Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

μ-Sulfato-1κO:2κO-μ-oxo-bis[tris(2-pyridylmethyl)amine-κ⁴N,N′,N″,N‴]-diiron(III) diperchlorate acetonitrile/water (0.75/0.25) solvate

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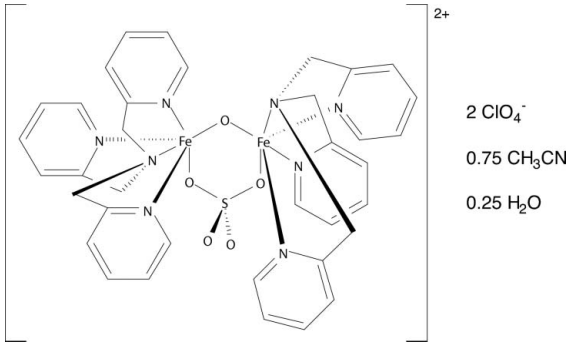
Received 16 July 2007; accepted 1 September 2007

Key indicators: single-crystal X-ray study; T = 90 K; mean σ(C–C) = 0.004 Å; disorder in solvent or counterion; R factor = 0.054; wR factor = 0.093; data-to-parameter ratio = 13.7.

The title complex, $[Fe_2(C_{18}H_{18}N_4)_2O(SO_4)](ClO_4)_2\cdot 0.75C_2H_3N\cdot 0.25H_2O$, consists of two perchlorate ions, a solvent cavity with acetonitrile and water (disordered 3/1), and an Fe complex dication. The dication is a diiron(III) unit containing an oxo bridge and a sulfato bridge. The iron(III) centers are pseudo-octahedral, six-coordinate, with tris(2-pyridylmethyl) amine (TPA) providing four N atoms. The distances and angles are typical for bent μ-oxo-bridged TPA complexes. The complex was the unexpected result of a reaction designed to produce a μ-sulfido–μ-carboxylato–diiron center.

Related literature

The preparation of the compound has been reported previously (Holz *et al.*, 1993; Hazell *et al.*, 1994). The structure is typical of a bent μ-oxo–diiron(III) complex with TPA (Norman *et al.*, 1997). The sulfato bridge was produced by oxidation of sulfide, a result similar to the oxidation of methanol to formate in an Fe^{III} TPA system (Norman *et al.*, 1998). For related literature, see: Mukherjee *et al.* (1988).



Experimental

Crystal data

$[Fe_2(C_{18}H_{18}N_4)_2O(SO_4)]_4(ClO_4)_8\cdot 3C_2H_3N\cdot H_2O$
M_r = 4154.72
Monoclinic, $P2_1/n$
a = 12.7031 (10) Å
b = 24.477 (3) Å
c = 13.6165 (11) Å
β = 103.357 (5)°
V = 4119.3 (6) Å³
Z = 1
Mo $K\alpha$ radiation
μ = 0.96 mm⁻¹
T = 90 K
0.30 × 0.17 × 0.05 mm

Data collection

Nonius KappaCCD (with Oxford Cryostream) diffractometer
Absorption correction: multi-scan *HKL SCALEPACK* (Otwinowski & Minor, 1997)
T_{min} = 0.728, T_{max} = 0.946
81911 measured reflections
14279 independent reflections
8172 reflections with $I > 3\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.093
S = 0.90
8172 reflections
595 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.78 e Å⁻³
$\Delta\rho_{min}$ = −0.71 e Å⁻³

Table 1
Selected geometric parameters (Å, °).

Fe1—O1	1.788 (2)	Fe2—O1	1.807 (2)
Fe1—O2	2.012 (2)	Fe2—O3	1.950 (2)
Fe1—N11	2.153 (2)	Fe2—N21	2.220 (2)
Fe1—N12	2.138 (2)	Fe2—N22	2.138 (2)
Fe1—N13	2.140 (2)	Fe2—N23	2.129 (2)
Fe1—N14	2.242 (2)	Fe2—N24	2.213 (2)
Fe1—O1—Fe2	133.0 (1)		

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *TEXSAN for Windows* (Molecular Structure Corporation, 1999); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *TEXSAN for Windows*.

We thank Frank Fronczek for data collection, and the Louisiana Board of Regents Support Fund and the Robert A. Welch Foundation (x-0011) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2197).

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supplementary materials

Acta Cryst. (2007). E**63**, m2480-m2481 [**doi:10.1107/S1600536807042857**]

μ-Sulfato-1κO:2κO-μ-oxo-bis[tris(2-pyridylmethyl)amine-$\kappa^4 N,N',N'',N'''$]diiron(III) diperchlorate acetonitrile/water (0.75/0.25) solvate

C. M. Smith and R. E. Norman

Comment

As the result of an attempt to synthesize a new class of diiron complexes with a µ-sulfido-µ-carboxylato diiron core using tris-(2-pyridylmethyl)amine (TPA), the title complex, (I), was prepared and structurally characterized. Since the replacement of a µ-oxo ligand by a µ-sulfido ligand has been little studied (Mukherjee *et al.*, 1988), we were not entirely sure what spectroscopic changes would accompany this replacement. To determine whether we had synthesized the desired sulfido-bridged species, we determined the structure. Surprisingly, instead of a µ-sulfido-µ-acetato diiron TPA species we had produced a µ-oxo-µ-sulfato diiron(III) TPA species. The sulfate must have been formed by oxidation of sulfide as no sulfate was added. The source of oxidant is undetermined, but presumably is either perchlorate or atmospheric oxygen. Similarly, a µ-oxo-µ-formato diiron(III) TPA species was produced by aerobic oxidation of a methanol solution of Fe(III) and TPA (Norman *et al.*, 1998).

The structures and spectral properties of several µ-oxo diiron(III) complexes with the TPA ligand have been previously reported (see for example, Norman *et al.*, 1997, or Norman *et al.*, 1998 and references therein). The title complex displays the typical pattern of inequivalent iron sites (Fe1 has the tertiary amine nitrogen atom of TPA *trans* to the oxo bridge, while Fe2 has the tertiary amine nitrogen atom of TPA *cis* to the oxo bridge) and a distinctly asymmetric oxo bridge [Fe1—O1 is 1.788 (2) Å and Fe2—O1 is 1.807 (2) Å], with pronounced lengthening of the bonds *trans* to the oxo bridge (Fig. 1).

Figure 2 is provided to indicate the numbering of atoms in the TPA ligands. N_{xy} provides the identifiers where *x* refers to the Fe number and the *y* identifies the ring. For both TPA ligands, N_{x1} is in the Fe1—O1—Fe2 plane. N_{x4} is the tertiary amine nitrogen atom.

The preparation of $[Fe_2(TPA)_2O(SO_4)](ClO_4)_2$ has been reported at least twice previously (Holz *et al.*, 1993; Hazell *et al.*, 1994), but its structure was not determined. Interestingly, the Fe—O—Fe angle was predicted, based on electronic spectroscopy, to be 134° (Holz *et al.*, 1993) which agrees well with the 133.0 (1)° reported here.

Experimental

Tris[(2-pyridinium)methyl]amine perchlorate (0.6017 g, 1.017 mmol), triethylamine (0.63 ml, 4.5 mmol) and sodium acetate (0.0417 g, 1.023 mmol) were dissolved in 40 ml MeOH. $Fe(ClO_4)_3.10H_2O$ (0.5465 g, 1.023 mmol) was dissolved in 2 ml MeOH and this solution was added to the ligand solution. $Na_2S{\cdot}9H_2O$ (0.1482 g, 0.6170 mmol) was then added. The mixture was stirred for approximately 20 minutes and then allowed to sit for 20 minutes until a yellow precipitate formed, which was removed by filtration. The resultant filtrate turned bright green and was allowed to sit for four days. Small green rectangular plates formed which were isolated with cold MeOH, dried and dissolved in CH_3CN. The solution was placed in a sealed vessel containing ethyl acetate. Yellow-green rectangular plates formed after two days, one of which was selected for structure determination.

Refinement

Initially the structure was modeled with a single acetonitrile in the asymmetric unit with full occupancy. During refinement, the thermal parameters for this acetontrile grew larger and there was a persistent peak of electron density near the nitrile carbon atom (C1). Since this feature was not in a chemically reasonable position, it was assigned as an oxygen atom (O6) of a water molecule at 25% occupancy and the occupancy of the acetonitrile atoms was fixed at 75%. This produces an apparent close contact between O6 and C1 of 1.15 (2) Å.

The populations of C1, C2, N1 and O6 were refined to evaluate the 3:1 acetonitrile:water ratio. All of the populations increased as did the thermal parameters for the acetonitrile atoms. At the same time *R* and *wR* decreased, but not significantly. This model was rejected and the populations were fixed to preserve the 3:1 ratio.

With the exception of the disordered water, the hydrogen atoms were placed in calculated positions and assigned thermal parameters 1.2 times larger than the atoms to which theyμ-Sulfato-1κ*O*:2κ*O*-μ-oxo-bis[tris(2-pyridylmethyl)amine-κ^4 *N*,*N*',*N*'',*N*''']diiron(III) diperchlorate acetonitrile/water (0.75/0.25) solvate are bound. The hydrogen atoms for the water were located in difference maps, and were also assigned thermal parameters 1.2 times larger than the oxygen atom to which they are bound.

Figures

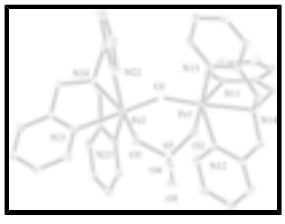


Fig. 1. Perspective drawing of the $[Fe_2(TPA)_2O(SO_4)]^{2+}$ cation with displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted.

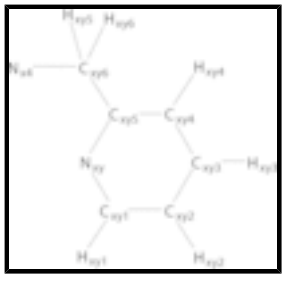


Fig. 2. The numbering of atoms in the TPA ligands.

μ-Sulfato-1κ*O*:2κ*O*-μ-oxo-bis[tris(2-pyridylmethyl)amine-κ^4 *N*,*N*',*N*'',*N*''']diiron(III) diperchlorate acetonitrile/water (0.75/0.25) solvate

Crystal data

$[Fe_2(C_{18}H_{18}N_4)_2O(SO_4)]_4(ClO_4)_8\cdot 3C_2H_3N\cdot H_2O$	F_{000} = 2132.00
M_r = 4154.72	D_x = 1.675 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.7107 Å
Hall symbol: -P 2yn	Cell parameters from 14215 reflections

a = 12.7031 (10) Å	θ = 2.5–32.0º
b = 24.477 (3) Å	μ = 0.96 mm^{-1}
c = 13.6165 (11) Å	T = 90 K
β = 103.357 (5)º	Lath, yellow-green
V = 4119.3 (6) Å^3	0.30 × 0.17 × 0.05 mm
Z = 1	

Data collection

Nonius KappaCCD (with Oxford Cryostream) diffractometer	14279 independent reflections
Radiation source: fine-focus sealed tube	8172 reflections with $I > 3\sigma(I)$
Monochromator: graphite	R_{int} = 0.042
T = 90 K	θ_{max} = 32.0º
ω scans with κ offsets	θ_{min} = 2.5º
Absorption correction: multi-scan *HKL SCALEPACK* (Otwinowski & Minor, 1997)	h = −18→18
T_{min} = 0.728, T_{max} = 0.946	k = −36→36
81911 measured reflections	l = −20→20

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	Weighting scheme based on measured s.u.'s $w = 1/[\sigma^2(F_o) + 0.000841\|F_o\|^2]$
$R[F^2 > 2\sigma(F^2)]$ = 0.054	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.093	$\Delta\rho_{max}$ = 0.78 e Å^{-3}
S = 0.90	$\Delta\rho_{min}$ = −0.71 e Å^{-3}
8172 reflections	Extinction correction: none
595 parameters	

Special details

Refinement. Refinement of F^2. The weighted R-factor wR and goodness of fit are based on F^2, conventional R-factors R are based on F. R-factors based on F^2 are statistically about twice as large as those based on F.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Fe1	0.22087 (3)	0.26340 (2)	0.93084 (2)	0.01043 (8)	
Fe2	0.29912 (3)	0.15787 (2)	0.81495 (2)	0.01094 (8)	
Cl1	0.35062 (5)	0.36704 (3)	0.38755 (4)	0.0136 (1)	
Cl2	0.16176 (5)	0.02549 (3)	0.36029 (4)	0.0150 (1)	
S5	0.46963 (5)	0.23004 (3)	0.96923 (4)	0.0123 (1)	
O1	0.20634 (13)	0.20867 (7)	0.84171 (11)	0.0124 (4)	
O2	0.37397 (13)	0.25008 (7)	1.00798 (11)	0.0129 (4)	
O3	0.43271 (13)	0.17723 (7)	0.91148 (12)	0.0161 (4)	

O4	0.55651 (13)	0.21686 (8)	1.05476 (12)	0.0166 (5)	
O5	0.4959 (1)	0.26959 (8)	0.89952 (12)	0.0198 (5)	
O6	0.0659 (13)	0.4065 (8)	0.6270 (8)	0.119 (6)	0.25
O11	0.4197 (1)	0.32356 (8)	0.36660 (12)	0.0185 (5)	
O12	0.24272 (13)	0.34587 (8)	0.37924 (13)	0.0204 (5)	
O13	0.3478 (2)	0.41082 (8)	0.31582 (13)	0.0223 (5)	
O14	0.3926 (2)	0.38753 (8)	0.48880 (12)	0.0215 (5)	
O21	0.0775 (1)	−0.00452 (8)	0.3920 (1)	0.0244 (5)	
O22	0.1767 (2)	0.07740 (8)	0.4111 (1)	0.0313 (6)	
O23	0.1307 (2)	0.03407 (9)	0.25307 (13)	0.0298 (6)	
O24	0.2609 (1)	−0.00557 (9)	0.3862 (1)	0.0264 (5)	
N1	0.0615 (5)	0.4712 (3)	0.6607 (5)	0.112 (3)	0.75
N11	0.0673 (2)	0.30205 (9)	0.8705 (1)	0.0125 (5)	
N12	0.2774 (2)	0.33111 (9)	0.8582 (1)	0.0130 (5)	
N13	0.1708 (2)	0.22604 (9)	1.0547 (1)	0.0119 (5)	
N14	0.2234 (2)	0.33223 (8)	1.03999 (13)	0.0121 (5)	
N21	0.3982 (2)	0.09698 (9)	0.7557 (2)	0.0153 (5)	
N22	0.2472 (2)	0.09465 (9)	0.9014 (1)	0.0135 (5)	
N23	0.3084 (2)	0.19461 (9)	0.6755 (1)	0.0134 (5)	
N24	0.1760 (2)	0.11150 (9)	0.7049 (1)	0.0124 (5)	
C1	0.0943 (4)	0.4470 (2)	0.5982 (4)	0.041 (1)	0.75
C2	0.1257 (3)	0.4167 (2)	0.5289 (3)	0.0231 (10)	0.75
C111	0.0045 (2)	0.28996 (11)	0.7787 (2)	0.0150 (6)	
C112	−0.0826 (2)	0.32136 (12)	0.7327 (2)	0.0189 (7)	
C113	−0.1098 (2)	0.36695 (12)	0.7842 (2)	0.0206 (7)	
C114	−0.0454 (2)	0.37946 (11)	0.8778 (2)	0.0181 (7)	
C115	0.0439 (2)	0.34687 (10)	0.9182 (2)	0.0132 (6)	
C116	0.1165 (2)	0.35992 (11)	1.0196 (2)	0.0153 (6)	
C121	0.2846 (2)	0.33099 (11)	0.7613 (2)	0.0157 (6)	
C122	0.3387 (2)	0.37159 (11)	0.7221 (2)	0.0184 (7)	
C123	0.3848 (2)	0.41413 (12)	0.7840 (2)	0.0191 (7)	
C124	0.3736 (2)	0.41542 (11)	0.8834 (2)	0.0168 (6)	
C125	0.3194 (2)	0.37323 (10)	0.9184 (2)	0.0144 (6)	
C126	0.3123 (2)	0.36916 (11)	1.0274 (2)	0.0164 (6)	
C131	0.1278 (2)	0.17545 (10)	1.0520 (2)	0.0130 (6)	
C132	0.1007 (2)	0.15191 (11)	1.1349 (2)	0.0146 (6)	
C133	0.1142 (2)	0.18243 (12)	1.2231 (2)	0.0163 (6)	
C134	0.1573 (2)	0.23451 (11)	1.2264 (2)	0.0146 (6)	
C135	0.1879 (2)	0.25491 (10)	1.1420 (2)	0.0128 (6)	
C136	0.2468 (2)	0.30805 (11)	1.1426 (2)	0.0144 (6)	
C211	0.5072 (2)	0.09782 (11)	0.7736 (2)	0.0181 (7)	
C212	0.5643 (2)	0.06486 (12)	0.7223 (2)	0.0189 (7)	
C213	0.5072 (2)	0.03167 (12)	0.6458 (2)	0.0217 (7)	
C214	0.3957 (2)	0.03125 (11)	0.6247 (2)	0.0194 (7)	
C215	0.3433 (2)	0.06357 (10)	0.6826 (2)	0.0149 (6)	
C216	0.2224 (2)	0.06104 (11)	0.6700 (2)	0.0145 (6)	
C221	0.3020 (2)	0.07783 (11)	0.9932 (2)	0.0190 (7)	
C222	0.2591 (2)	0.03969 (12)	1.0487 (2)	0.0229 (7)	
C223	0.1578 (2)	0.01815 (12)	1.0076 (2)	0.0229 (7)	

C224	0.1017 (2)	0.03533 (11)	0.9122 (2)	0.0191 (7)	
C225	0.1484 (2)	0.07404 (11)	0.8619 (2)	0.0156 (6)	
C226	0.0923 (2)	0.09717 (11)	0.7605 (2)	0.0151 (6)	
C231	0.3918 (2)	0.22496 (11)	0.6615 (2)	0.0152 (6)	
C232	0.4004 (2)	0.24110 (11)	0.5658 (2)	0.0160 (6)	
C233	0.3215 (2)	0.22475 (11)	0.4830 (2)	0.0157 (6)	
C234	0.2350 (2)	0.19409 (11)	0.4975 (2)	0.0143 (6)	
C235	0.2300 (2)	0.18008 (10)	0.5949 (2)	0.0128 (6)	
C236	0.1359 (2)	0.14990 (11)	0.6194 (2)	0.0146 (6)	
H1	0.1659	0.3862	0.5606	0.028*	0.75
H2	0.1698	0.4380	0.4960	0.028*	0.75
H3	0.0639	0.4042	0.4807	0.028*	0.75
H4	0.0786	0.4258	0.6894	0.143*	0.25
H5	0.1336	0.3869	0.6254	0.143*	0.25
H111	0.0213	0.2584	0.7445	0.018*	
H112	−0.1237	0.3124	0.6672	0.023*	
H113	−0.1711	0.3887	0.7554	0.025*	
H114	−0.0619	0.4101	0.9144	0.022*	
H115	0.0804	0.3492	1.0703	0.018*	
H116	0.1284	0.3983	1.0231	0.018*	
H121	0.2516	0.3022	0.7184	0.019*	
H122	0.3440	0.3703	0.6537	0.022*	
H123	0.4236	0.4421	0.7592	0.023*	
H124	0.4027	0.4449	0.9266	0.020*	
H125	0.2996	0.4046	1.0508	0.020*	
H126	0.3789	0.3555	1.0663	0.020*	
H131	0.1156	0.1553	0.9908	0.016*	
H132	0.0735	0.1157	1.1318	0.018*	
H133	0.0940	0.1676	1.2806	0.020*	
H134	0.1659	0.2561	1.2857	0.018*	
H135	0.3224	0.3018	1.1646	0.017*	
H136	0.2241	0.3327	1.1875	0.017*	
H211	0.5461	0.1220	0.8235	0.022*	
H212	0.6411	0.0649	0.7389	0.023*	
H213	0.5447	0.0093	0.6081	0.026*	
H214	0.3554	0.0093	0.5716	0.023*	
H215	0.2059	0.0309	0.7078	0.017*	
H216	0.1898	0.0557	0.6005	0.017*	
H221	0.3718	0.0925	1.0207	0.023*	
H222	0.2986	0.0286	1.1136	0.027*	
H223	0.1268	−0.0081	1.0440	0.027*	
H224	0.0325	0.0206	0.8823	0.023*	
H225	0.0526	0.1289	0.7697	0.018*	
H226	0.0443	0.0707	0.7235	0.018*	
H231	0.4463	0.2357	0.7185	0.018*	
H232	0.4595	0.2630	0.5574	0.019*	
H233	0.3267	0.2345	0.4168	0.019*	
H234	0.1798	0.1828	0.4416	0.017*	
H235	0.0993	0.1299	0.5619	0.018*	

H236	0.0875	0.1754	0.6379	0.018*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0114 (2)	0.0108 (2)	0.0095 (2)	−0.0013 (1)	0.00342 (12)	−0.00123 (13)
Fe2	0.0098 (2)	0.0122 (2)	0.0114 (2)	−0.0019 (1)	0.00351 (12)	−0.00255 (13)
Cl1	0.0139 (3)	0.0142 (3)	0.0123 (3)	0.0003 (2)	0.0022 (2)	0.0000 (2)
Cl2	0.0176 (3)	0.0125 (3)	0.0155 (3)	0.0005 (2)	0.0050 (2)	−0.0008 (2)
S5	0.0105 (3)	0.0150 (3)	0.0115 (3)	−0.0023 (2)	0.0024 (2)	−0.0025 (2)
O1	0.0120 (8)	0.0125 (9)	0.0129 (8)	−0.0013 (7)	0.0036 (6)	−0.0017 (7)
O2	0.0113 (8)	0.0155 (9)	0.0117 (8)	0.0003 (7)	0.0025 (6)	−0.0022 (7)
O3	0.0128 (8)	0.0158 (10)	0.0185 (9)	−0.0016 (7)	0.0013 (7)	−0.0064 (7)
O4	0.0133 (8)	0.0214 (10)	0.0140 (8)	−0.0006 (8)	0.0006 (7)	−0.0029 (7)
O5	0.0187 (9)	0.0236 (11)	0.0189 (9)	−0.0047 (8)	0.0076 (7)	0.0028 (8)
O6	0.122 (12)	0.21 (2)	0.032 (6)	0.14 (1)	0.034 (7)	0.041 (9)
O11	0.0195 (9)	0.0171 (10)	0.0204 (9)	0.0031 (8)	0.0077 (7)	−0.0017 (7)
O12	0.0131 (9)	0.0247 (11)	0.0242 (9)	−0.0046 (8)	0.0060 (7)	−0.0014 (8)
O13	0.0272 (10)	0.0174 (10)	0.0215 (10)	−0.0002 (8)	0.0037 (8)	0.0055 (8)
O14	0.0242 (10)	0.0238 (11)	0.0143 (9)	0.0007 (9)	0.0000 (7)	−0.0058 (8)
O21	0.0178 (10)	0.0219 (11)	0.0356 (11)	−0.0002 (8)	0.0106 (8)	0.0062 (9)
O22	0.0470 (13)	0.0149 (11)	0.0315 (11)	−0.0017 (10)	0.0077 (10)	−0.0082 (9)
O23	0.0487 (13)	0.0268 (12)	0.0147 (9)	0.0088 (10)	0.0090 (9)	0.0040 (8)
O24	0.0153 (9)	0.0271 (12)	0.0364 (11)	0.0071 (9)	0.0048 (8)	0.0000 (9)
N1	0.115 (5)	0.126 (6)	0.117 (5)	−0.037 (4)	0.072 (4)	−0.091 (5)
N11	0.0140 (10)	0.0121 (11)	0.0121 (9)	−0.0021 (8)	0.0045 (8)	−0.0008 (8)
N12	0.0132 (10)	0.0111 (11)	0.0147 (10)	−0.0012 (8)	0.0030 (8)	−0.0017 (8)
N13	0.0102 (9)	0.0138 (11)	0.0117 (9)	0.0004 (8)	0.0027 (8)	0.0002 (8)
N14	0.0138 (10)	0.0117 (11)	0.0103 (9)	−0.0017 (8)	0.0015 (7)	−0.0004 (8)
N21	0.0121 (10)	0.0167 (12)	0.0173 (10)	−0.0013 (9)	0.0040 (8)	−0.0027 (8)
N22	0.0141 (10)	0.0131 (11)	0.0144 (10)	0.0002 (9)	0.0054 (8)	−0.0019 (8)
N23	0.0122 (10)	0.0158 (11)	0.0130 (9)	−0.0022 (8)	0.0044 (8)	−0.0035 (8)
N24	0.0118 (10)	0.0115 (11)	0.0145 (10)	−0.0006 (8)	0.0046 (8)	−0.0012 (8)
C1	0.031 (2)	0.039 (3)	0.051 (3)	−0.014 (2)	0.007 (2)	0.000 (2)
C2	0.023 (2)	0.023 (2)	0.021 (2)	−0.003 (2)	0.000 (1)	−0.002 (2)
C111	0.0164 (12)	0.0146 (13)	0.0147 (11)	−0.0034 (10)	0.0053 (10)	−0.0024 (10)
C112	0.0143 (12)	0.024 (2)	0.0167 (12)	−0.0028 (11)	−0.0002 (9)	−0.0003 (11)
C113	0.0162 (13)	0.017 (1)	0.027 (1)	0.0021 (11)	0.0021 (10)	0.0022 (11)
C114	0.0199 (13)	0.015 (1)	0.0186 (12)	0.0004 (11)	0.0031 (10)	−0.0016 (10)
C115	0.0153 (11)	0.0123 (12)	0.0135 (11)	−0.0013 (10)	0.0063 (9)	0.0011 (9)
C116	0.0155 (12)	0.0146 (13)	0.0164 (12)	0.0030 (10)	0.0048 (10)	−0.0027 (10)
C121	0.0164 (12)	0.0146 (13)	0.0170 (12)	0.0012 (10)	0.0056 (10)	0.0009 (10)
C122	0.0206 (13)	0.020 (2)	0.0154 (12)	0.0015 (11)	0.0066 (10)	0.0047 (10)
C123	0.0175 (13)	0.018 (1)	0.0229 (13)	−0.0010 (11)	0.0072 (10)	0.0059 (11)
C124	0.0150 (12)	0.0124 (13)	0.0213 (13)	−0.0010 (10)	0.0006 (10)	0.0000 (10)
C125	0.0129 (12)	0.0132 (13)	0.0168 (12)	0.0003 (10)	0.0029 (9)	0.0005 (10)
C126	0.0197 (13)	0.0134 (13)	0.0159 (12)	−0.0062 (11)	0.0040 (10)	−0.0034 (10)
C131	0.0093 (11)	0.0166 (13)	0.0127 (11)	0.0004 (10)	0.0020 (9)	−0.0017 (9)

C132	0.0106 (11)	0.0142 (13)	0.0179 (12)	0.0007 (10)	0.0010 (9)	0.0035 (10)
C133	0.0132 (12)	0.023 (2)	0.0118 (11)	0.0006 (11)	0.0021 (9)	0.0037 (10)
C134	0.0132 (11)	0.022 (1)	0.0091 (11)	0.0022 (11)	0.0028 (9)	−0.0003 (10)
C135	0.0113 (11)	0.0137 (13)	0.0128 (11)	0.0024 (10)	0.0018 (9)	−0.0003 (9)
C136	0.0176 (12)	0.0146 (13)	0.0109 (11)	−0.0007 (10)	0.0030 (9)	−0.0009 (9)
C211	0.0135 (12)	0.020 (2)	0.0210 (13)	−0.0023 (11)	0.0043 (10)	−0.0063 (10)
C212	0.0128 (12)	0.018 (1)	0.027 (1)	0.0010 (11)	0.0070 (10)	−0.0025 (11)
C213	0.0197 (13)	0.020 (2)	0.030 (1)	0.0000 (11)	0.0130 (11)	−0.0070 (11)
C214	0.0169 (12)	0.018 (1)	0.0239 (13)	−0.0013 (11)	0.0061 (10)	−0.0084 (11)
C215	0.0155 (12)	0.0116 (13)	0.0192 (12)	−0.0018 (10)	0.0070 (10)	−0.0027 (10)
C216	0.0136 (11)	0.0141 (13)	0.0160 (11)	−0.0030 (10)	0.0038 (9)	−0.0039 (9)
C221	0.0190 (13)	0.015 (1)	0.0239 (13)	0.0029 (11)	0.0065 (10)	0.0002 (11)
C222	0.029 (2)	0.018 (2)	0.0222 (13)	0.0064 (12)	0.0086 (12)	0.0051 (11)
C223	0.030 (2)	0.015 (1)	0.030 (1)	0.0012 (12)	0.0183 (12)	0.0026 (11)
C224	0.0188 (13)	0.016 (1)	0.0263 (13)	−0.0020 (11)	0.0130 (11)	−0.0030 (11)
C225	0.0166 (12)	0.0124 (13)	0.0201 (12)	0.0009 (10)	0.0089 (10)	−0.0043 (10)
C226	0.0111 (11)	0.0153 (13)	0.0203 (12)	−0.0023 (10)	0.0066 (9)	−0.0044 (10)
C231	0.0139 (12)	0.017 (1)	0.0158 (12)	−0.0032 (10)	0.0048 (9)	−0.0028 (10)
C232	0.0143 (12)	0.018 (1)	0.0164 (12)	−0.0036 (10)	0.0058 (9)	−0.0019 (10)
C233	0.0192 (13)	0.0144 (13)	0.0139 (11)	0.0023 (10)	0.0049 (10)	0.0013 (9)
C234	0.0149 (12)	0.0156 (13)	0.0119 (11)	0.0022 (10)	0.0017 (9)	−0.0011 (9)
C235	0.0100 (11)	0.0130 (13)	0.0155 (11)	0.0010 (9)	0.0035 (9)	−0.0023 (9)
C236	0.0106 (11)	0.017 (1)	0.0154 (11)	−0.0008 (10)	0.0016 (9)	−0.0031 (10)

Geometric parameters (Å, °)

Fe1—O1	1.788 (2)	C135—C136	1.499 (3)
Fe1—O2	2.012 (2)	C211—C212	1.379 (3)
Fe1—N11	2.153 (2)	C212—C213	1.386 (4)
Fe1—N12	2.138 (2)	C213—C214	1.379 (4)
Fe1—N13	2.140 (2)	C214—C215	1.391 (3)
Fe1—N14	2.242 (2)	C215—C216	1.506 (3)
Fe2—O1	1.807 (2)	C221—C222	1.389 (4)
Fe2—O3	1.950 (2)	C222—C223	1.384 (4)
Fe2—N21	2.220 (2)	C223—C224	1.395 (4)
Fe2—N22	2.138 (2)	C224—C225	1.380 (3)
Fe2—N23	2.129 (2)	C225—C226	1.511 (4)
Fe2—N24	2.213 (2)	C231—C232	1.390 (3)
Cl1—O11	1.449 (2)	C232—C233	1.383 (3)
Cl1—O12	1.445 (2)	C233—C234	1.382 (3)
Cl1—O13	1.445 (2)	C234—C235	1.385 (3)
Cl1—O14	1.448 (2)	C235—C236	1.507 (3)
Cl2—O21	1.444 (2)	O6—H4	0.951
Cl2—O22	1.438 (2)	O6—H5	0.991
Cl2—O23	1.437 (2)	C2—H1	0.950
Cl2—O24	1.444 (2)	C2—H2	0.950
S5—O2	1.514 (2)	C2—H3	0.950
S5—O3	1.529 (2)	C111—H111	0.950
S5—O4	1.444 (2)	C112—H112	0.950

S5—O5	1.448 (2)	C113—H113	0.950
N1—C1	1.188 (7)	C114—H114	0.950
N11—C111	1.351 (3)	C116—H115	0.950
N11—C115	1.343 (3)	C116—H116	0.950
N12—C121	1.344 (3)	C121—H121	0.950
N12—C125	1.348 (3)	C122—H122	0.950
N13—C131	1.351 (3)	C123—H123	0.950
N13—C135	1.356 (3)	C124—H124	0.950
N14—C116	1.486 (3)	C126—H125	0.950
N14—C126	1.487 (3)	C126—H126	0.950
N14—C136	1.482 (3)	C131—H131	0.950
N21—C211	1.349 (3)	C132—H132	0.950
N21—C215	1.351 (3)	C133—H133	0.950
N22—C221	1.347 (3)	C134—H134	0.950
N22—C225	1.345 (3)	C136—H135	0.950
N23—C231	1.343 (3)	C136—H136	0.950
N23—C235	1.348 (3)	C211—H211	0.950
N24—C216	1.492 (3)	C212—H212	0.950
N24—C226	1.483 (3)	C213—H213	0.950
N24—C236	1.491 (3)	C214—H214	0.950
C1—C2	1.332 (6)	C216—H215	0.950
C111—C112	1.373 (4)	C216—H216	0.950
C112—C113	1.403 (4)	C221—H221	0.950
C113—C114	1.380 (4)	C222—H222	0.950
C114—C115	1.392 (4)	C223—H223	0.950
C115—C116	1.506 (3)	C224—H224	0.950
C121—C122	1.383 (3)	C226—H225	0.950
C122—C123	1.382 (4)	C226—H226	0.950
C123—C124	1.392 (3)	C231—H231	0.950
C124—C125	1.385 (3)	C232—H232	0.950
C125—C126	1.511 (3)	C233—H233	0.950
C131—C132	1.379 (3)	C234—H234	0.950
C132—C133	1.390 (4)	C236—H235	0.950
C133—C134	1.384 (4)	C236—H236	0.950
C134—C135	1.389 (3)		
O14···C132^{i}	3.074 (3)	O14···C223^{iv}	3.263 (4)
O22···C234	3.113 (3)	O4···C111^{ii}	3.269 (3)
O4···O6^{ii}	3.17 (2)	O24···C212^{iii}	3.277 (3)
O24···C213^{iii}	3.141 (3)	O12···C2	3.281 (4)
O5···C234^{ii}	3.150 (3)	N1···N21^{iv}	3.282 (7)
N1···C215^{iv}	3.152 (6)	O23···C132^{vi}	3.282 (3)
O13···O23^{v}	3.190 (3)	O11···C233	3.291 (3)
N1···C214^{iv}	3.204 (6)	O14···C131^{i}	3.294 (3)
O11···C131^{i}	3.206 (3)		
O1—Fe1—O2	99.71 (7)	C212—C213—C214	119.6 (2)
O1—Fe1—N11	97.34 (8)	C213—C214—C215	118.8 (2)
O1—Fe1—N12	105.07 (7)	N21—C215—C214	121.9 (2)

O1—Fe1—N13	102.23 (8)	N21—C215—C216	116.7 (2)
O1—Fe1—N14	175.05 (7)	C214—C215—C216	121.4 (2)
O2—Fe1—N11	162.14 (8)	N24—C216—C215	113.4 (2)
O2—Fe1—N12	88.82 (7)	N22—C221—C222	121.8 (2)
O2—Fe1—N13	86.95 (7)	C221—C222—C223	118.8 (2)
O2—Fe1—N14	84.91 (7)	C222—C223—C224	119.2 (2)
N11—Fe1—N12	81.63 (8)	C223—C224—C225	118.9 (2)
N11—Fe1—N13	94.63 (7)	N22—C225—C224	121.9 (2)
N11—Fe1—N14	78.23 (7)	N22—C225—C226	115.1 (2)
N12—Fe1—N13	152.70 (8)	C224—C225—C226	123.0 (2)
N12—Fe1—N14	76.64 (7)	N24—C226—C225	108.2 (2)
N13—Fe1—N14	76.12 (7)	N23—C231—C232	121.8 (2)
O1—Fe2—O3	101.74 (7)	C231—C232—C233	118.8 (2)
O1—Fe2—N21	170.51 (7)	C232—C233—C234	119.4 (2)
O1—Fe2—N22	95.09 (7)	C233—C234—C235	119.0 (2)
O1—Fe2—N23	93.57 (8)	N23—C235—C234	121.7 (2)
O1—Fe2—N24	95.61 (7)	N23—C235—C236	115.1 (2)
O3—Fe2—N21	85.97 (7)	C234—C235—C236	123.2 (2)
O3—Fe2—N22	97.82 (7)	N24—C236—C235	109.7 (2)
O3—Fe2—N23	106.23 (8)	H4—O6—H5	106.94
O3—Fe2—N24	161.81 (8)	C1—C2—H1	109.47
N21—Fe2—N22	89.26 (8)	C1—C2—H2	109.47
N21—Fe2—N23	78.83 (8)	C1—C2—H3	109.47
N21—Fe2—N24	77.34 (7)	H1—C2—H2	109.47
N22—Fe2—N23	152.16 (8)	H1—C2—H3	109.47
N22—Fe2—N24	75.04 (7)	H2—C2—H3	109.47
N23—Fe2—N24	77.81 (7)	N11—C111—H111	118.65
O11—Cl1—O12	109.2 (1)	C112—C111—H111	118.65
O11—Cl1—O13	109.4 (1)	C111—C112—H112	120.57
O11—Cl1—O14	109.6 (1)	C113—C112—H112	120.57
O12—Cl1—O13	109.8 (1)	C112—C113—H113	120.78
O12—Cl1—O14	109.5 (1)	C114—C113—H113	120.78
O13—Cl1—O14	109.4 (1)	C113—C114—H114	120.23
O21—Cl2—O22	109.3 (1)	C115—C114—H114	120.23
O21—Cl2—O23	109.2 (1)	N14—C116—H115	108.21
O21—Cl2—O24	108.9 (1)	N14—C116—H116	108.21
O22—Cl2—O23	109.5 (1)	C115—C116—H115	108.21
O22—Cl2—O24	109.7 (1)	C115—C116—H116	108.21
O23—Cl2—O24	110.2 (1)	H115—C116—H116	109.46
O2—S5—O3	106.1 (1)	N12—C121—H121	119.01
O2—S5—O4	108.47 (9)	C122—C121—H121	119.02
O2—S5—O5	109.7 (1)	C121—C122—H122	120.51
O3—S5—O4	108.2 (1)	C123—C122—H122	120.51
O3—S5—O5	108.5 (1)	C122—C123—H123	120.48
O4—S5—O5	115.4 (1)	C124—C123—H123	120.48
Fe1—O1—Fe2	133.0 (1)	C123—C124—H124	120.40
Fe1—O2—S5	128.9 (1)	C125—C124—H124	120.40
Fe2—O3—S5	131.9 (1)	N14—C126—H125	108.86
Fe1—N11—C111	123.1 (2)	N14—C126—H126	108.86

Fe1—N11—C115	117.1 (2)	C125—C126—H125	108.86
C111—N11—C115	118.5 (2)	C125—C126—H126	108.86
Fe1—N12—C121	124.0 (2)	H125—C126—H126	109.46
Fe1—N12—C125	116.1 (2)	N13—C131—H131	118.78
C121—N12—C125	119.4 (2)	C132—C131—H131	118.78
Fe1—N13—C131	124.2 (2)	C131—C132—H132	120.73
Fe1—N13—C135	116.8 (2)	C133—C132—H132	120.73
C131—N13—C135	118.9 (2)	C132—C133—H133	120.26
Fe1—N14—C116	110.2 (1)	C134—C133—H133	120.26
Fe1—N14—C126	106.0 (1)	C133—C134—H134	120.38
Fe1—N14—C136	107.1 (1)	C135—C134—H134	120.38
C116—N14—C126	112.8 (2)	N14—C136—H135	109.22
C116—N14—C136	109.5 (2)	N14—C136—H136	109.22
C126—N14—C136	111.1 (2)	C135—C136—H135	109.22
Fe2—N21—C211	124.6 (2)	C135—C136—H136	109.22
Fe2—N21—C215	115.7 (2)	H135—C136—H136	109.46
C211—N21—C215	118.5 (2)	N21—C211—H211	118.75
Fe2—N22—C221	125.0 (2)	C212—C211—H211	118.75
Fe2—N22—C225	115.5 (2)	C211—C212—H212	120.69
C221—N22—C225	119.4 (2)	C213—C212—H212	120.69
Fe2—N23—C231	124.7 (2)	C212—C213—H213	120.18
Fe2—N23—C235	115.6 (2)	C214—C213—H213	120.18
C231—N23—C235	119.3 (2)	C213—C214—H214	120.62
Fe2—N24—C216	111.8 (1)	C215—C214—H214	120.62
Fe2—N24—C226	104.7 (1)	N24—C216—H215	108.49
Fe2—N24—C236	105.4 (1)	N24—C216—H216	108.49
C216—N24—C226	110.4 (2)	C215—C216—H215	108.49
C216—N24—C236	111.2 (2)	C215—C216—H216	108.49
C226—N24—C236	113.0 (2)	H215—C216—H216	109.46
N1—C1—C2	175.5 (6)	N22—C221—H221	119.10
N11—C111—C112	122.7 (2)	C222—C221—H221	119.10
C111—C112—C113	118.9 (2)	C221—C222—H222	120.61
C112—C113—C114	118.4 (2)	C223—C222—H222	120.61
C113—C114—C115	119.5 (2)	C222—C223—H223	120.38
N11—C115—C114	121.8 (2)	C224—C223—H223	120.38
N11—C115—C116	117.4 (2)	C223—C224—H224	120.54
C114—C115—C116	120.7 (2)	C225—C224—H224	120.54
N14—C116—C115	114.5 (2)	N24—C226—H225	109.78
N12—C121—C122	122.0 (2)	N24—C226—H226	109.78
C121—C122—C123	119.0 (2)	C225—C226—H225	109.78
C122—C123—C124	119.0 (2)	C225—C226—H226	109.78
C123—C124—C125	119.2 (2)	H225—C226—H226	109.46
N12—C125—C124	121.3 (2)	N23—C231—H231	119.12
N12—C125—C126	116.2 (2)	C232—C231—H231	119.12
C124—C125—C126	122.3 (2)	C231—C232—H232	120.59
N14—C126—C125	111.9 (2)	C233—C232—H232	120.59
N13—C131—C132	122.4 (2)	C232—C233—H233	120.30
C131—C132—C133	118.5 (2)	C234—C233—H233	120.30
C132—C133—C134	119.5 (2)	C233—C234—H234	120.49

C133—C134—C135	119.2 (2)	C235—C234—H234	120.49
N13—C135—C134	121.3 (2)	N24—C236—H235	109.42
N13—C135—C136	115.8 (2)	N24—C236—H236	109.42
C134—C135—C136	122.8 (2)	C235—C236—H235	109.42
N14—C136—C135	110.5 (2)	C235—C236—H236	109.42
N21—C211—C212	122.5 (2)	H235—C236—H236	109.46
C211—C212—C213	118.6 (2)		
Fe1—O1—Fe2—O3	−0.8 (1)	N13—Fe1—N11—C111	−116.5 (2)
Fe1—O1—Fe2—N21	−144.7 (4)	N13—Fe1—N11—C115	76.4 (2)
Fe1—O1—Fe2—N22	98.3 (1)	N13—Fe1—N12—C121	−171.6 (2)
Fe1—O1—Fe2—N23	−108.2 (1)	N13—Fe1—N12—C125	16.3 (3)
Fe1—O1—Fe2—N24	173.7 (1)	N13—Fe1—N14—C116	−90.0 (1)
Fe1—O2—S5—O3	−53.0 (2)	N13—Fe1—N14—C126	147.7 (2)
Fe1—O2—S5—O4	−169.0 (1)	N13—Fe1—N14—C136	29.0 (1)
Fe1—O2—S5—O5	64.1 (2)	N13—C131—C132—C133	2.8 (4)
Fe1—N11—C111—C112	−167.5 (2)	N13—C135—C134—C133	3.7 (4)
Fe1—N11—C115—C114	170.6 (2)	N13—C135—C136—N14	30.5 (3)
Fe1—N11—C115—C116	−11.2 (3)	N14—Fe1—N11—C111	168.8 (2)
Fe1—N12—C121—C122	−168.6 (2)	N14—Fe1—N11—C115	1.6 (2)
Fe1—N12—C125—C124	169.9 (2)	N14—Fe1—N12—C121	−167.6 (2)
Fe1—N12—C125—C126	−5.1 (3)	N14—Fe1—N12—C125	20.4 (2)
Fe1—N13—C131—C132	177.2 (2)	N14—Fe1—N13—C131	168.2 (2)
Fe1—N13—C135—C134	179.3 (2)	N14—Fe1—N13—C135	−14.4 (2)
Fe1—N13—C135—C136	−3.9 (3)	N14—C116—C115—C114	−163.5 (2)
Fe1—N14—C116—C115	−15.7 (2)	N14—C126—C125—C124	161.7 (2)
Fe1—N14—C126—C125	37.3 (2)	N14—C136—C135—C134	−152.8 (2)
Fe1—N14—C136—C135	−39.7 (2)	N21—Fe2—N22—C221	84.7 (2)
Fe2—O1—Fe1—O2	−4.8 (1)	N21—Fe2—N22—C225	−100.5 (2)
Fe2—O1—Fe1—N11	169.9 (1)	N21—Fe2—N23—C231	−82.7 (2)
Fe2—O1—Fe1—N12	86.6 (1)	N21—Fe2—N23—C235	89.0 (2)
Fe2—O1—Fe1—N13	−93.7 (1)	N21—Fe2—N24—C216	11.2 (1)
Fe2—O1—Fe1—N14	−163.8 (8)	N21—Fe2—N24—C226	130.8 (2)
Fe2—O3—S5—O2	43.9 (2)	N21—Fe2—N24—C236	−109.8 (1)
Fe2—O3—S5—O4	160.1 (1)	N21—C211—C212—C213	3.4 (4)
Fe2—O3—S5—O5	−73.9 (2)	N21—C215—C214—C213	2.9 (4)
Fe2—N21—C211—C212	−169.0 (2)	N21—C215—C216—N24	25.8 (3)
Fe2—N21—C215—C214	166.9 (2)	N22—Fe2—N21—C211	−115.4 (2)
Fe2—N21—C215—C216	−15.8 (3)	N22—Fe2—N21—C215	77.2 (2)
Fe2—N22—C221—C222	174.5 (2)	N22—Fe2—N23—C231	−149.0 (2)
Fe2—N22—C225—C224	−176.1 (2)	N22—Fe2—N23—C235	22.7 (3)
Fe2—N22—C225—C226	2.7 (3)	N22—Fe2—N24—C216	−81.4 (2)
Fe2—N23—C231—C232	170.4 (2)	N22—Fe2—N24—C226	38.1 (1)
Fe2—N23—C235—C234	−170.0 (2)	N22—Fe2—N24—C236	157.6 (1)
Fe2—N23—C235—C236	12.4 (3)	N22—C221—C222—C223	0.6 (4)
Fe2—N24—C216—C215	−22.5 (2)	N22—C225—C224—C223	1.5 (4)
Fe2—N24—C226—C225	−47.8 (2)	N22—C225—C226—N24	31.7 (3)
Fe2—N24—C236—C235	43.0 (2)	N23—Fe2—N21—C211	89.9 (2)
S5—O2—Fe1—O1	36.1 (1)	N23—Fe2—N21—C215	−77.5 (2)
S5—O2—Fe1—N11	−126.4 (2)	N23—Fe2—N22—C221	148.7 (2)

S5—O2—Fe1—N12	−68.9 (1)	N23—Fe2—N22—C225	−36.5 (3)
S5—O2—Fe1—N13	138.0 (1)	N23—Fe2—N24—C216	92.3 (2)
S5—O2—Fe1—N14	−145.6 (1)	N23—Fe2—N24—C226	−148.1 (2)
S5—O3—Fe2—O1	−20.1 (1)	N23—Fe2—N24—C236	−28.6 (1)
S5—O3—Fe2—N21	154.3 (1)	N23—C231—C232—C233	−0.8 (4)
S5—O3—Fe2—N22	−117.0 (1)	N23—C235—C234—C233	−1.4 (4)
S5—O3—Fe2—N23	77.2 (1)	N23—C235—C236—N24	−38.6 (3)
S5—O3—Fe2—N24	177.6 (2)	N24—Fe2—N21—C211	169.8 (2)
O1—Fe1—N11—C111	−13.5 (2)	N24—Fe2—N21—C215	2.3 (2)
O1—Fe1—N11—C115	179.4 (2)	N24—Fe2—N22—C221	161.8 (2)
O1—Fe1—N12—C121	7.6 (2)	N24—Fe2—N22—C225	−23.4 (2)
O1—Fe1—N12—C125	−164.4 (2)	N24—Fe2—N23—C231	−162.0 (2)
O1—Fe1—N13—C131	−7.0 (2)	N24—Fe2—N23—C235	9.7 (2)
O1—Fe1—N13—C135	170.4 (2)	N24—C216—C215—C214	−156.9 (2)
O1—Fe1—N14—C116	−18.8 (9)	N24—C226—C225—C224	−149.5 (2)
O1—Fe1—N14—C126	−141.2 (8)	N24—C236—C235—C234	143.8 (2)
O1—Fe1—N14—C136	100.2 (8)	C111—N11—C115—C114	2.9 (3)
O1—Fe2—N21—C211	127.2 (4)	C111—N11—C115—C116	−178.9 (2)
O1—Fe2—N21—C215	−40.2 (6)	C111—C112—C113—C114	2.2 (4)
O1—Fe2—N22—C221	−103.7 (2)	C112—C111—N11—C115	−0.5 (3)
O1—Fe2—N22—C225	71.1 (2)	C112—C113—C114—C115	0.0 (4)
O1—Fe2—N23—C231	103.0 (2)	C113—C114—C115—C116	179.2 (2)
O1—Fe2—N23—C235	−85.2 (2)	C115—C116—N14—C126	102.6 (2)
O1—Fe2—N24—C216	−175.2 (1)	C115—C116—N14—C136	−133.2 (2)
O1—Fe2—N24—C226	−55.7 (2)	C116—N14—C126—C125	−83.4 (2)
O1—Fe2—N24—C236	63.8 (1)	C116—N14—C136—C135	79.8 (2)
O2—Fe1—N11—C111	149.1 (2)	C121—N12—C125—C124	−2.5 (4)
O2—Fe1—N11—C115	−18.0 (3)	C121—N12—C125—C126	−177.5 (2)
O2—Fe1—N12—C121	107.3 (2)	C121—C122—C123—C124	−1.3 (4)
O2—Fe1—N12—C125	−64.7 (2)	C122—C121—N12—C125	3.2 (4)
O2—Fe1—N13—C131	−106.3 (2)	C122—C123—C124—C125	1.9 (4)
O2—Fe1—N13—C135	71.1 (2)	C123—C124—C125—C126	174.6 (2)
O2—Fe1—N14—C116	−178.1 (1)	C125—C126—N14—C136	153.3 (2)
O2—Fe1—N14—C126	59.6 (1)	C126—N14—C136—C135	−155.0 (2)
O2—Fe1—N14—C136	−59.1 (1)	C131—N13—C135—C134	−3.1 (3)
O3—Fe2—N21—C211	−17.5 (2)	C131—N13—C135—C136	173.6 (2)
O3—Fe2—N21—C215	175.1 (2)	C131—C132—C133—C134	−2.1 (4)
O3—Fe2—N22—C221	−1.1 (2)	C132—C131—N13—C135	−0.2 (3)
O3—Fe2—N22—C225	173.7 (2)	C132—C133—C134—C135	−1.1 (4)
O3—Fe2—N23—C231	−0.3 (2)	C133—C134—C135—C136	−172.8 (2)
O3—Fe2—N23—C235	171.4 (2)	C211—N21—C215—C214	−1.4 (4)
O3—Fe2—N24—C216	−12.7 (3)	C211—N21—C215—C216	175.9 (2)
O3—Fe2—N24—C226	106.9 (2)	C211—C212—C213—C214	−1.7 (4)
O3—Fe2—N24—C236	−133.6 (2)	C212—C211—N21—C215	−1.8 (4)
N11—Fe1—N12—C121	−87.8 (2)	C212—C213—C214—C215	−1.3 (4)
N11—Fe1—N12—C125	100.2 (2)	C213—C214—C215—C216	−174.2 (2)
N11—Fe1—N13—C131	91.5 (2)	C215—C216—N24—C226	−138.6 (2)
N11—Fe1—N13—C135	−91.1 (2)	C215—C216—N24—C236	95.0 (2)
N11—Fe1—N14—C116	7.8 (1)	C216—N24—C226—C225	72.6 (2)

N11—Fe1—N14—C126	−114.5 (2)	C216—N24—C236—C235	−78.3 (2)
N11—Fe1—N14—C136	126.9 (1)	C221—N22—C225—C224	−1.0 (4)
N11—C111—C112—C113	−2.0 (4)	C221—N22—C225—C226	177.8 (2)
N11—C115—C114—C113	−2.6 (4)	C221—C222—C223—C224	−0.1 (4)
N11—C115—C116—N14	18.3 (3)	C222—C221—N22—C225	−0.1 (4)
N12—Fe1—N11—C111	90.8 (2)	C222—C223—C224—C225	−0.9 (4)
N12—Fe1—N11—C115	−76.4 (2)	C223—C224—C225—C226	−177.2 (2)
N12—Fe1—N13—C131	172.2 (2)	C225—C226—N24—C236	−162.0 (2)
N12—Fe1—N13—C135	−10.4 (3)	C226—N24—C236—C235	156.8 (2)
N12—Fe1—N14—C116	91.9 (2)	C231—N23—C235—C234	2.2 (4)
N12—Fe1—N14—C126	−30.4 (1)	C231—N23—C235—C236	−175.4 (2)
N12—Fe1—N14—C136	−149.1 (2)	C231—C232—C233—C234	1.6 (4)
N12—C121—C122—C123	−1.3 (4)	C232—C231—N23—C235	−1.1 (4)
N12—C125—C124—C123	−0.1 (4)	C232—C233—C234—C235	−0.6 (4)
N12—C125—C126—N14	−23.4 (3)	C233—C234—C235—C236	176.0 (2)

Symmetry codes: (i) *x*+1/2, −*y*+1/2, *z*−1/2; (ii) *x*+1/2, −*y*+1/2, *z*+1/2; (iii) −*x*+1, −*y*, −*z*+1; (iv) −*x*+1/2, *y*+1/2, −*z*+3/2; (v) −*x*+1/2, *y*+1/2, −*z*+1/2; (vi) *x*, *y*, *z*−1.

Fig. 1

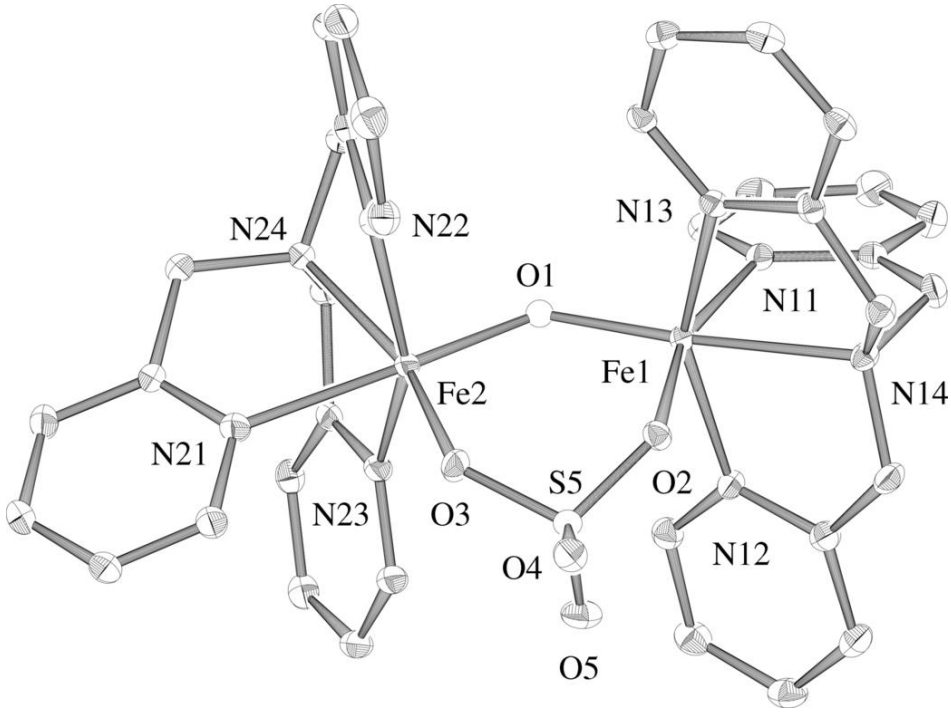
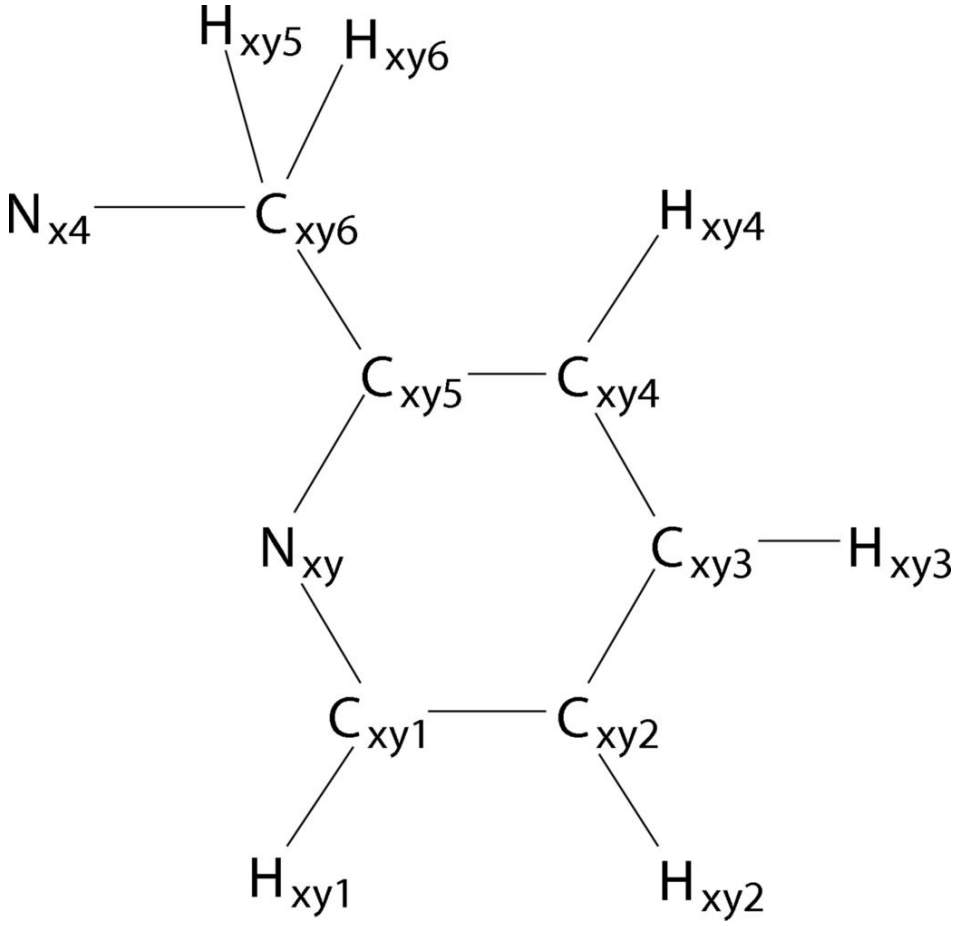


Fig. 2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