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ISSN 2414-3146

Bis(1-phenylimidazole)[5,10,15,20-tetrakis(2-pivalamidophenyl)porphinato]iron(III) trifluoromethanesulfonate chlorobenzene disolvate

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Received 13 December 2018
Accepted 4 January 2019

Edited by S. Parkin, University of Kentucky, USA

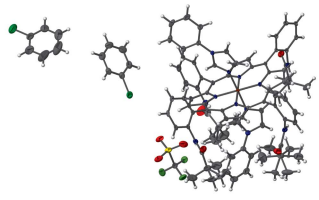
Keywords: crystal structure; iron(III)porphyrin; teraphenylporphyrin; bis(imidazole) complex.

CCDC reference: 1888676

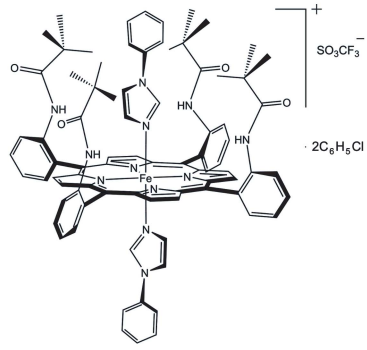
Structural data: full structural data are available from iucrdata.iucr.org

The title complex, $[Fe(C_{64}H_{64}N_8O_4)(C_9H_8N_2)_2](CF_3O_3S)\cdot 2C_6H_5Cl$, has an unusual relative orientation of the two planar axial ligands [dihedral angle between the two imidazole planes = 46.55 (9)°]. The average equatorial Fe—N bond length is 1.974 (3) Å; the axial distances are 1.9628 (19) and 1.9932 (19) Å. The porphyrin core displays modest ruffling. Disorder is modeled for three of the *tert*-butyl groups of the pickets. In the crystal, a modest π–π interaction exists between adjacent phenyl rings related by an inversion center, and hydrogen bonds connect the trifluoromethanesulfonate oxygen atoms to the amide groups of the picket substituents.

3D view



Chemical scheme



Structure description

A widespread function of heme proteins in biology is that of electron transfer. One common class of electron-transfer proteins are those in which the central iron of the porphyrin is further coordinated by two axial histidine (imidazole) ligands (Scheidt *et al.*, 1987; Safo *et al.*, 1997). The iron shuttles between the +2 and +3 oxidation states; a major question is control of the redox potential. The relative orientation of the two planar axial ligands has been suggested as a structural feature capable of modulating redox potentials (Walker, 2004). Previous structure determinations of iron(III) porphyrinates show that such planar axial ligands are commonly in a relatively parallel orientation, which can be achieved by steric hindrance effects (Safo *et al.*, 1991). The structure of the bis(1-phenylimidazole)(tetra-*o*-pivalamidophenylporphinato)iron(III) cation (Fig. 1), however, shows that an unusual ligand orientation midway between the limiting cases can be obtained.

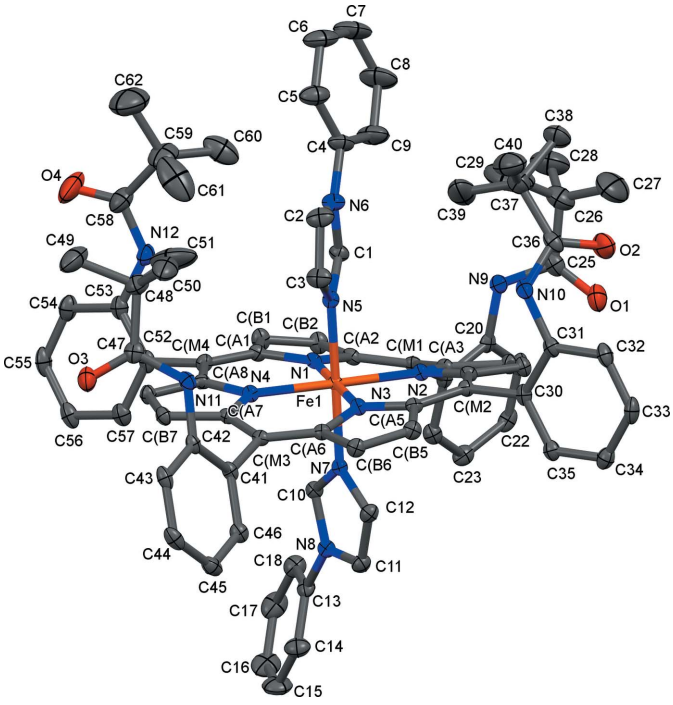


Figure 1
Displacement ellipsoid plot of the bis(1-phenylimidazole)(tetraphenylporphinato)iron(III) cation with atom labeling and displacement ellipsoids drawn at the 50% probability level. H atoms are not displayed for clarity.

The average Fe-to-porphyrin-nitrogen bond length is 1.974 (3) Å, a value that is on the low side compared to other six-coordinate low-spin iron(III) porphyrinates. This low value can be expected given that the porphyrin core displays modest ruffling, with the average observed displacement of the methine carbon atoms of 0.29 (8) Å from the mean plane of the 24-atom core. The two axial Fe—N bond length of 1.9628 (19) and 1.9632 (19) Å are within expected values. The only unusual feature of the structure is the dihedral angle between the two axial ligand planes, which is 46.55 (9)°. This dihedral angle is typically close to either 0° or 90°. The individual dihedral angles of the two ligands are 26.53 (6) and 20.03 (12)° with the same in-plane Fe–N vector.

In the crystal, hydrogen bonds connect the trifluoromethanesulfonate oxygen atoms to amide groups of the picket substituents and a modest π–π interaction exists between adjacent phenyl rings (C41–C46) related by an inversion center. Aside from typical van der Waals contacts, there are no other significant supramolecular interactions. Two molecules of chlorobenzene are also present in the asymmetric unit.

A large number of six-coordinate iron(III) porphyrinates with two planar axial ligands have been reported. The axial ligands have been both pyridines and imidazoles. A recent review (Scheidt, 2012) has provided structural details for these, including values for the relative orientation angle between the planar ligands and the dihedral angle between the ligand plane and the closest iron to porphinato nitrogen vector (see Table 6 of the review).

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Fe(C_{64}H_{64}N_8O_4)(C_9H_8N_2)_2]$-$(CF_3O_3S)\cdot 2C_6H_5Cl$
M_r	1727.59
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, b, c (Å)	12.2257 (4), 19.3422 (8), 19.5199 (8)
α, β, γ (°)	88.061 (2), 72.058 (2), 77.104 (2)
V (Å^3)	4277.6 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.33
Crystal size (mm)	0.50 × 0.13 × 0.05
Data collection	
Diffractometer	Bruker SMART APEX CCD area detector
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.949, 0.983
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	113863, 18189, 12915
R_{int}	0.052
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.636
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.124, 1.03
No. of reflections	18189
No. of parameters	1135
No. of restraints	133
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.05, −0.68

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*), *ORTEPIII* (Burnett & Johnson, 1996) and *publCIF* (Westrip, 2010).

Synthesis and crystallization

H_2TpivPP was prepared by the method of Adler *et al.* (1967). The μ-oxo derivative $[Fe(TpivPP)]_2O$ was prepared by a modified version of the procedure described by Hoffman *et al.* (1972). The oxido bridge was cleaved with HO_3SCF_3 (triflic acid) to yield $[Fe(TpivPP)(OSO_2CF_3)]$, which was then reacted with a tenfold excess of 1-phenylimidazole. Crystals were obtained by liquid diffusion of hexanes into a chlorobenzene solution of the complex.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The two chlorobenzene solvates and the trifluoromethanesulfonate counter-ion are completely ordered. Three of the four *t*-butyl groups are disordered over two sets of sites with half occupancy and some SIMU and SADI restrains were applied along with some bond-length constraints.

Funding information

We thank the US National Institutes of Health for support under grant GM-38401.

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full crystallographic data

IUCrData (2019). **4**, x190015 [https://doi.org/10.1107/S2414314619000154]

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Crystal data

$[Fe(C_{64}H_{64}N_8O_4)(C_9H_8N_2)_2](CF_3O_3S)\cdot 2C_6H_5Cl$
M_r = 1727.59
Triclinic, $P\overline{1}$
a = 12.2257 (4) Å
b = 19.3422 (8) Å
c = 19.5199 (8) Å
α = 88.061 (2)°
β = 72.058 (2)°
γ = 77.104 (2)°
V = 4277.6 (3) Å^3
Z = 2
$F(000)$ = 1806
D_x = 1.341 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9744 reflections
θ = 2.3–26.9°
μ = 0.33 mm^{-1}
T = 100 K
Needle, black
0.50 × 0.13 × 0.05 mm

Data collection

Bruker SMART APEX CCD area detector diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 8.33 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.949, T_{max} = 0.983
113863 measured reflections
18189 independent reflections
12915 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 26.9°, θ_{min} = 1.1°
h = −15→11
k = −24→24
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.124
S = 1.03
18189 reflections
1135 parameters
133 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0436P)^2 + 5.9854P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.05 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 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. The Large Non-Solvent C/H are one of the terminal methyl groups of 1,2-dimethyl-imidazole: C4.
ADP similarity restraints and same distance restraints were applied to carbon atoms in the disordered t-Bu groups.
All H atoms were placed in calculated positions and refined as riding atoms; for aryl H atoms, C–H = 0.95 Å and U_{iso} (H) = 1.2 U_{eq}(C), for methyl H atoms, C–H = 0.98 Å and U_{iso} (H) = 1.5 U_{eq}(C), and amide H atoms, N–H = 0.88 Å and U_{iso} (H) = 1.2 U_{eq}(N).

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Fe1	0.93950 (3)	0.75015 (2)	0.63711 (2)	0.01074 (8)	
N1	0.78809 (16)	0.72388 (10)	0.64703 (10)	0.0123 (4)	
N2	0.86067 (16)	0.85140 (10)	0.64050 (10)	0.0122 (4)	
N3	1.09012 (16)	0.77709 (10)	0.62626 (10)	0.0123 (4)	
N4	1.01776 (16)	0.64883 (10)	0.63486 (10)	0.0121 (4)	
N5	0.90366 (16)	0.75372 (10)	0.74229 (10)	0.0133 (4)	
N6	0.80318 (18)	0.76676 (11)	0.85683 (11)	0.0203 (4)	
N7	0.97438 (16)	0.74543 (10)	0.53204 (10)	0.0127 (4)	
N8	0.96989 (17)	0.71990 (10)	0.42456 (10)	0.0148 (4)	
N9	0.45521 (17)	0.94748 (11)	0.70142 (11)	0.0177 (4)	
H9A	0.451504	0.914169	0.733357	0.021*	
N10	1.00682 (18)	0.98738 (11)	0.76731 (11)	0.0193 (4)	
H10A	1.041310	0.945419	0.778348	0.023*	
N11	1.35206 (17)	0.58124 (10)	0.69671 (10)	0.0169 (4)	
H11A	1.321549	0.622192	0.720893	0.020*	
N12	0.7180 (2)	0.53529 (11)	0.77801 (11)	0.0239 (5)	
H12A	0.720816	0.580372	0.774378	0.029*	
O1	0.45350 (18)	1.06302 (10)	0.68223 (11)	0.0312 (4)	
O2	0.85973 (18)	1.08432 (10)	0.80426 (11)	0.0361 (5)	
O3	1.37302 (17)	0.46263 (9)	0.70258 (10)	0.0271 (4)	
O4	0.6706 (3)	0.45394 (13)	0.86069 (13)	0.0581 (7)	
C(A1	0.7647 (2)	0.65742 (12)	0.65465 (12)	0.0140 (5)	
C(A2	0.68793 (19)	0.76795 (12)	0.63857 (12)	0.0141 (5)	
C(A3	0.75130 (19)	0.87917 (12)	0.63296 (12)	0.0136 (5)	
C(A4	0.9078 (2)	0.90904 (12)	0.64430 (12)	0.0135 (4)	
C(A5	1.1091 (2)	0.84386 (12)	0.62972 (12)	0.0130 (4)	
C(A6	1.20033 (19)	0.73253 (12)	0.60811 (12)	0.0125 (4)	
C(A7	1.13631 (19)	0.62089 (12)	0.62138 (12)	0.0131 (4)	
C(A8	0.9655 (2)	0.59181 (12)	0.64406 (12)	0.0136 (5)	
C(B1	0.6456 (2)	0.66096 (13)	0.65649 (13)	0.0187 (5)	
H(BA	0.606704	0.622661	0.664286	0.022*	
C(B2	0.5990 (2)	0.72842 (13)	0.64517 (13)	0.0180 (5)	
H(BB	0.521806	0.746569	0.642101	0.022*	
C(B3	0.7296 (2)	0.95499 (12)	0.63294 (13)	0.0164 (5)	
H(BC	0.661283	0.986508	0.627587	0.020*	
C(B4	0.8248 (2)	0.97318 (12)	0.64197 (12)	0.0161 (5)	

H(BD	0.834640	1.020057	0.646023	0.019*
C(B5	1.2328 (2)	0.84081 (12)	0.61406 (12)	0.0156 (5)
H(BE	1.268116	0.879785	0.614407	0.019*
C(B6	1.2888 (2)	0.77294 (12)	0.59891 (12)	0.0151 (5)
H(BF	1.371733	0.754760	0.584696	0.018*
C(B7	1.1577 (2)	0.54518 (12)	0.62501 (12)	0.0153 (5)
H(BG	1.231943	0.513478	0.618562	0.018*
C(B8	1.0527 (2)	0.52738 (12)	0.63928 (12)	0.0160 (5)
H(BH	1.039078	0.480762	0.645107	0.019*
C(M1	0.67276 (19)	0.83982 (12)	0.62630 (12)	0.0140 (5)
C(M2	1.0239 (2)	0.90646 (12)	0.64069 (12)	0.0134 (4)
C(M3	1.22433 (19)	0.65934 (12)	0.60419 (11)	0.0123 (4)
C(M4	0.8473 (2)	0.59447 (12)	0.65275 (12)	0.0144 (5)
C1	0.7973 (2)	0.76725 (12)	0.78911 (12)	0.0174 (5)
H1A	0.726097	0.776134	0.776848	0.021*
C2	0.9206 (2)	0.75124 (15)	0.85209 (14)	0.0261 (6)
H2A	0.952419	0.746629	0.891130	0.031*
C3	0.9818 (2)	0.74382 (14)	0.78149 (13)	0.0229 (5)
H3A	1.065338	0.733434	0.761893	0.027*
C4	0.7042 (2)	0.78096 (15)	0.92079 (13)	0.0257 (6)
C5	0.7174 (3)	0.75546 (17)	0.98558 (14)	0.0327 (7)
H5A	0.791972	0.729818	0.988051	0.039*
C6	0.6201 (3)	0.76804 (19)	1.04663 (15)	0.0415 (8)
H6A	0.627986	0.750937	1.091449	0.050*
C7	0.5123 (3)	0.8049 (2)	1.04330 (16)	0.0487 (9)
H7A	0.446067	0.813150	1.085599	0.058*
C8	0.5003 (3)	0.8298 (2)	0.97862 (17)	0.0497 (9)
H8A	0.425502	0.854848	0.976083	0.060*
C9	0.5975 (3)	0.81835 (18)	0.91698 (16)	0.0401 (8)
H9B	0.589790	0.836418	0.872429	0.048*
C10	0.9264 (2)	0.71164 (12)	0.49569 (12)	0.0147 (5)
H10B	0.868715	0.684991	0.516925	0.018*
C11	1.0516 (2)	0.76081 (13)	0.41534 (13)	0.0182 (5)
H11B	1.097728	0.775282	0.370849	0.022*
C12	1.0538 (2)	0.77641 (12)	0.48149 (12)	0.0172 (5)
H12B	1.102174	0.804256	0.491749	0.021*
C13	0.9392 (2)	0.69018 (12)	0.36889 (12)	0.0175 (5)
C14	1.0222 (2)	0.67407 (15)	0.30215 (14)	0.0267 (6)
H14A	1.098712	0.682900	0.293279	0.032*
C15	0.9934 (3)	0.64506 (17)	0.24843 (15)	0.0359 (7)
H15A	1.050234	0.633878	0.202242	0.043*
C16	0.8829 (3)	0.63217 (17)	0.26120 (16)	0.0377 (7)
H16A	0.863653	0.612300	0.223760	0.045*
C17	0.8001 (3)	0.64787 (16)	0.32788 (16)	0.0324 (7)
H17A	0.724021	0.638488	0.336520	0.039*
C18	0.8275 (2)	0.67742 (14)	0.38263 (14)	0.0238 (6)
H18A	0.770493	0.688713	0.428760	0.029*
C19	0.5779 (2)	0.87392 (12)	0.59471 (12)	0.0149 (5)

C20	0.4808 (2)	0.92779 (12)	0.62789 (12)	0.0148 (5)	
C21	0.4066 (2)	0.96134 (12)	0.58949 (13)	0.0176 (5)	
H21A	0.341239	0.998762	0.612043	0.021*	
C22	0.4269 (2)	0.94075 (13)	0.51900 (13)	0.0194 (5)	
H22A	0.376227	0.964484	0.493037	0.023*	
C23	0.5206 (2)	0.88579 (13)	0.48579 (13)	0.0203 (5)	
H23A	0.533937	0.870778	0.437492	0.024*	
C24	0.5944 (2)	0.85314 (13)	0.52403 (13)	0.0186 (5)	
H24A	0.658732	0.815188	0.501378	0.022*	
C25	0.4362 (2)	1.01582 (14)	0.72430 (14)	0.0229 (5)	
C26	0.3934 (3)	1.02978 (17)	0.80550 (17)	0.0397 (7)	
C27	0.4285 (10)	1.0940 (5)	0.8236 (6)	0.071 (3)	0.5
H27A	0.400621	1.102660	0.875956	0.106*	0.5
H27B	0.514663	1.086627	0.806172	0.106*	0.5
H27C	0.393442	1.135123	0.800548	0.106*	0.5
C27B	0.3653 (9)	1.1120 (4)	0.8183 (6)	0.062 (3)	0.5
H27D	0.337268	1.123551	0.870211	0.093*	0.5
H27E	0.436956	1.129622	0.796028	0.093*	0.5
H27F	0.304201	1.134439	0.796777	0.093*	0.5
C28	0.2655 (3)	1.0194 (2)	0.8345 (2)	0.0639 (11)	
H28A	0.261740	0.973791	0.816101	0.096*	
H28B	0.240828	1.020091	0.887282	0.096*	
H28C	0.212784	1.057912	0.818490	0.096*	
C29	0.4624 (4)	0.9731 (3)	0.8428 (2)	0.0852 (16)	
H29A	0.447336	0.926689	0.835217	0.128*	
H29B	0.546938	0.971401	0.822396	0.128*	
H29C	0.436942	0.984960	0.894538	0.128*	
C30	1.0628 (2)	0.97496 (12)	0.63673 (13)	0.0151 (5)	
C31	1.0538 (2)	1.01341 (12)	0.69799 (13)	0.0167 (5)	
C32	1.0901 (2)	1.07689 (13)	0.69149 (14)	0.0212 (5)	
H32A	1.083983	1.102730	0.733548	0.025*	
C33	1.1349 (2)	1.10282 (13)	0.62478 (15)	0.0225 (5)	
H33A	1.160707	1.146034	0.620802	0.027*	
C34	1.1424 (2)	1.06607 (13)	0.56351 (14)	0.0210 (5)	
H34A	1.171564	1.084481	0.517363	0.025*	
C35	1.1072 (2)	1.00235 (12)	0.56953 (13)	0.0178 (5)	
H35A	1.113423	0.976916	0.527198	0.021*	
C36	0.9096 (2)	1.02590 (14)	0.81702 (14)	0.0226 (5)	
C37	0.8650 (3)	0.99098 (15)	0.88829 (15)	0.0315 (6)	
C38	0.7537 (6)	1.0400 (3)	0.9340 (3)	0.0358 (14)	0.5
H38A	0.770887	1.085573	0.942376	0.054*	0.5
H38B	0.693905	1.047777	0.909020	0.054*	0.5
H38C	0.724034	1.018571	0.980311	0.054*	0.5
C39	0.8442 (8)	0.9216 (4)	0.8740 (4)	0.062 (2)	0.5
H39A	0.918142	0.891291	0.844295	0.093*	0.5
H39B	0.815383	0.899026	0.919751	0.093*	0.5
H39C	0.785253	0.928233	0.848460	0.093*	0.5
C40	0.9623 (6)	0.9841 (4)	0.9259 (4)	0.0515 (17)	0.5

H40A	0.973277	1.031353	0.934364	0.077*	0.5
H40B	0.938231	0.961244	0.972040	0.077*	0.5
H40C	1.036668	0.955229	0.894923	0.077*	0.5
C38B	0.8238 (8)	1.0476 (4)	0.9482 (4)	0.0571 (19)	0.5
H38D	0.767286	1.087552	0.937313	0.086*	0.5
H38E	0.785846	1.027705	0.993874	0.086*	0.5
H38F	0.891780	1.064291	0.952188	0.086*	0.5
C39B	0.7590 (7)	0.9628 (5)	0.8838 (5)	0.0632 (19)	0.5
H39D	0.702105	1.001295	0.871266	0.095*	0.5
H39E	0.786279	0.924393	0.846869	0.095*	0.5
H39F	0.721027	0.944645	0.930588	0.095*	0.5
C40B	0.9517 (6)	0.9309 (4)	0.9077 (3)	0.0385 (14)	0.5
H40D	0.980140	0.893240	0.869980	0.058*	0.5
H40E	1.018473	0.948605	0.912041	0.058*	0.5
H40F	0.912539	0.912019	0.953726	0.058*	0.5
C41	1.35014 (19)	0.62121 (12)	0.57741 (12)	0.0138 (5)	
C42	1.4096 (2)	0.58184 (12)	0.62156 (12)	0.0150 (5)	
C43	1.5264 (2)	0.54604 (12)	0.59258 (14)	0.0189 (5)	
H43A	1.565600	0.517851	0.622499	0.023*	
C44	1.5858 (2)	0.55102 (13)	0.52089 (14)	0.0204 (5)	
H44A	1.666015	0.526754	0.501613	0.025*	
C45	1.5290 (2)	0.59128 (13)	0.47688 (14)	0.0213 (5)	
H45A	1.570152	0.595207	0.427462	0.026*	
C46	1.4122 (2)	0.62573 (12)	0.50505 (13)	0.0171 (5)	
H46A	1.373313	0.653076	0.474496	0.021*	
C47	1.3415 (2)	0.52103 (13)	0.73327 (13)	0.0190 (5)	
C48	1.2868 (2)	0.53172 (15)	0.81470 (14)	0.0269 (6)	
C49	1.2879 (4)	0.45944 (18)	0.84835 (17)	0.0469 (9)	
H49A	1.369414	0.431856	0.836713	0.070*	
H49B	1.253122	0.465889	0.900777	0.070*	
H49C	1.241967	0.434086	0.829218	0.070*	
C50	1.3608 (3)	0.56876 (17)	0.84500 (16)	0.0404 (8)	
H50A	1.441081	0.539498	0.833847	0.061*	
H50B	1.363313	0.615013	0.823247	0.061*	
H50C	1.325420	0.575537	0.897367	0.061*	
C51	1.1623 (3)	0.5762 (3)	0.83141 (19)	0.0725 (14)	
H51A	1.164126	0.622249	0.809175	0.109*	
H51B	1.115446	0.551602	0.812164	0.109*	
H51C	1.126601	0.583404	0.883723	0.109*	
C52	0.8111 (2)	0.52591 (12)	0.65032 (13)	0.0159 (5)	
C53	0.7445 (2)	0.49823 (13)	0.71262 (14)	0.0200 (5)	
C54	0.7070 (2)	0.43628 (13)	0.70741 (15)	0.0244 (6)	
H54A	0.659969	0.418112	0.749261	0.029*	
C55	0.7381 (2)	0.40132 (13)	0.64149 (16)	0.0256 (6)	
H55A	0.712241	0.359067	0.638246	0.031*	
C56	0.8063 (2)	0.42700 (13)	0.58012 (15)	0.0227 (5)	
H56A	0.829207	0.401961	0.535078	0.027*	
C57	0.8410 (2)	0.48958 (13)	0.58488 (14)	0.0197 (5)	

H57A	0.886280	0.507943	0.542491	0.024*	
C58	0.6885 (3)	0.51220 (16)	0.84629 (16)	0.0330 (7)	
C59	0.6815 (3)	0.56753 (19)	0.90287 (17)	0.0437 (8)	
C60	0.5958 (3)	0.63529 (19)	0.89839 (19)	0.0476 (9)	
H60A	0.612784	0.649522	0.848202	0.071*	
H60B	0.515196	0.627836	0.915925	0.071*	
H60C	0.603378	0.672690	0.928114	0.071*	
C61	0.8052 (4)	0.5815 (2)	0.8887 (3)	0.0707 (13)	
H61A	0.827853	0.604728	0.842745	0.106*	
H61B	0.804924	0.612228	0.927695	0.106*	
H61C	0.861936	0.536293	0.886751	0.106*	
C62	0.6760 (10)	0.5335 (7)	0.9734 (6)	0.074 (3)	0.5
H62A	0.738347	0.490132	0.965856	0.111*	0.5
H62B	0.687105	0.566484	1.006425	0.111*	0.5
H62C	0.598924	0.521629	0.994236	0.111*	0.5
C62B	0.6085 (8)	0.5450 (6)	0.9801 (5)	0.058 (2)	0.5
H62D	0.652412	0.500134	0.992617	0.087*	0.5
H62E	0.596506	0.581996	1.016407	0.087*	0.5
H62F	0.531753	0.539076	0.978453	0.087*	0.5
Cl1	0.30235 (6)	0.85783 (4)	0.41245 (4)	0.03351 (16)	
C1S	0.3514 (2)	0.80218 (14)	0.33610 (15)	0.0266 (6)	
C2S	0.4458 (3)	0.74531 (15)	0.32949 (16)	0.0321 (6)	
H2SA	0.485009	0.738011	0.365136	0.039*	
C3S	0.4820 (3)	0.69942 (16)	0.27036 (17)	0.0391 (7)	
H3SA	0.546473	0.659870	0.265071	0.047*	
C4S	0.4245 (3)	0.71092 (17)	0.21860 (17)	0.0401 (8)	
H4SA	0.449306	0.679258	0.177813	0.048*	
C5S	0.3309 (3)	0.76865 (17)	0.22646 (16)	0.0371 (7)	
H5SA	0.291415	0.776199	0.190974	0.044*	
C6S	0.2946 (2)	0.81488 (15)	0.28447 (15)	0.0297 (6)	
H6SA	0.231428	0.855051	0.289154	0.036*	
Cl2	−0.03510 (10)	0.61394 (6)	0.03481 (5)	0.0669 (3)	
C7S	0.0233 (3)	0.67744 (18)	0.06266 (16)	0.0402 (8)	
C8S	−0.0485 (4)	0.7405 (2)	0.0915 (2)	0.0681 (13)	
H8SA	−0.130308	0.750223	0.096470	0.082*	
C9S	0.0005 (5)	0.7901 (2)	0.1136 (3)	0.0895 (18)	
H9SA	−0.048140	0.834859	0.133265	0.107*	
C10S	0.1162 (6)	0.7760 (3)	0.1076 (3)	0.0839 (16)	
H10C	0.148177	0.810733	0.123281	0.101*	
C11S	0.1867 (4)	0.7132 (3)	0.0797 (2)	0.0658 (12)	
H11C	0.267951	0.703431	0.076114	0.079*	
C12S	0.1412 (3)	0.6632 (2)	0.05624 (17)	0.0492 (9)	
H12C	0.190909	0.618944	0.035733	0.059*	
C13S	0.2419 (2)	0.78784 (14)	0.88701 (14)	0.0246 (6)	
F1	0.14186 (15)	0.76576 (10)	0.91300 (9)	0.0411 (4)	
F2	0.32612 (15)	0.74030 (9)	0.90245 (9)	0.0351 (4)	
F3	0.22865 (16)	0.84806 (9)	0.92232 (9)	0.0379 (4)	
O1S	0.1759 (2)	0.85349 (10)	0.78548 (11)	0.0387 (5)	

O2S	0.28187 (19)	0.73105 (10)	0.76257 (10)	0.0325 (5)
O3S	0.38448 (19)	0.82205 (11)	0.77249 (11)	0.0409 (5)
S1	0.27464 (6)	0.80022 (3)	0.79058 (3)	0.02572 (15)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.00788 (16)	0.01159 (16)	0.01288 (16)	−0.00152 (12)	−0.00373 (12)	−0.00079 (12)
N1	0.0087 (9)	0.0133 (9)	0.0144 (9)	−0.0014 (7)	−0.0038 (7)	−0.0011 (7)
N2	0.0090 (9)	0.0131 (9)	0.0148 (9)	−0.0024 (7)	−0.0043 (7)	−0.0003 (7)
N3	0.0101 (9)	0.0129 (9)	0.0149 (9)	−0.0025 (7)	−0.0053 (7)	−0.0004 (7)
N4	0.0085 (9)	0.0135 (9)	0.0152 (9)	−0.0031 (7)	−0.0046 (7)	−0.0002 (7)
N5	0.0121 (10)	0.0142 (9)	0.0148 (9)	−0.0030 (7)	−0.0061 (8)	0.0011 (7)
N6	0.0187 (11)	0.0269 (11)	0.0152 (10)	−0.0064 (9)	−0.0041 (8)	−0.0001 (8)
N7	0.0110 (9)	0.0125 (9)	0.0149 (9)	−0.0024 (7)	−0.0045 (8)	−0.0002 (7)
N8	0.0132 (10)	0.0159 (10)	0.0156 (10)	−0.0028 (8)	−0.0053 (8)	−0.0001 (8)
N9	0.0152 (10)	0.0181 (10)	0.0185 (10)	−0.0015 (8)	−0.0051 (8)	0.0011 (8)
N10	0.0221 (11)	0.0152 (10)	0.0203 (10)	−0.0010 (8)	−0.0080 (9)	−0.0024 (8)
N11	0.0157 (10)	0.0161 (10)	0.0187 (10)	−0.0001 (8)	−0.0068 (8)	−0.0026 (8)
N12	0.0336 (13)	0.0171 (11)	0.0238 (11)	−0.0116 (9)	−0.0092 (10)	0.0035 (9)
O1	0.0383 (12)	0.0193 (10)	0.0388 (11)	−0.0056 (8)	−0.0163 (9)	−0.0011 (8)
O2	0.0316 (11)	0.0299 (11)	0.0362 (11)	0.0091 (9)	−0.0064 (9)	0.0002 (9)
O3	0.0356 (11)	0.0178 (9)	0.0310 (10)	−0.0055 (8)	−0.0153 (9)	0.0012 (8)
O4	0.105 (2)	0.0409 (14)	0.0443 (14)	−0.0374 (14)	−0.0326 (14)	0.0238 (11)
C(A1	0.0119 (11)	0.0159 (11)	0.0151 (11)	−0.0049 (9)	−0.0041 (9)	−0.0014 (9)
C(A2	0.0104 (11)	0.0163 (11)	0.0154 (11)	−0.0014 (9)	−0.0046 (9)	−0.0032 (9)
C(A3	0.0113 (11)	0.0157 (11)	0.0132 (11)	−0.0012 (9)	−0.0043 (9)	−0.0006 (9)
C(A4	0.0119 (11)	0.0142 (11)	0.0143 (11)	−0.0030 (9)	−0.0035 (9)	−0.0011 (9)
C(A5	0.0132 (11)	0.0153 (11)	0.0126 (11)	−0.0051 (9)	−0.0055 (9)	−0.0004 (9)
C(A6	0.0108 (11)	0.0155 (11)	0.0126 (11)	−0.0033 (9)	−0.0055 (9)	0.0005 (9)
C(A7	0.0109 (11)	0.0153 (11)	0.0128 (11)	−0.0013 (9)	−0.0040 (9)	−0.0008 (9)
C(A8	0.0122 (11)	0.0150 (11)	0.0125 (11)	−0.0034 (9)	−0.0020 (9)	0.0001 (9)
C(B1	0.0131 (12)	0.0176 (12)	0.0270 (13)	−0.0056 (9)	−0.0067 (10)	−0.0009 (10)
C(B2	0.0128 (12)	0.0185 (12)	0.0255 (13)	−0.0048 (9)	−0.0088 (10)	−0.0001 (10)
C(B3	0.0127 (12)	0.0152 (12)	0.0209 (12)	−0.0011 (9)	−0.0059 (9)	0.0012 (9)
C(B4	0.0143 (12)	0.0126 (11)	0.0212 (12)	−0.0017 (9)	−0.0058 (9)	−0.0018 (9)
C(B5	0.0136 (12)	0.0175 (12)	0.0182 (12)	−0.0055 (9)	−0.0072 (9)	0.0008 (9)
C(B6	0.0109 (11)	0.0176 (12)	0.0185 (11)	−0.0046 (9)	−0.0062 (9)	0.0012 (9)
C(B7	0.0134 (11)	0.0135 (11)	0.0183 (11)	0.0004 (9)	−0.0063 (9)	−0.0011 (9)
C(B8	0.0139 (12)	0.0138 (11)	0.0200 (12)	−0.0033 (9)	−0.0046 (9)	0.0003 (9)
C(M1	0.0092 (11)	0.0169 (11)	0.0144 (11)	−0.0015 (9)	−0.0024 (9)	−0.0002 (9)
C(M2	0.0138 (11)	0.0145 (11)	0.0135 (11)	−0.0053 (9)	−0.0049 (9)	−0.0004 (9)
C(M3	0.0097 (11)	0.0150 (11)	0.0124 (10)	−0.0011 (9)	−0.0045 (8)	−0.0002 (8)
C(M4	0.0120 (11)	0.0146 (11)	0.0175 (11)	−0.0042 (9)	−0.0051 (9)	0.0016 (9)
C1	0.0148 (12)	0.0200 (12)	0.0171 (12)	−0.0036 (9)	−0.0044 (9)	−0.0010 (9)
C2	0.0200 (13)	0.0408 (16)	0.0205 (13)	−0.0077 (12)	−0.0101 (11)	0.0036 (11)
C3	0.0156 (13)	0.0328 (15)	0.0212 (13)	−0.0021 (11)	−0.0093 (10)	0.0011 (11)
C4	0.0214 (14)	0.0360 (15)	0.0174 (12)	−0.0109 (11)	0.0006 (10)	−0.0025 (11)

C5	0.0333 (16)	0.0490 (18)	0.0206 (14)	−0.0201 (14)	−0.0070 (12)	−0.0009 (12)
C6	0.046 (2)	0.068 (2)	0.0159 (14)	−0.0323 (17)	−0.0030 (13)	−0.0011 (14)
C7	0.040 (2)	0.077 (3)	0.0222 (15)	−0.0238 (18)	0.0088 (14)	−0.0103 (16)
C8	0.0287 (17)	0.074 (3)	0.0323 (17)	−0.0012 (16)	0.0046 (14)	−0.0071 (17)
C9	0.0314 (17)	0.056 (2)	0.0223 (14)	−0.0011 (15)	0.0016 (12)	0.0002 (14)
C10	0.0134 (11)	0.0156 (11)	0.0156 (11)	−0.0030 (9)	−0.0055 (9)	0.0003 (9)
C11	0.0174 (12)	0.0194 (12)	0.0185 (12)	−0.0066 (10)	−0.0047 (10)	0.0024 (9)
C12	0.0153 (12)	0.0187 (12)	0.0191 (12)	−0.0059 (9)	−0.0059 (9)	0.0030 (9)
C13	0.0214 (13)	0.0168 (12)	0.0173 (12)	−0.0033 (10)	−0.0114 (10)	0.0019 (9)
C14	0.0270 (15)	0.0354 (16)	0.0198 (13)	−0.0077 (12)	−0.0097 (11)	0.0020 (11)
C15	0.0473 (19)	0.0479 (19)	0.0156 (13)	−0.0141 (15)	−0.0114 (13)	−0.0012 (12)
C16	0.054 (2)	0.0457 (19)	0.0259 (15)	−0.0215 (16)	−0.0237 (14)	0.0008 (13)
C17	0.0378 (17)	0.0378 (17)	0.0353 (16)	−0.0195 (13)	−0.0237 (14)	0.0084 (13)
C18	0.0240 (14)	0.0263 (14)	0.0246 (13)	−0.0085 (11)	−0.0103 (11)	0.0025 (11)
C19	0.0115 (11)	0.0138 (11)	0.0207 (12)	−0.0047 (9)	−0.0057 (9)	0.0023 (9)
C20	0.0120 (11)	0.0139 (11)	0.0209 (12)	−0.0068 (9)	−0.0058 (9)	0.0025 (9)
C21	0.0125 (12)	0.0144 (11)	0.0280 (13)	−0.0053 (9)	−0.0080 (10)	0.0041 (10)
C22	0.0168 (12)	0.0212 (13)	0.0273 (13)	−0.0101 (10)	−0.0139 (10)	0.0094 (10)
C23	0.0213 (13)	0.0247 (13)	0.0208 (12)	−0.0116 (10)	−0.0105 (10)	0.0035 (10)
C24	0.0145 (12)	0.0184 (12)	0.0232 (12)	−0.0040 (9)	−0.0060 (10)	−0.0012 (10)
C25	0.0167 (13)	0.0225 (13)	0.0301 (14)	−0.0019 (10)	−0.0092 (11)	−0.0045 (11)
C26	0.0425 (18)	0.0429 (18)	0.0309 (15)	−0.0052 (14)	−0.0087 (13)	−0.0110 (13)
C27	0.105 (6)	0.057 (5)	0.048 (4)	−0.025 (5)	−0.015 (5)	−0.019 (4)
C27B	0.074 (5)	0.049 (4)	0.049 (4)	−0.025 (4)	0.012 (5)	−0.031 (4)
C28	0.056 (2)	0.080 (3)	0.040 (2)	−0.009 (2)	0.0050 (17)	−0.0094 (19)
C29	0.072 (3)	0.134 (4)	0.040 (2)	0.018 (3)	−0.030 (2)	−0.019 (2)
C30	0.0095 (11)	0.0135 (11)	0.0239 (12)	−0.0005 (9)	−0.0088 (9)	0.0009 (9)
C31	0.0137 (12)	0.0154 (12)	0.0214 (12)	0.0002 (9)	−0.0080 (10)	−0.0015 (9)
C32	0.0219 (13)	0.0147 (12)	0.0304 (14)	−0.0027 (10)	−0.0136 (11)	−0.0044 (10)
C33	0.0208 (13)	0.0120 (12)	0.0384 (15)	−0.0050 (10)	−0.0136 (11)	0.0037 (10)
C34	0.0186 (13)	0.0190 (12)	0.0264 (13)	−0.0044 (10)	−0.0086 (10)	0.0057 (10)
C35	0.0154 (12)	0.0160 (12)	0.0225 (12)	−0.0017 (9)	−0.0076 (10)	−0.0004 (9)
C36	0.0211 (13)	0.0225 (13)	0.0252 (13)	−0.0015 (10)	−0.0101 (11)	−0.0072 (10)
C37	0.0306 (15)	0.0268 (14)	0.0296 (14)	−0.0015 (11)	−0.0021 (12)	−0.0015 (11)
C38	0.026 (3)	0.038 (3)	0.033 (3)	−0.001 (3)	0.002 (2)	−0.005 (2)
C39	0.068 (4)	0.040 (3)	0.053 (4)	−0.022 (3)	0.027 (3)	−0.006 (3)
C40	0.051 (4)	0.062 (4)	0.029 (3)	0.004 (3)	−0.007 (3)	0.008 (3)
C38B	0.069 (4)	0.043 (3)	0.033 (3)	0.006 (3)	0.009 (3)	−0.005 (3)
C39B	0.050 (4)	0.070 (4)	0.071 (4)	−0.024 (3)	−0.016 (3)	0.023 (4)
C40B	0.042 (3)	0.042 (3)	0.022 (3)	−0.002 (3)	−0.002 (2)	0.007 (2)
C41	0.0094 (11)	0.0130 (11)	0.0197 (12)	−0.0025 (9)	−0.0049 (9)	−0.0037 (9)
C42	0.0132 (11)	0.0126 (11)	0.0209 (12)	−0.0036 (9)	−0.0065 (9)	−0.0031 (9)
C43	0.0154 (12)	0.0141 (12)	0.0297 (13)	−0.0008 (9)	−0.0118 (10)	−0.0056 (10)
C44	0.0101 (12)	0.0198 (13)	0.0301 (14)	−0.0026 (9)	−0.0038 (10)	−0.0094 (10)
C45	0.0172 (13)	0.0225 (13)	0.0218 (13)	−0.0069 (10)	−0.0002 (10)	−0.0063 (10)
C46	0.0137 (12)	0.0177 (12)	0.0210 (12)	−0.0044 (9)	−0.0061 (9)	−0.0015 (9)
C47	0.0157 (12)	0.0209 (13)	0.0240 (13)	−0.0038 (10)	−0.0118 (10)	0.0023 (10)
C48	0.0299 (15)	0.0293 (15)	0.0225 (13)	−0.0066 (12)	−0.0098 (11)	0.0046 (11)

C49	0.079 (3)	0.046 (2)	0.0301 (16)	−0.0370 (19)	−0.0234 (17)	0.0149 (14)
C50	0.069 (2)	0.0356 (17)	0.0247 (15)	−0.0182 (16)	−0.0211 (15)	0.0006 (13)
C51	0.033 (2)	0.123 (4)	0.0340 (19)	0.014 (2)	0.0066 (15)	0.019 (2)
C52	0.0093 (11)	0.0128 (11)	0.0273 (13)	−0.0017 (9)	−0.0084 (10)	0.0009 (9)
C53	0.0155 (12)	0.0168 (12)	0.0290 (14)	−0.0023 (9)	−0.0096 (10)	0.0009 (10)
C54	0.0199 (13)	0.0194 (13)	0.0366 (15)	−0.0080 (10)	−0.0102 (11)	0.0046 (11)
C55	0.0208 (13)	0.0142 (12)	0.0467 (17)	−0.0054 (10)	−0.0160 (12)	−0.0010 (11)
C56	0.0177 (13)	0.0175 (12)	0.0349 (15)	0.0001 (10)	−0.0133 (11)	−0.0064 (11)
C57	0.0125 (12)	0.0188 (12)	0.0275 (13)	−0.0015 (9)	−0.0069 (10)	−0.0018 (10)
C58	0.0402 (18)	0.0341 (16)	0.0306 (15)	−0.0139 (13)	−0.0167 (13)	0.0128 (13)
C59	0.064 (2)	0.0507 (19)	0.0278 (15)	−0.0221 (16)	−0.0247 (15)	0.0086 (14)
C60	0.0342 (18)	0.063 (2)	0.0478 (19)	−0.0094 (16)	−0.0140 (15)	−0.0228 (17)
C61	0.059 (2)	0.069 (3)	0.100 (3)	0.006 (2)	−0.056 (2)	−0.036 (2)
C62	0.104 (6)	0.088 (5)	0.035 (4)	−0.035 (6)	−0.021 (5)	0.010 (4)
C62B	0.073 (5)	0.074 (5)	0.023 (3)	−0.015 (5)	−0.011 (4)	0.016 (3)
Cl1	0.0324 (4)	0.0317 (4)	0.0398 (4)	−0.0109 (3)	−0.0130 (3)	0.0000 (3)
C1S	0.0252 (14)	0.0264 (14)	0.0310 (15)	−0.0123 (11)	−0.0087 (12)	0.0070 (11)
C2S	0.0302 (16)	0.0292 (15)	0.0419 (17)	−0.0095 (12)	−0.0172 (13)	0.0096 (13)
C3S	0.0403 (18)	0.0268 (16)	0.0448 (18)	−0.0061 (13)	−0.0072 (15)	0.0076 (13)
C4S	0.051 (2)	0.0352 (17)	0.0318 (16)	−0.0185 (15)	−0.0025 (14)	0.0024 (13)
C5S	0.0404 (18)	0.0454 (19)	0.0307 (16)	−0.0194 (15)	−0.0127 (13)	0.0111 (14)
C6S	0.0254 (15)	0.0312 (15)	0.0345 (15)	−0.0100 (12)	−0.0105 (12)	0.0107 (12)
Cl2	0.0787 (7)	0.0849 (8)	0.0502 (5)	−0.0437 (6)	−0.0195 (5)	−0.0066 (5)
C7S	0.051 (2)	0.050 (2)	0.0228 (15)	−0.0162 (16)	−0.0133 (14)	0.0024 (14)
C8S	0.067 (3)	0.079 (3)	0.059 (2)	0.018 (2)	−0.044 (2)	−0.015 (2)
C9S	0.137 (5)	0.049 (3)	0.099 (4)	0.020 (3)	−0.086 (4)	−0.020 (2)
C10S	0.140 (5)	0.059 (3)	0.095 (4)	−0.040 (3)	−0.088 (4)	0.026 (3)
C11S	0.072 (3)	0.091 (3)	0.053 (2)	−0.045 (3)	−0.029 (2)	0.022 (2)
C12S	0.050 (2)	0.063 (2)	0.0316 (17)	−0.0172 (18)	−0.0049 (15)	0.0018 (16)
C13S	0.0253 (14)	0.0262 (14)	0.0234 (13)	−0.0041 (11)	−0.0103 (11)	0.0005 (11)
F1	0.0337 (10)	0.0618 (12)	0.0308 (9)	−0.0210 (9)	−0.0081 (8)	0.0112 (8)
F2	0.0379 (10)	0.0368 (9)	0.0319 (9)	0.0005 (8)	−0.0191 (8)	0.0031 (7)
F3	0.0506 (11)	0.0346 (9)	0.0270 (9)	−0.0015 (8)	−0.0143 (8)	−0.0103 (7)
O1S	0.0569 (14)	0.0263 (11)	0.0297 (11)	0.0090 (10)	−0.0214 (10)	−0.0020 (8)
O2S	0.0518 (13)	0.0211 (10)	0.0241 (10)	−0.0026 (9)	−0.0146 (9)	−0.0020 (8)
O3S	0.0449 (13)	0.0313 (11)	0.0374 (12)	−0.0147 (10)	0.0045 (10)	0.0023 (9)
S1	0.0371 (4)	0.0187 (3)	0.0183 (3)	−0.0023 (3)	−0.0070 (3)	0.0006 (2)

Geometric parameters (Å, º)

Fe1—N7	1.9628 (19)	C28—H28A	0.9800
Fe1—N5	1.9632 (19)	C28—H28B	0.9800
Fe1—N3	1.9719 (19)	C28—H28C	0.9800
Fe1—N2	1.9737 (18)	C29—H29A	0.9800
Fe1—N4	1.9752 (18)	C29—H29B	0.9800
Fe1—N1	1.9785 (19)	C29—H29C	0.9800
N1—C(A1	1.371 (3)	C30—C31	1.392 (3)
N1—C(A2	1.379 (3)	C30—C35	1.393 (3)

N2—C(A3	1.376 (3)	C31—C32	1.385 (3)
N2—C(A4	1.378 (3)	C32—C33	1.373 (4)
N3—C(A5	1.369 (3)	C32—H32A	0.9500
N3—C(A6	1.376 (3)	C33—C34	1.380 (4)
N4—C(A7	1.374 (3)	C33—H33A	0.9500
N4—C(A8	1.374 (3)	C34—C35	1.383 (3)
N5—C1	1.314 (3)	C34—H34A	0.9500
N5—C3	1.376 (3)	C35—H35A	0.9500
N6—C1	1.346 (3)	C36—C37	1.524 (4)
N6—C2	1.374 (3)	C37—C39	1.471 (8)
N6—C4	1.429 (3)	C37—C38	1.510 (6)
N7—C10	1.317 (3)	C37—C40B	1.511 (7)
N7—C12	1.380 (3)	C37—C38B	1.517 (7)
N8—C10	1.343 (3)	C37—C39B	1.541 (8)
N8—C11	1.375 (3)	C37—C40	1.560 (8)
N8—C13	1.429 (3)	C38—H38A	0.9800
N9—C25	1.356 (3)	C38—H38B	0.9800
N9—C20	1.418 (3)	C38—H38C	0.9800
N9—H9A	0.8800	C39—H39A	0.9800
N10—C36	1.361 (3)	C39—H39B	0.9800
N10—C31	1.421 (3)	C39—H39C	0.9800
N10—H10A	0.8800	C40—H40A	0.9800
N11—C47	1.355 (3)	C40—H40B	0.9800
N11—C42	1.419 (3)	C40—H40C	0.9800
N11—H11A	0.8800	C38B—H38D	0.9800
N12—C58	1.357 (3)	C38B—H38E	0.9800
N12—C53	1.397 (3)	C38B—H38F	0.9800
N12—H12A	0.8800	C39B—H39D	0.9800
O1—C25	1.217 (3)	C39B—H39E	0.9800
O2—C36	1.216 (3)	C39B—H39F	0.9800
O3—C47	1.222 (3)	C40B—H40D	0.9800
O4—C58	1.203 (4)	C40B—H40E	0.9800
C(A1—C(M4	1.391 (3)	C40B—H40F	0.9800
C(A1—C(B1	1.432 (3)	C41—C46	1.393 (3)
C(A2—C(M1	1.383 (3)	C41—C42	1.395 (3)
C(A2—C(B2	1.436 (3)	C42—C43	1.388 (3)
C(A3—C(M1	1.389 (3)	C43—C44	1.375 (4)
C(A3—C(B3	1.431 (3)	C43—H43A	0.9500
C(A4—C(M2	1.388 (3)	C44—C45	1.381 (4)
C(A4—C(B4	1.426 (3)	C44—H44A	0.9500
C(A5—C(M2	1.383 (3)	C45—C46	1.379 (3)
C(A5—C(B5	1.436 (3)	C45—H45A	0.9500
C(A6—C(M3	1.380 (3)	C46—H46A	0.9500
C(A6—C(B6	1.436 (3)	C47—C48	1.524 (4)
C(A7—C(M3	1.393 (3)	C48—C51	1.514 (4)
C(A7—C(B7	1.432 (3)	C48—C49	1.523 (4)
C(A8—C(M4	1.391 (3)	C48—C50	1.526 (4)
C(A8—C(B8	1.433 (3)	C49—H49A	0.9800

C(B1—C(B2	1.343 (3)	C49—H49B	0.9800
C(B1—H(BA	0.9500	C49—H49C	0.9800
C(B2—H(BB	0.9500	C50—H50A	0.9800
C(B3—C(B4	1.350 (3)	C50—H50B	0.9800
C(B3—H(BC	0.9500	C50—H50C	0.9800
C(B4—H(BD	0.9500	C51—H51A	0.9800
C(B5—C(B6	1.334 (3)	C51—H51B	0.9800
C(B5—H(BE	0.9500	C51—H51C	0.9800
C(B6—H(BF	0.9500	C52—C57	1.385 (3)
C(B7—C(B8	1.346 (3)	C52—C53	1.403 (3)
C(B7—H(BG	0.9500	C53—C54	1.392 (3)
C(B8—H(BH	0.9500	C54—C55	1.378 (4)
C(M1—C19	1.494 (3)	C54—H54A	0.9500
C(M2—C30	1.496 (3)	C55—C56	1.381 (4)
C(M3—C41	1.486 (3)	C55—H55A	0.9500
C(M4—C52	1.496 (3)	C56—C57	1.384 (3)
C1—H1A	0.9500	C56—H56A	0.9500
C2—C3	1.345 (4)	C57—H57A	0.9500
C2—H2A	0.9500	C58—C59	1.534 (4)
C3—H3A	0.9500	C59—C62	1.495 (11)
C4—C9	1.366 (4)	C59—C60	1.504 (5)
C4—C5	1.384 (4)	C59—C61	1.535 (5)
C5—C6	1.383 (4)	C59—C62B	1.599 (9)
C5—H5A	0.9500	C60—H60A	0.9800
C6—C7	1.370 (5)	C60—H60B	0.9800
C6—H6A	0.9500	C60—H60C	0.9800
C7—C8	1.375 (5)	C61—H61A	0.9800
C7—H7A	0.9500	C61—H61B	0.9800
C8—C9	1.388 (4)	C61—H61C	0.9800
C8—H8A	0.9500	C62—H62A	0.9800
C9—H9B	0.9500	C62—H62B	0.9800
C10—H10B	0.9500	C62—H62C	0.9800
C11—C12	1.345 (3)	C62B—H62D	0.9800
C11—H11B	0.9500	C62B—H62E	0.9800
C12—H12B	0.9500	C62B—H62F	0.9800
C13—C14	1.377 (4)	Cl1—C1S	1.735 (3)
C13—C18	1.385 (4)	C1S—C6S	1.377 (4)
C14—C15	1.377 (4)	C1S—C2S	1.382 (4)
C14—H14A	0.9500	C2S—C3S	1.377 (4)
C15—C16	1.374 (4)	C2S—H2SA	0.9500
C15—H15A	0.9500	C3S—C4S	1.385 (5)
C16—C17	1.374 (4)	C3S—H3SA	0.9500
C16—H16A	0.9500	C4S—C5S	1.383 (5)
C17—C18	1.389 (4)	C4S—H4SA	0.9500
C17—H17A	0.9500	C5S—C6S	1.364 (4)
C18—H18A	0.9500	C5S—H5SA	0.9500
C19—C20	1.390 (3)	C6S—H6SA	0.9500
C19—C24	1.391 (3)	Cl2—C7S	1.729 (3)

C20—C21	1.389 (3)	C7S—C8S	1.356 (5)
C21—C22	1.377 (3)	C7S—C12S	1.371 (5)
C21—H21A	0.9500	C8S—C9S	1.382 (6)
C22—C23	1.381 (4)	C8S—H8SA	0.9500
C22—H22A	0.9500	C9S—C10S	1.349 (7)
C23—C24	1.378 (3)	C9S—H9SA	0.9500
C23—H23A	0.9500	C10S—C11S	1.343 (7)
C24—H24A	0.9500	C10S—H10C	0.9500
C25—C26	1.521 (4)	C11S—C12S	1.372 (5)
C26—C27	1.488 (9)	C11S—H11C	0.9500
C26—C29	1.535 (5)	C12S—H12C	0.9500
C26—C28	1.547 (5)	C13S—F2	1.322 (3)
C26—C27B	1.562 (8)	C13S—F3	1.326 (3)
C27—H27A	0.9800	C13S—F1	1.331 (3)
C27—H27B	0.9800	C13S—S1	1.819 (3)
C27—H27C	0.9800	O1S—S1	1.429 (2)
C27B—H27D	0.9800	O2S—S1	1.4367 (19)
C27B—H27E	0.9800	O3S—S1	1.434 (2)
C27B—H27F	0.9800		

N7—Fe1—N5	179.21 (8)	H29B—C29—H29C	109.5
N7—Fe1—N3	90.63 (8)	C31—C30—C35	118.5 (2)
N5—Fe1—N3	89.98 (8)	C31—C30—C(M2	122.4 (2)
N7—Fe1—N2	90.57 (8)	C35—C30—C(M2	119.1 (2)
N5—Fe1—N2	89.92 (8)	C32—C31—C30	120.2 (2)
N3—Fe1—N2	89.82 (8)	C32—C31—N10	120.1 (2)
N7—Fe1—N4	90.05 (8)	C30—C31—N10	119.7 (2)
N5—Fe1—N4	89.46 (8)	C33—C32—C31	120.6 (2)
N3—Fe1—N4	90.27 (8)	C33—C32—H32A	119.7
N2—Fe1—N4	179.38 (8)	C31—C32—H32A	119.7
N7—Fe1—N1	88.84 (8)	C32—C33—C34	120.0 (2)
N5—Fe1—N1	90.55 (8)	C32—C33—H33A	120.0
N3—Fe1—N1	179.31 (8)	C34—C33—H33A	120.0
N2—Fe1—N1	89.74 (8)	C33—C34—C35	119.8 (2)
N4—Fe1—N1	90.18 (8)	C33—C34—H34A	120.1
C(A1—N1—C(A2	105.44 (18)	C35—C34—H34A	120.1
C(A1—N1—Fe1	127.76 (15)	C34—C35—C30	121.0 (2)
C(A2—N1—Fe1	126.36 (15)	C34—C35—H35A	119.5
C(A3—N2—C(A4	105.52 (18)	C30—C35—H35A	119.5
C(A3—N2—Fe1	127.11 (15)	O2—C36—N10	121.5 (2)
C(A4—N2—Fe1	127.13 (15)	O2—C36—C37	122.1 (2)
C(A5—N3—C(A6	105.26 (18)	N10—C36—C37	116.5 (2)
C(A5—N3—Fe1	127.89 (15)	C39—C37—C38	111.8 (5)
C(A6—N3—Fe1	126.69 (15)	C40B—C37—C38B	107.3 (5)
C(A7—N4—C(A8	105.95 (18)	C39—C37—C36	109.3 (4)
C(A7—N4—Fe1	126.91 (15)	C38—C37—C36	108.3 (3)
C(A8—N4—Fe1	127.11 (15)	C40B—C37—C36	116.9 (3)
C1—N5—C3	106.7 (2)	C38B—C37—C36	108.1 (4)

C1—N5—Fe1	125.35 (16)	C40B—C37—C39B	108.8 (5)
C3—N5—Fe1	127.97 (16)	C38B—C37—C39B	109.5 (5)
C1—N6—C2	107.2 (2)	C36—C37—C39B	106.1 (4)
C1—N6—C4	125.4 (2)	C39—C37—C40	112.2 (5)
C2—N6—C4	127.4 (2)	C38—C37—C40	108.8 (4)
C10—N7—C12	106.21 (19)	C36—C37—C40	106.2 (3)
C10—N7—Fe1	126.56 (16)	C37—C38—H38A	109.5
C12—N7—Fe1	127.22 (15)	C37—C38—H38B	109.5
C10—N8—C11	107.07 (19)	H38A—C38—H38B	109.5
C10—N8—C13	126.4 (2)	C37—C38—H38C	109.5
C11—N8—C13	126.5 (2)	H38A—C38—H38C	109.5
C25—N9—C20	122.4 (2)	H38B—C38—H38C	109.5
C25—N9—H9A	118.8	C37—C39—H39A	109.5
C20—N9—H9A	118.8	C37—C39—H39B	109.5
C36—N10—C31	121.5 (2)	H39A—C39—H39B	109.5
C36—N10—H10A	119.3	C37—C39—H39C	109.5
C31—N10—H10A	119.3	H39A—C39—H39C	109.5
C47—N11—C42	123.6 (2)	H39B—C39—H39C	109.5
C47—N11—H11A	118.2	C37—C40—H40A	109.5
C42—N11—H11A	118.2	C37—C40—H40B	109.5
C58—N12—C53	129.7 (2)	H40A—C40—H40B	109.5
C58—N12—H12A	115.2	C37—C40—H40C	109.5
C53—N12—H12A	115.2	H40A—C40—H40C	109.5
N1—C(A1—C(M4	125.4 (2)	H40B—C40—H40C	109.5
N1—C(A1—C(B1	110.1 (2)	C37—C38B—H38D	109.5
C(M4—C(A1—C(B1	124.1 (2)	C37—C38B—H38E	109.5
N1—C(A2—C(M1	126.0 (2)	H38D—C38B—H38E	109.5
N1—C(A2—C(B2	109.9 (2)	C37—C38B—H38F	109.5
C(M1—C(A2—C(B2	124.1 (2)	H38D—C38B—H38F	109.5
N2—C(A3—C(M1	125.3 (2)	H38E—C38B—H38F	109.5
N2—C(A3—C(B3	110.14 (19)	C37—C39B—H39D	109.5
C(M1—C(A3—C(B3	124.5 (2)	C37—C39B—H39E	109.5
N2—C(A4—C(M2	125.9 (2)	H39D—C39B—H39E	109.5
N2—C(A4—C(B4	109.97 (19)	C37—C39B—H39F	109.5
C(M2—C(A4—C(B4	123.6 (2)	H39D—C39B—H39F	109.5
N3—C(A5—C(M2	125.7 (2)	H39E—C39B—H39F	109.5
N3—C(A5—C(B5	110.32 (19)	C37—C40B—H40D	109.5
C(M2—C(A5—C(B5	123.8 (2)	C37—C40B—H40E	109.5
N3—C(A6—C(M3	126.0 (2)	H40D—C40B—H40E	109.5
N3—C(A6—C(B6	110.06 (19)	C37—C40B—H40F	109.5
C(M3—C(A6—C(B6	123.8 (2)	H40D—C40B—H40F	109.5
N4—C(A7—C(M3	125.8 (2)	H40E—C40B—H40F	109.5
N4—C(A7—C(B7	109.86 (19)	C46—C41—C42	118.4 (2)
C(M3—C(A7—C(B7	124.3 (2)	C46—C41—C(M3	118.5 (2)
N4—C(A8—C(M4	126.1 (2)	C42—C41—C(M3	123.1 (2)
N4—C(A8—C(B8	109.72 (19)	C43—C42—C41	120.1 (2)
C(M4—C(A8—C(B8	124.1 (2)	C43—C42—N11	120.1 (2)
C(B2—C(B1—C(A1	107.3 (2)	C41—C42—N11	119.8 (2)

C(B2—C(B1—H(BA	126.3	C44—C43—C42	120.5 (2)
C(A1—C(B1—H(BA	126.3	C44—C43—H43A	119.7
C(B1—C(B2—C(A2	107.0 (2)	C42—C43—H43A	119.7
C(B1—C(B2—H(BB	126.5	C43—C44—C45	120.1 (2)
C(A2—C(B2—H(BB	126.5	C43—C44—H44A	120.0
C(B4—C(B3—C(A3	106.9 (2)	C45—C44—H44A	120.0
C(B4—C(B3—H(BC	126.6	C46—C45—C44	119.7 (2)
C(A3—C(B3—H(BC	126.6	C46—C45—H45A	120.2
C(B3—C(B4—C(A4	107.4 (2)	C44—C45—H45A	120.2
C(B3—C(B4—H(BD	126.3	C45—C46—C41	121.3 (2)
C(A4—C(B4—H(BD	126.3	C45—C46—H46A	119.4
C(B6—C(B5—C(A5	107.1 (2)	C41—C46—H46A	119.4
C(B6—C(B5—H(BE	126.4	O3—C47—N11	121.9 (2)
C(A5—C(B5—H(BE	126.4	O3—C47—C48	122.8 (2)
C(B5—C(B6—C(A6	107.2 (2)	N11—C47—C48	115.2 (2)
C(B5—C(B6—H(BF	126.4	C51—C48—C49	111.2 (3)
C(A6—C(B6—H(BF	126.4	C51—C48—C47	109.0 (2)
C(B8—C(B7—C(A7	107.1 (2)	C49—C48—C47	109.0 (2)
C(B8—C(B7—H(BG	126.4	C51—C48—C50	110.3 (3)
C(A7—C(B7—H(BG	126.4	C49—C48—C50	107.7 (2)
C(B7—C(B8—C(A8	107.3 (2)	C47—C48—C50	109.6 (2)
C(B7—C(B8—H(BH	126.4	C48—C49—H49A	109.5
C(A8—C(B8—H(BH	126.4	C48—C49—H49B	109.5
C(A2—C(M1—C(A3	122.7 (2)	H49A—C49—H49B	109.5
C(A2—C(M1—C19	118.3 (2)	C48—C49—H49C	109.5
C(A3—C(M1—C19	118.5 (2)	H49A—C49—H49C	109.5
C(A5—C(M2—C(A4	123.0 (2)	H49B—C49—H49C	109.5
C(A5—C(M2—C30	118.1 (2)	C48—C50—H50A	109.5
C(A4—C(M2—C30	118.2 (2)	C48—C50—H50B	109.5
C(A6—C(M3—C(A7	122.9 (2)	H50A—C50—H50B	109.5
C(A6—C(M3—C41	117.4 (2)	C48—C50—H50C	109.5
C(A7—C(M3—C41	119.6 (2)	H50A—C50—H50C	109.5
C(A8—C(M4—C(A1	123.3 (2)	H50B—C50—H50C	109.5
C(A8—C(M4—C52	118.0 (2)	C48—C51—H51A	109.5
C(A1—C(M4—C52	118.2 (2)	C48—C51—H51B	109.5
N5—C1—N6	110.5 (2)	H51A—C51—H51B	109.5
N5—C1—H1A	124.7	C48—C51—H51C	109.5
N6—C1—H1A	124.7	H51A—C51—H51C	109.5
C3—C2—N6	106.7 (2)	H51B—C51—H51C	109.5
C3—C2—H2A	126.6	C57—C52—C53	118.9 (2)
N6—C2—H2A	126.6	C57—C52—C(M4	119.5 (2)
C2—C3—N5	108.9 (2)	C53—C52—C(M4	121.6 (2)
C2—C3—H3A	125.6	C54—C53—N12	122.7 (2)
N5—C3—H3A	125.6	C54—C53—C52	119.8 (2)
C9—C4—C5	120.9 (3)	N12—C53—C52	117.5 (2)
C9—C4—N6	119.6 (2)	C55—C54—C53	120.0 (2)
C5—C4—N6	119.5 (2)	C55—C54—H54A	120.0
C6—C5—C4	118.7 (3)	C53—C54—H54A	120.0

C6—C5—H5A	120.6	C54—C55—C56	120.8 (2)
C4—C5—H5A	120.6	C54—C55—H55A	119.6
C7—C6—C5	120.8 (3)	C56—C55—H55A	119.6
C7—C6—H6A	119.6	C55—C56—C57	119.3 (2)
C5—C6—H6A	119.6	C55—C56—H56A	120.3
C6—C7—C8	119.8 (3)	C57—C56—H56A	120.3
C6—C7—H7A	120.1	C56—C57—C52	121.2 (2)
C8—C7—H7A	120.1	C56—C57—H57A	119.4
C7—C8—C9	120.0 (3)	C52—C57—H57A	119.4
C7—C8—H8A	120.0	O4—C58—N12	123.2 (3)
C9—C8—H8A	120.0	O4—C58—C59	123.6 (3)
C4—C9—C8	119.6 (3)	N12—C58—C59	113.2 (2)
C4—C9—H9B	120.2	C62—C59—C60	121.0 (5)
C8—C9—H9B	120.2	C62—C59—C58	110.0 (5)
N7—C10—N8	110.9 (2)	C60—C59—C58	110.6 (3)
N7—C10—H10B	124.5	C62—C59—C61	95.5 (5)
N8—C10—H10B	124.5	C60—C59—C61	110.1 (3)
C12—C11—N8	106.8 (2)	C58—C59—C61	108.1 (3)
C12—C11—H11B	126.6	C60—C59—C62B	97.6 (4)
N8—C11—H11B	126.6	C58—C59—C62B	108.1 (5)
C11—C12—N7	109.0 (2)	C61—C59—C62B	121.7 (5)
C11—C12—H12B	125.5	C59—C60—H60A	109.5
N7—C12—H12B	125.5	C59—C60—H60B	109.5
C14—C13—C18	120.9 (2)	H60A—C60—H60B	109.5
C14—C13—N8	119.1 (2)	C59—C60—H60C	109.5
C18—C13—N8	120.0 (2)	H60A—C60—H60C	109.5
C15—C14—C13	119.4 (3)	H60B—C60—H60C	109.5
C15—C14—H14A	120.3	C59—C61—H61A	109.5
C13—C14—H14A	120.3	C59—C61—H61B	109.5
C16—C15—C14	120.4 (3)	H61A—C61—H61B	109.5
C16—C15—H15A	119.8	C59—C61—H61C	109.5
C14—C15—H15A	119.8	H61A—C61—H61C	109.5
C15—C16—C17	120.3 (3)	H61B—C61—H61C	109.5
C15—C16—H16A	119.8	C59—C62—H62A	109.5
C17—C16—H16A	119.8	C59—C62—H62B	109.5
C16—C17—C18	120.1 (3)	H62A—C62—H62B	109.5
C16—C17—H17A	120.0	C59—C62—H62C	109.5
C18—C17—H17A	120.0	H62A—C62—H62C	109.5
C13—C18—C17	118.9 (3)	H62B—C62—H62C	109.5
C13—C18—H18A	120.5	C59—C62B—H62D	109.5
C17—C18—H18A	120.5	C59—C62B—H62E	109.5
C20—C19—C24	118.1 (2)	H62D—C62B—H62E	109.5
C20—C19—C(M1	125.5 (2)	C59—C62B—H62F	109.5
C24—C19—C(M1	116.2 (2)	H62D—C62B—H62F	109.5
C21—C20—C19	120.0 (2)	H62E—C62B—H62F	109.5
C21—C20—N9	119.6 (2)	C6S—C1S—C2S	121.8 (3)
C19—C20—N9	120.4 (2)	C6S—C1S—Cl1	119.5 (2)
C22—C21—C20	120.5 (2)	C2S—C1S—Cl1	118.7 (2)

C22—C21—H21A	119.8	C3S—C2S—C1S	118.9 (3)
C20—C21—H21A	119.8	C3S—C2S—H2SA	120.6
C21—C22—C23	120.4 (2)	C1S—C2S—H2SA	120.6
C21—C22—H22A	119.8	C2S—C3S—C4S	120.0 (3)
C23—C22—H22A	119.8	C2S—C3S—H3SA	120.0
C24—C23—C22	118.8 (2)	C4S—C3S—H3SA	120.0
C24—C23—H23A	120.6	C5S—C4S—C3S	119.8 (3)
C22—C23—H23A	120.6	C5S—C4S—H4SA	120.1
C23—C24—C19	122.2 (2)	C3S—C4S—H4SA	120.1
C23—C24—H24A	118.9	C6S—C5S—C4S	120.9 (3)
C19—C24—H24A	118.9	C6S—C5S—H5SA	119.6
O1—C25—N9	121.8 (2)	C4S—C5S—H5SA	119.6
O1—C25—C26	122.1 (2)	C5S—C6S—C1S	118.7 (3)
N9—C25—C26	116.1 (2)	C5S—C6S—H6SA	120.7
C27—C26—C25	110.0 (5)	C1S—C6S—H6SA	120.7
C27—C26—C29	100.3 (5)	C8S—C7S—C12S	120.8 (4)
C25—C26—C29	111.0 (3)	C8S—C7S—Cl2	119.4 (3)
C27—C26—C28	122.8 (5)	C12S—C7S—Cl2	119.7 (3)
C25—C26—C28	108.1 (3)	C7S—C8S—C9S	118.2 (4)
C29—C26—C28	104.0 (3)	C7S—C8S—H8SA	120.9
C25—C26—C27B	106.6 (5)	C9S—C8S—H8SA	120.9
C29—C26—C27B	127.2 (5)	C10S—C9S—C8S	121.0 (4)
C28—C26—C27B	97.9 (4)	C10S—C9S—H9SA	119.5
C26—C27—H27A	109.5	C8S—C9S—H9SA	119.5
C26—C27—H27B	109.5	C11S—C10S—C9S	120.5 (4)
H27A—C27—H27B	109.5	C11S—C10S—H10C	119.8
C26—C27—H27C	109.5	C9S—C10S—H10C	119.8
H27A—C27—H27C	109.5	C10S—C11S—C12S	119.9 (4)
H27B—C27—H27C	109.5	C10S—C11S—H11C	120.0
C26—C27B—H27D	109.5	C12S—C11S—H11C	120.0
C26—C27B—H27E	109.5	C7S—C12S—C11S	119.5 (4)
H27D—C27B—H27E	109.5	C7S—C12S—H12C	120.2
C26—C27B—H27F	109.5	C11S—C12S—H12C	120.2
H27D—C27B—H27F	109.5	F2—C13S—F3	107.8 (2)
H27E—C27B—H27F	109.5	F2—C13S—F1	107.7 (2)
C26—C28—H28A	109.5	F3—C13S—F1	107.4 (2)
C26—C28—H28B	109.5	F2—C13S—S1	112.02 (18)
H28A—C28—H28B	109.5	F3—C13S—S1	111.33 (18)
C26—C28—H28C	109.5	F1—C13S—S1	110.49 (18)
H28A—C28—H28C	109.5	O1S—S1—O3S	115.42 (14)
H28B—C28—H28C	109.5	O1S—S1—O2S	114.89 (13)
C26—C29—H29A	109.5	O3S—S1—O2S	115.08 (13)
C26—C29—H29B	109.5	O1S—S1—C13S	103.34 (12)
H29A—C29—H29B	109.5	O3S—S1—C13S	102.42 (13)
C26—C29—H29C	109.5	O2S—S1—C13S	103.08 (12)
H29A—C29—H29C	109.5		