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Retraction of articles

This article reports the retraction of articles published in *Acta Crystallographica Section E* between 2007 and 2009.

After further thorough investigation (see Harrison *et al.*, 2010), articles are retracted as a result of problems with the data sets or incorrect atom assignments. Full details of all the articles are given in Table 1.

Table 1
Details of articles to be retracted, in order of publication.

Title	Reference	DOI	Refcode
catena-Poly[[aqua(pyrazine-2-carboxylato)iron(II)]-μ-pyrazine-2-carboxylato]	Hao & Liu (2007)	10.1107/S1600536806053207	NEVLUW
Poly[aquabis(μ-pyrazine-2-carboxylato)nickel(II)]	Hao, Mu & Liu (2007)	10.1107/S1600536806054225	TEVQUH
catena-Poly[[(2,2′-bipyridine-κ^2N,N')zinc(II)]-μ-imidazole-4,5-dicarboxylato-$\kappa^4N^1,O^5:N^3,O^4$]	Li, Dong *et al.* (2007)	10.1107/S1600536807014420	XIBPAA
Poly[[aqua(2,2-bipyridyl)(μ$_3$-pyridine-3,4-dicarboxylato)manganese(II)] monohydrate]	Li, Niu *et al.* (2007)	10.1107/S1600536807023586	GIGYAX
Poly[chlorido-μ$_3$-1,2,4-triazolato-nickel(II)]	Gao, Wang & Hao (2007*a*)	10.1107/S1600536807025962	WIGTEM
Poly[[(μ$_4$-carbonyldibenzene-3,3′,4,4′-tetracarboxylato)tetrakis(1,10-phenanthroline)-dicadmium(II)] dihydrate]	Gao, Wang & Niu (2007*a*)	10.1107/S1600536807028425	EDUNUN
Tetraaquabis(4,4′-bipyridine)iron(II) pyridine-2,6-dicarboxylate tetrahydrate	Gao, Wang & Niu (2007*b*)	10.1107/S1600536807027973	EDUPAV
catena-Poly[[(2,2-bipyridine)cobalt(II)]-μ-imidazole-4,5-dicarboxylato]	Hao, Bao & Yu (2007)	10.1107/S1600536807027699	EDURUR
catena-Poly[[aqua(pyrazine-2-carboxylato)cobalt(II)]-μ-pyrazine-2-carboxylato]	Gao, Wang, Niu & Hao (2007*a*)	10.1107/S1600536807027961	ODOJIA01
Poly[[[aqua(2,2-bipyridine)iron(II)]-μ$_3$-pyridine-3,4-dicarboxylato] monohydrate]	Hao & Yu (2007*a*)	10.1107/S160053680702867X	RIGRUV
catena-Poly[[[diaqua(6-carboxypyridine-2-carboxylato-κ^3O,N,O')gadolinium(III)]-μ-pyridine-2,6-dicarboxylato-$\kappa^4N,O,O':O''$] tetrahydrate]	Hao & Yu (2007*b*)	10.1107/S1600536807029789	MIGDOW
Poly[[aqua(pyrazine-2-carboxylato)copper(II)]-μ-pyrazine-2-carboxylato]	Gao, Wang, Niu & Hao (2007*b*)	10.1107/S1600536807030528	MIGKUJ
cyclo-Tetrakis[μ-N-(2-hydroxybenzoyl)-N′-(2-hydroxy-3-methoxybenzylidene)hydrazinate(2−)]tetracobalt(II) N,N-dimethylformamide tetrasolvate	Gao, Wang & Niu (2007*c*)	10.1107/S1600536807033338	UDUXOH
Poly[chlorido(μ$_3$-1,2,4-triazolato)manganese(II)]	Gao, Wang & Hao (2007*b*)	10.1107/S1600536807032886	UDUZAV
catena-Poly[[aqua(pyrazine-2-carboxylato-κ^2N^1,O)zinc(II)]-μ-pyrazine-2-carboxylato-$\kappa^2N^1,O:N^4$]	Gao, Wang, Niu & Hao (2007*c*)	10.1107/S1600536807033041	UDUZEZ
cyclo-Tetrakis[μ-N-(2-hydroxybenzoyl)-N′-(2-hydroxy-3-methoxybenzylidene)hydrazine(2−)]tetrazinc(II) N,N-dimethylformamide tetrasolvate	Gao, Wang & Niu (2007*d*)	10.1107/S1600536807034514	TIFZIS
catena-Poly[[[diaqua(6-carboxypyridine-2-carboxylato)terbium(III)]-μ-pyridine-2,6-dicarboxylato] tetrahydrate]	Hao & Yu (2007*c*)	10.1107/S1600536807034629	TIFZUE
catena-Poly[[aqua(pyrazine-2-carboxylato-κ^2N^1,O)manganese(II)]-μ-pyrazine-2-carboxylato-$\kappa^3N^1,O:N^4$]	Gao, Wang, Niu & Hao (2007*d*)	10.1107/S1600536807034496	TIGBER
Poly[chlorido-μ$_3$-1,2,4-triazolato-iron(II)]	Gao, Wang & Hao (2007*c*)	10.1107/S1600536807036239	TIGHIB
Tetraaquabis(4,4′-bipyridine)manganese(II) pyridine-2,6-dicarboxylate tetrahydrate	Gao, Wang & Niu (2007*e*)	10.1107/S160053680703766X	AFEGIC
Poly[chlorido(μ$_3$-1,2,4-triazolato)copper(II)]	Gao, Wang & Niu (2007*f*)	10.1107/S1600536807040007	VIKBAT
catena-Poly[[(2,2′-bipyridine)nickel(II)]-μ-imidazole-4,5-dicarboxylato]	Hao & Yu (2007*d*)	10.1107/S1600536807040330	VIKCOI
Poly[[[(2,2′-bipyridine)cadmium(II)]-μ$_3$-pyridine-2,4-dicarboxylato] monohydrate]	Li, Wang & Liu (2007)	10.1107/S160053680704202X	XIKVOD
Poly[aqua(μ$_4$-benzene-1,3-dicarboxylato-$\kappa^4O:O':O'':O'''$)bis(imidazole-κN)palladium(II)]	Hao & Yu (2007*e*)	10.1107/S1600536807044315	SILKII
Tetraaquabis(4,4′-bipyridine)cobalt(II) pyridine-2,6-dicarboxylate tetrahydrate	Guan, Gao, Wang & Wang (2007*a*)	10.1107/S1600536807046107	XILPOY
cyclo-Tetrakis[μ-N-(2-hydroxybenzoyl)-N′-(2-hydroxy-3-methoxybenzylidene)hydrazinato(2−)]tetranickel(II) N,N-dimethylformamide tetrasolvate	Guan, Gao, Wang & Wang (2007*b*)	10.1107/S1600536807048325	SILZOD
Bis(cyanido-κC)bis(1,10-phenanthroline-κ^2N,N')chromium(III) bis(azido-κN)[N,N′-(o-phenylene)bis(pyridine-2-carboxamide)-κ^4N]chromate(III) monohydrate	Guan, Gao, Wang & Wang (2007*c*)	10.1107/S1600536807049872	GIMVUU
Tris[2-(propyliminomethyl)phenolato-κ^2N,O]iron(III)	Hao, Mu & Kong (2008*a*)	10.1107/S1600536808018540	MODFIV
Bis{μ-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}bis[(thiocyanato-κN)-iron(III)]	Hao, Mu & Kong (2008*b*)	10.1107/S1600536808021892	YODCAW
catena-Poly[[aqua(2,2′-bipyridine-κ^2N,N')copper(II)]-μ-5-nitroisophthalato-$\kappa^3O^1,O^{1'}:O^3$]	Hao & Liu (2008)	10.1107/S1600536808035150	COLVEF
Tetrakis(μ-2,4-difluorobenzoato)bis[(2,2′-bipyridine)(2,4-difluorobenzoato)terbium(III)]	Hao & Liu (2009)	10.1107/S1600536808043936	WOQLAQ

  doi:10.1107/S1600536811037597

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Bis{μ-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}bis[(thiocyanato-κN)iron(III)]

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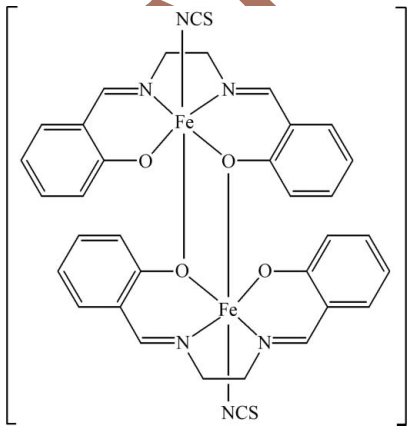
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.009 Å; R factor = 0.058; wR factor = 0.181; data-to-parameter ratio = 14.7.

The title compound, $[Fe_2(C_{16}H_{14}N_2O_2)_2(NCS)_2]$, is isostructural with the Mn^{III}-containing analogue. Each Fe^{III} atom is chelated by a tetradentate 2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolate ligand and by the N atom of a thiocyanate anion, in a square-pyramidal arrangement. The complex molecules form centrosymmetric dimers, with an Fe—O contact of 2.549 (3) Å, *trans* to each thiocyanate anion, completing a distorted octahedral coordination geometry.

Related literature

For related literature, see: Garnovskii *et al.* (1993); Huang *et al.* (2002); Bhadbhade & Srinivas (1993); Bunce *et al.* (1998). For the isostructural Mn^{III}-containing compound, see: Wang *et al.* (2008).



Experimental

Crystal data

$[Fe_2(C_{16}H_{14}N_2O_2)_2(NCS)_2]$
M_r = 380.23
Monoclinic, $P2_1/n$
a = 8.9231 (10) Å
b = 14.0779 (10) Å
c = 14.9716 (10) Å
β = 106.844 (1)°
V = 1800.0 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.97 mm^{-1}
T = 293 (2) K
0.12 × 0.11 × 0.09 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.893, T_{max} = 0.918
12796 measured reflections
3191 independent reflections
2535 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.180
S = 1.00
3191 reflections
217 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2293).

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supporting information

Acta Cryst. (2008). E**64**, m1034 [doi:10.1107/S1600536808021892]

Bis{μ-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}bis[(thiocyanato-κN)iron(III)]

Lujiang Hao, Chunhua Mu and Binbin Kong

S1. Comment

The design of Schiff-base complexes has received long-lasting research interest not only because of their appealing structural and topological novelty but also due to their potential medical value derived from their antiviral and the inhibition of angiogenesis (Garnovskii *et al.*, 1993; Huang *et al.*, 2002). The related Fe complexes with multidentate Schiff-base ligands have aroused particular interest because this metal can exhibit several oxidation states and may provide the basis of models for active sites of biological systems (Bhadbhade & Srinivas, 1993; Bunce *et al.*, 1998).

The title compound is isostructural with its Mn^{III}-containing analogue (Wang *et al.*, 2008). Each Fe^{III} atom is chelated by a tetradentate 2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolate ligand and by the N atom of a thiocyanate anion, in a square-pyramidal arrangement. The maximum atomic deviation from the least-square plane of the equatorially located atoms, Fe1, N1, N2, O1 and O2, is 0.077 Å. The Fe—N(isothiocyanato) bond length (2.178 (4) Å) is longer than the other two Fe—N bonds (1.985 (4) and 1.988 (4) Å). The complexes form centrosymmetric dimers, with an Fe—O contact of 2.549 (3)Å *trans* to each thiocyanate anion, completing a distorted octahedral coordination geometry.

S2. Experimental

A mixture of iron(III) 2,4-pentanedionate (0.5 mmol), *N*,*N*′-disalicylidene-ethylenediamine (0.5 mmoL), and sodium isothiocyanate (1 mmoL) in 20 ml methanol was refluxed for two hours. The resulting solution was cooled and filtered and the filtrate was evaporated naturally at room temperature to yield brown blocks after a few days with a yield of 11%. Elemental analysis calculated: C 53.65, H 3.68, N 11.05%; found: C 53.60, H 3.64, N 11.02%.

S3. Refinement

All H atoms were placed in calculated positions with C—H = 0.93 Å and refined as riding with U_{iso}(H) = 1.2U_{eq}(C).

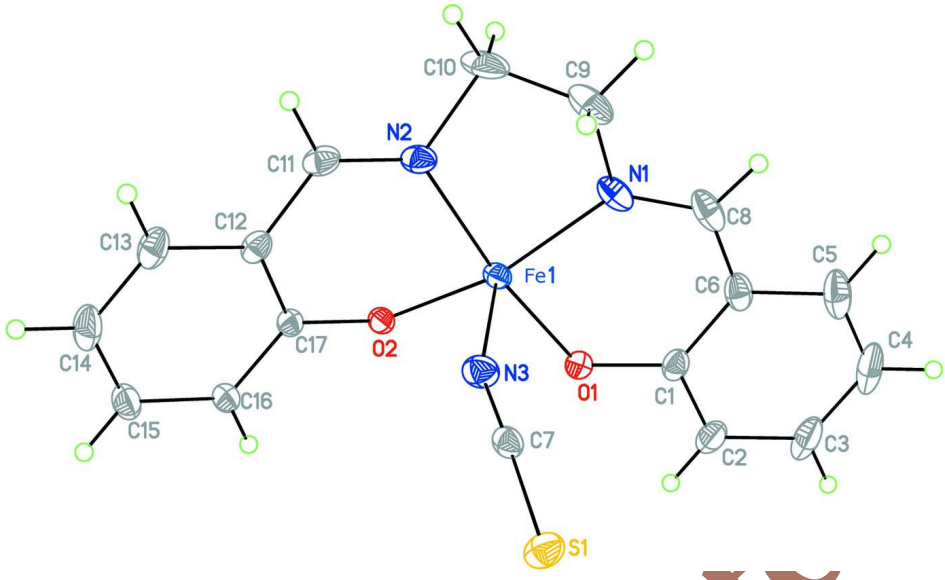

Figure 1

The asymmetric unit drawn with 30% probability displacement ellipsoids for the non-H atoms.

Bis{μ-2,2′-[ethane-1,2- diylbis(nitrilomethylidyne)]diphenolato}bis[(thiocyanato-κN)iron(III)]

Crystal data

$[Fe_2(C_{16}H_{14}N_2O_2)_2(NCS)_2]$
$M_r = 380.23$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 8.9231$ (10) Å
$b = 14.0779$ (10) Å
$c = 14.9716$ (10) Å
$\beta = 106.844$ (1)°
$V = 1800.0$ (3) Å^3
$Z = 4$
$F(000) = 780$
$D_x = 1.403$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4497 reflections
$\theta = 2.4$–24.4°
$\mu = 0.97$ mm^{-1}
$T = 293$ K
Block, brown
0.12 × 0.11 × 0.09 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.893$, $T_{max} = 0.918$
12796 measured reflections
3191 independent reflections
2535 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 25.3°$, $\theta_{min} = 2.4°$
$h = -10\rightarrow10$
$k = -16\rightarrow16$
$l = -18\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.180$
$S = 1.00$
3191 reflections
217 parameters
0 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

$w = 1/[\sigma^2(F_o^2) + (0.114P)^2 + 1.289P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 1.12$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.64494 (7)	0.01030 (4)	0.10343 (4)	0.0586 (3)
C1	0.9422 (5)	−0.0874 (3)	0.2499 (3)	0.0612 (10)
C2	0.5250 (4)	−0.1763 (3)	0.0554 (3)	0.0563 (9)
C3	0.5503 (5)	−0.2621 (3)	0.0151 (4)	0.0690 (11)
H3	0.6005	−0.2622	−0.0314	0.083*
C4	0.5012 (7)	−0.3464 (4)	0.0441 (5)	0.0905 (15)
H4	0.5190	−0.4032	0.0171	0.109*
C5	0.4258 (7)	−0.3475 (4)	0.1126 (5)	0.103 (2)
H5	0.3939	−0.4049	0.1318	0.124*
C6	0.3974 (7)	−0.2631 (4)	0.1529 (4)	0.0895 (16)
H6	0.3438	−0.2638	0.1977	0.107*
C7	0.4493 (5)	−0.1778 (3)	0.1262 (3)	0.0665 (11)
C8	0.4150 (6)	−0.0914 (4)	0.1685 (3)	0.0757 (13)
H8	0.3416	−0.0948	0.2016	0.091*
C9	0.4311 (10)	0.0777 (5)	0.2043 (5)	0.117 (2)
H9A	0.3827	0.0625	0.2528	0.141*
H9B	0.3577	0.1145	0.1563	0.141*
C10	0.5833 (10)	0.1335 (4)	0.2450 (4)	0.109 (2)
H10A	0.5603	0.1986	0.2577	0.130*
H10B	0.6451	0.1046	0.3027	0.130*
C11	0.7504 (8)	0.2036 (4)	0.1629 (4)	0.0936 (18)
H11	0.7469	0.2578	0.1977	0.112*
C12	0.8444 (6)	0.2076 (3)	0.1012 (4)	0.0801 (13)
C13	0.8633 (5)	0.1309 (3)	0.0459 (3)	0.0684 (11)
C14	0.9632 (6)	0.1410 (4)	−0.0104 (4)	0.0900 (16)
H14	0.9784	0.0901	−0.0464	0.108*
C15	1.0394 (7)	0.2261 (6)	−0.0128 (7)	0.125 (3)
H15	1.1052	0.2319	−0.0507	0.150*
C16	1.0191 (9)	0.3026 (6)	0.0405 (7)	0.136 (3)
H16	1.0706	0.3596	0.0382	0.163*
C17	0.9219 (9)	0.2942 (5)	0.0971 (5)	0.123 (3)
H17	0.9076	0.3457	0.1326	0.148*

N1	0.8171 (5)	−0.0695 (3)	0.2098 (3)	0.0785 (10)
N2	0.6685 (6)	0.1309 (3)	0.1752 (3)	0.0796 (11)
N3	0.4771 (5)	−0.0113 (3)	0.1639 (3)	0.0721 (10)
O1	0.5684 (3)	−0.09420 (17)	0.02262 (18)	0.0553 (6)
O2	0.7880 (3)	0.0489 (2)	0.0418 (2)	0.0660 (7)
S1	1.11963 (15)	−0.11760 (11)	0.30804 (10)	0.0858 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0672 (4)	0.0522 (4)	0.0613 (4)	0.0061 (2)	0.0262 (3)	−0.0013 (2)
C1	0.075 (3)	0.048 (2)	0.065 (2)	0.0050 (19)	0.028 (2)	0.0093 (17)
C2	0.053 (2)	0.050 (2)	0.066 (2)	0.0008 (16)	0.0163 (17)	0.0063 (17)
C3	0.064 (2)	0.051 (2)	0.090 (3)	0.0037 (18)	0.020 (2)	0.005 (2)
C4	0.087 (3)	0.055 (3)	0.120 (4)	0.000 (2)	0.016 (3)	0.011 (3)
C5	0.104 (4)	0.074 (4)	0.120 (5)	−0.018 (3)	0.014 (4)	0.040 (3)
C6	0.084 (3)	0.096 (4)	0.087 (3)	−0.019 (3)	0.023 (3)	0.034 (3)
C7	0.056 (2)	0.079 (3)	0.064 (2)	−0.002 (2)	0.0153 (19)	0.021 (2)
C8	0.075 (3)	0.095 (4)	0.068 (3)	0.011 (3)	0.038 (2)	0.021 (2)
C9	0.149 (6)	0.116 (5)	0.122 (5)	0.046 (5)	0.093 (5)	−0.003 (4)
C10	0.177 (7)	0.081 (4)	0.078 (3)	0.032 (4)	0.052 (4)	−0.008 (3)
C11	0.127 (5)	0.056 (3)	0.070 (3)	0.007 (3)	−0.015 (3)	−0.014 (2)
C12	0.084 (3)	0.067 (3)	0.071 (3)	−0.011 (2)	−0.006 (2)	−0.001 (2)
C13	0.051 (2)	0.065 (3)	0.079 (3)	−0.0061 (18)	0.002 (2)	0.012 (2)
C14	0.059 (3)	0.089 (4)	0.120 (4)	−0.006 (2)	0.023 (3)	0.024 (3)
C15	0.075 (4)	0.118 (6)	0.164 (7)	−0.038 (4)	0.006 (4)	0.045 (5)
C16	0.104 (5)	0.109 (6)	0.156 (7)	−0.057 (5)	−0.024 (5)	0.032 (5)
C17	0.129 (6)	0.082 (4)	0.117 (5)	−0.037 (4)	−0.032 (4)	−0.001 (3)
N1	0.077 (3)	0.075 (2)	0.082 (3)	0.017 (2)	0.020 (2)	0.012 (2)
N2	0.113 (3)	0.063 (2)	0.057 (2)	0.019 (2)	0.015 (2)	−0.0085 (16)
N3	0.080 (2)	0.079 (3)	0.069 (2)	0.0157 (19)	0.040 (2)	0.0052 (17)
O1	0.0636 (15)	0.0482 (13)	0.0608 (14)	0.0017 (11)	0.0284 (12)	0.0024 (11)
O2	0.0625 (16)	0.0566 (16)	0.084 (2)	−0.0024 (13)	0.0289 (14)	−0.0006 (14)
S1	0.0658 (7)	0.0956 (9)	0.0968 (9)	0.0082 (6)	0.0248 (6)	0.0267 (7)

Geometric parameters (Å, º)

Fe1—O2	1.860 (3)	C9—N3	1.500 (7)
Fe1—O1	1.902 (3)	C9—C10	1.534 (11)
Fe1—N3	1.985 (4)	C9—H9A	0.970
Fe1—N2	1.988 (4)	C9—H9B	0.970
Fe1—N1	2.178 (4)	C10—N2	1.459 (7)
C1—N1	1.132 (5)	C10—H10A	0.970
C1—S1	1.627 (5)	C10—H10B	0.970
C2—O1	1.355 (4)	C11—N2	1.302 (7)
C2—C7	1.412 (6)	C11—C12	1.418 (8)
C2—C3	1.397 (6)	C11—H11	0.930
C3—C4	1.378 (7)	C12—C13	1.401 (7)

C3—H3	0.930	C12—C17	1.412 (8)
C4—C5	1.380 (9)	C13—O2	1.328 (5)
C4—H4	0.930	C13—C14	1.400 (7)
C5—C6	1.388 (9)	C14—C15	1.383 (9)
C5—H5	0.930	C14—H14	0.930
C6—C7	1.387 (7)	C15—C16	1.384 (13)
C6—H6	0.930	C15—H15	0.930
C7—C8	1.445 (7)	C16—C17	1.382 (12)
C8—N3	1.267 (6)	C16—H16	0.930
C8—H8	0.930	C17—H17	0.930

O2—Fe1—O1	94.72 (12)	H9A—C9—H9B	108.7
O2—Fe1—N3	171.11 (14)	N2—C10—C9	106.7 (5)
O1—Fe1—N3	89.55 (14)	N2—C10—H10A	110.4
O2—Fe1—N2	92.21 (17)	C9—C10—H10A	110.4
O1—Fe1—N2	165.26 (15)	N2—C10—H10B	110.4
N3—Fe1—N2	81.92 (19)	C9—C10—H10B	110.4
O2—Fe1—N1	94.22 (14)	H10A—C10—H10B	108.6
O1—Fe1—N1	96.51 (14)	N2—C11—C12	125.9 (5)
N3—Fe1—N1	93.03 (16)	N2—C11—H11	117.0
N2—Fe1—N1	95.94 (16)	C12—C11—H11	117.0
N1—C1—S1	177.6 (4)	C13—C12—C17	119.7 (6)
O1—C2—C7	122.3 (4)	C13—C12—C11	123.4 (4)
O1—C2—C3	118.8 (4)	C17—C12—C11	116.9 (6)
C7—C2—C3	118.9 (4)	O2—C13—C14	117.6 (5)
C2—C3—C4	120.2 (5)	O2—C13—C12	123.4 (4)
C2—C3—H3	119.9	C14—C13—C12	119.0 (5)
C4—C3—H3	119.9	C13—C14—C15	120.5 (7)
C5—C4—C3	120.7 (5)	C13—C14—H14	119.8
C5—C4—H4	119.6	C15—C14—H14	119.7
C3—C4—H4	119.6	C16—C15—C14	120.8 (8)
C4—C5—C6	120.2 (5)	C16—C15—H15	119.6
C4—C5—H5	119.9	C14—C15—H15	119.6
C6—C5—H5	119.9	C17—C16—C15	119.8 (6)
C7—C6—C5	119.8 (5)	C17—C16—H16	120.1
C7—C6—H6	120.1	C15—C16—H16	120.1
C5—C6—H6	120.1	C16—C17—C12	120.2 (8)
C2—C7—C6	120.1 (5)	C16—C17—H17	119.9
C2—C7—C8	121.6 (4)	C12—C17—H17	119.9
C6—C7—C8	118.2 (4)	C1—N1—Fe1	151.7 (4)
N3—C8—C7	125.0 (4)	C11—N2—C10	120.8 (5)
N3—C8—H8	117.5	C11—N2—Fe1	124.8 (4)
C7—C8—H8	117.5	C10—N2—Fe1	114.4 (4)
N3—C9—C10	105.9 (5)	C8—N3—C9	123.1 (5)
N3—C9—H9A	110.6	C8—N3—Fe1	124.1 (3)
C10—C9—H9A	110.6	C9—N3—Fe1	112.8 (4)
N3—C9—H9B	110.6	C2—O1—Fe1	121.1 (2)
C10—C9—H9B	110.6	C13—O2—Fe1	130.0 (3)