−177.2 (2)	C48—C49—C50—C51	−4.5 (11)
C6—N8—C9—C10	88.3 (4)	C49—C50—C51—C52	1.9 (10)
C8—N8—C9—C10	−82.6 (5)	C48—C47—C52—C51	2.7 (9)
N1—C(A1—C(B1—C(B2	1.1 (4)	Cl1—C47—C52—C51	−176.0 (4)
C(M4—C(A1—C(B1—C(B2	−176.6 (3)	C50—C51—C52—C47	−0.9 (9)
C(A1—C(B1—C(B2—C(A2	−0.3 (4)	C3S^{i}—Cl1S—C1S—C4S^{i}	−90 (8)
N1—C(A2—C(B2—C(B1	−0.5 (4)	C5S^{i}—Cl1S—C1S—C4S^{i}	78 (8)
C(M1—C(A2—C(B2—C(B1	−180.0 (3)	C4S^{i}—Cl1S—C1S—C3S^{i}	90 (8)
N2—C(A3—C(B3—C(B4	−1.9 (4)	C5S^{i}—Cl1S—C1S—C3S^{i}	167.8 (14)
C(M1—C(A3—C(B3—C(B4	176.1 (3)	C4S^{i}—Cl1S—C1S—C5S^{i}	−78 (8)
C16—C11—C12—C13	1.4 (4)	C3S^{i}—Cl1S—C1S—C5S^{i}	−167.8 (14)
C(M1—C11—C12—C13	−179.3 (3)	C4S^{i}—Cl1S—C1S—C6S	95 (8)
C16—C11—C12—C17	−176.8 (3)	C3S^{i}—Cl1S—C1S—C6S	5.4 (10)
C(M1—C11—C12—C17	2.5 (4)	C5S^{i}—Cl1S—C1S—C6S	173.2 (15)
C(A3—C(B3—C(B4—C(A4	2.2 (4)	C4S^{i}—Cl1S—C1S—C2S	−83 (8)
N2—C(A4—C(B4—C(B3	−1.8 (4)	C3S^{i}—Cl1S—C1S—C2S	−173.1 (14)
C(M2—C(A4—C(B4—C(B3	173.3 (3)	C5S^{i}—Cl1S—C1S—C2S	−5.3 (9)
C11—C12—C13—C14	−1.5 (5)	C4S^{i}—Cl1S—C1S—C2S^{i}	91 (8)
C17—C12—C13—C14	176.7 (3)	C3S^{i}—Cl1S—C1S—C2S^{i}	1.5 (10)
N3—C(A5—C(B5—C(B6	0.7 (4)	C5S^{i}—Cl1S—C1S—C2S^{i}	169.3 (15)
C(M2—C(A5—C(B5—C(B6	−177.7 (3)	C4S^{i}—Cl1S—C1S—C6S^{i}	−80 (8)
C12—C13—C14—C15	0.6 (5)	C3S^{i}—Cl1S—C1S—C6S^{i}	−169.2 (16)
C12—C13—C14—C18	179.4 (3)	C5S^{i}—Cl1S—C1S—C6S^{i}	−1.4 (10)
C(A5—C(B5—C(B6—C(A6	−1.5 (4)	C4S^{i}—C1S—C2S—C3S	168 (2)
N3—C(A6—C(B6—C(B5	1.8 (4)	C3S^{i}—C1S—C2S—C3S	14 (3)
C(M3—C(A6—C(B6—C(B5	−172.5 (3)	C5S^{i}—C1S—C2S—C3S	170 (2)
C13—C14—C15—C16	0.5 (5)	C6S—C1S—C2S—C3S	2.8 (17)
C18—C14—C15—C16	−178.2 (3)	Cl1S—C1S—C2S—C3S	−178.7 (10)
N4—C(A7—C(B7—C(B8	0.2 (4)	C2S^{i}—C1S—C2S—C3S	4.8 (11)
C(M3—C(A7—C(B7—C(B8	179.7 (3)	C6S^{i}—C1S—C2S—C3S	8.8 (14)
C14—C15—C16—C11	−0.6 (5)	C4S^{i}—C1S—C2S—C1S^{i}	163 (2)
C14—C15—C16—C19	−178.7 (3)	C3S^{i}—C1S—C2S—C1S^{i}	10 (2)
C12—C11—C16—C15	−0.3 (4)	C5S^{i}—C1S—C2S—C1S^{i}	166 (2)
C(M1—C11—C16—C15	−179.6 (3)	C6S—C1S—C2S—C1S^{i}	−2.1 (9)
C12—C11—C16—C19	177.7 (3)	Cl1S—C1S—C2S—C1S^{i}	176.4 (9)
C(M1—C11—C16—C19	−1.6 (4)	C2S^{i}—C1S—C2S—C1S^{i}	0.000 (1)
C(A7—C(B7—C(B8—C(A8	1.1 (4)	C6S^{i}—C1S—C2S—C1S^{i}	4.0 (17)
N4—C(A8—C(B8—C(B7	−2.1 (4)	C3S^{i}—C1S—C2S—C4S^{i}	−153 (4)
C(M4—C(A8—C(B8—C(B7	171.6 (3)	C5S^{i}—C1S—C2S—C4S^{i}	3 (3)
N2—C(A3—C(M1—C(A2	5.2 (5)	C6S—C1S—C2S—C4S^{i}	−165 (3)
C(B3—C(A3—C(M1—C(A2	−172.5 (3)	Cl1S—C1S—C2S—C4S^{i}	13.5 (16)
N2—C(A3—C(M1—C11	−174.3 (3)	C2S^{i}—C1S—C2S—C4S^{i}	−163 (2)
C(B3—C(A3—C(M1—C11	8.0 (5)	C6S^{i}—C1S—C2S—C4S^{i}	−159 (2)
N1—C(A2—C(M1—C(A3	−2.3 (5)	C1S—C2S—C3S—C4S	−1 (2)
C(B2—C(A2—C(M1—C(A3	177.1 (3)	C1S^{i}—C2S—C3S—C4S	6.3 (10)

N1—C(A2—C(M1—C11	177.2 (3)	C4S^{i}—C2S—C3S—C4S	5 (3)
C(B2—C(A2—C(M1—C11	−3.4 (5)	C1S—C2S—C3S—Cl1S^{i}	−9 (3)
C16—C11—C(M1—C(A3	−82.7 (4)	C1S^{i}—C2S—C3S—Cl1S^{i}	−1.8 (13)
C12—C11—C(M1—C(A3	98.0 (3)	C4S^{i}—C2S—C3S—Cl1S^{i}	−3 (3)
C16—C11—C(M1—C(A2	97.8 (4)	C2S—C3S—C4S—C5S	0 (2)
C12—C11—C(M1—C(A2	−81.5 (4)	Cl1S^{i}—C3S—C4S—C5S	169 (2)
N2—C(A4—C(M2—C(A5	3.8 (5)	C2S—C3S—C4S—C6S^{i}	−9.4 (16)
C(B4—C(A4—C(M2—C(A5	−170.5 (3)	Cl1S^{i}—C3S—C4S—C6S^{i}	160 (2)
N2—C(A4—C(M2—C20	−176.1 (3)	C2S—C3S—C4S—C2S^{i}	−3.2 (18)
C(B4—C(A4—C(M2—C20	9.6 (5)	Cl1S^{i}—C3S—C4S—C2S^{i}	166.3 (18)
N3—C(A5—C(M2—C(A4	−6.1 (5)	C3S—C4S—C5S—C6S	0 (2)
C(B5—C(A5—C(M2—C(A4	172.2 (3)	C6S^{i}—C4S—C5S—C6S	3.2 (18)
N3—C(A5—C(M2—C20	173.8 (3)	C2S^{i}—C4S—C5S—C6S	9.4 (15)
C(B5—C(A5—C(M2—C20	−7.9 (5)	C3S—C4S—C5S—Cl1S^{i}	−169 (2)
N3—C(A6—C(M3—C(A7	−2.0 (5)	C6S^{i}—C4S—C5S—Cl1S^{i}	−166.0 (18)
C(B6—C(A6—C(M3—C(A7	171.4 (3)	C2S^{i}—C4S—C5S—Cl1S^{i}	−160 (2)
N3—C(A6—C(M3—C29	179.8 (3)	C4S^{i}—C1S—C6S—C5S	−168 (2)
C(B6—C(A6—C(M3—C29	−6.7 (5)	C3S^{i}—C1S—C6S—C5S	−171 (3)
N4—C(A7—C(M3—C(A6	6.0 (5)	C5S^{i}—C1S—C6S—C5S	−14 (3)
C(B7—C(A7—C(M3—C(A6	−173.5 (3)	C2S—C1S—C6S—C5S	−2.8 (17)
N4—C(A7—C(M3—C29	−175.9 (3)	Cl1S—C1S—C6S—C5S	178.7 (10)
C(B7—C(A7—C(M3—C29	4.7 (5)	C2S^{i}—C1S—C6S—C5S	−8.9 (14)
C(A4—C(M2—C20—C21	−90.1 (4)	C6S^{i}—C1S—C6S—C5S	−4.8 (11)
C(A5—C(M2—C20—C21	90.0 (4)	C3S^{i}—C1S—C6S—C4S^{i}	−3 (3)
C(A4—C(M2—C20—C25	90.1 (4)	C5S^{i}—C1S—C6S—C4S^{i}	153 (4)
C(A5—C(M2—C20—C25	−89.8 (4)	C2S—C1S—C6S—C4S^{i}	165 (3)
N1—C(A1—C(M4—C(A8	−3.2 (5)	Cl1S—C1S—C6S—C4S^{i}	−13.7 (16)
C(B1—C(A1—C(M4—C(A8	174.0 (3)	C2S^{i}—C1S—C6S—C4S^{i}	159 (2)
N1—C(A1—C(M4—C38	179.9 (3)	C6S^{i}—C1S—C6S—C4S^{i}	163 (2)
C(B1—C(A1—C(M4—C38	−2.9 (5)	C4S^{i}—C1S—C6S—C1S^{i}	−163 (2)
N4—C(A8—C(M4—C(A1	−3.8 (5)	C3S^{i}—C1S—C6S—C1S^{i}	−166 (2)
C(B8—C(A8—C(M4—C(A1	−176.5 (3)	C5S^{i}—C1S—C6S—C1S^{i}	−9 (2)
N4—C(A8—C(M4—C38	173.1 (3)	C2S—C1S—C6S—C1S^{i}	2.0 (9)
C(B8—C(A8—C(M4—C38	0.4 (5)	Cl1S—C1S—C6S—C1S^{i}	−176.5 (9)
C25—C20—C21—C22	0.8 (5)	C2S^{i}—C1S—C6S—C1S^{i}	−4.1 (17)
C(M2—C20—C21—C22	−179.0 (3)	C6S^{i}—C1S—C6S—C1S^{i}	0.000 (1)
C25—C20—C21—C26	−178.4 (3)	C4S—C5S—C6S—C1S	1 (2)
C(M2—C20—C21—C26	1.8 (5)	Cl1S^{i}—C5S—C6S—C1S	9 (3)
C20—C21—C22—C23	0.1 (5)	C4S—C5S—C6S—C4S^{i}	−5 (3)
C26—C21—C22—C23	179.3 (4)	Cl1S^{i}—C5S—C6S—C4S^{i}	3 (3)
C21—C22—C23—C24	−0.2 (5)	C4S—C5S—C6S—C1S^{i}	−6.1 (10)
C21—C22—C23—C27	−178.2 (3)	Cl1S^{i}—C5S—C6S—C1S^{i}	1.7 (12)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

C(*B*4—H(*B*4···Cl1*S*^{ii}	0.95	2.91	3.713 (4)	143

Symmetry code: (ii) $x+1/2, -y+1/2, z+1/2$.