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Retraction of articles by T. Liu *et al.*

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A series of 29 papers by Liu *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 29 papers by Liu *et al.* are retracted. 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
Tetrakis(pyrazine-κN)bis(thiocyanato-κN)manganese(II)	Liu & Xie (2007*a*)	10.1107/S1600536807026852	EDUMAS
(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')copper(II) dinitrate dihydrate	Liu, Wang, Wang & Xie (2007*b*)	10.1107/S1600536807028255	EDUVAB
Tetrakis(pyrazine-κN)bis(thiocyanato-κN)zinc(II)	Liu & Xie (2007*b*)	10.1107/S1600536807028735	RIGQAA
Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-lanthanum(III)]	Liu, Wang, Wang & Xie (2007*c*)	10.1107/S1600536807030917	UDUMIQ
Polymeric $KNOF_2$	Liu Wang, Wang & Xie (2007*a*)	10.1107/S1600536807027195	ICSD 240891
(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')cobalt(II) dinitrate dihydrate	Liu, Wang, Wang & Xie (2007*d*)	10.1107/S1600536807031224	WIHJED
Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-praseodymium(III)]	Liu, Wang, Wang & Xie (2007*e*)	10.1107/S1600536807032679	WIHQEK
Tetrakis[μ-(2-pyridyloxy)acetato-$\kappa^2O:O'$]bis{(1,10-phenanthroline-κ^2N,N')-[(2-pyridyloxy)acetato-κO]neodymium(III)}	Liu, Wang, Wang & Xie (2007*f*)	10.1107/S1600536807035349	TIGDAP
(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')manganese(II) dinitrate dihydrate	Liu, Wang, Wang & Xie (2007*g*)	10.1107/S1600536807035076	TIGDET
2-Amino-3,5-dinitrobenzoic acid–ammonia (1/1)	Liu & Zhu (2007*j*)	10.1107/S1600536807040068	KIKQAX
2-Hydroxy-3,5-dinitrobenzamide monohydrate	Liu & Zhu (2007*k*)	10.1107/S1600536807039712	KIKQEB
2-(1-Hydroxy-2-pyridyl)acetamide monohydrate	Liu & Zhu (2007*l*)	10.1107/S1600536807040652	CIKQOD
Bis(2,2′-bipyridine-κN,N′)bis(thiocyanato-κN)iron(II)	Liu & Zhu (2007*a*)	10.1107/S1600536807043486	XIFXOA
catena-Poly[hexakis(μ_2-anilinoacetamide)bis(1,10-phenanthroline)disamarium(III]	Liu & Zhu (2007*b*)	10.1107/S1600536807045485	XILNAI
3-Hydroxy-2,4,6-trinitropyridine monohydrate	Liu & Zhu (2007*m*)	10.1107/S1600536807045230	PILNOO
catena-Poly[hexakis(μ_2-anilinoacetamide)bis(1,10-phenanthroline)-dipraseodymium(III)]	Liu & Zhu (2007*c*)	10.1107/S1600536807047733	SILZET
catena-Poly[[tetra-μ-anilinoacetamidato-bis(1,10-phenanthroline)dicerium(III)]-di-μ-anilinoacetamidato]	Liu & Zhu (2007*d*)	10.1107/S1600536807050969	GIMZOS
Tetrakis(pyridine-κN)bis(thiocyanato-κN)chromium(II)	Liu & Zhu (2007*e*)	10.1107/S1600536807051756	WINFAB
2-Ammonio-3-carboxy-5-nitrobenzoate monohydrate	Liu & Zhu (2007*n*)	10.1107/S1600536807048477	GINFEP
2-(Benzoylhydrazinocarbonyl)benzoic acid	Liu & Zhu (2007*o*)	10.1107/S160053680705204X	TINZIA
Tetrakis(pyridine-κN)bis(thiocyanato-κN)vanadium(II)	Liu & Zhu (2007*f*)	10.1107/S1600536807054529	HIPZIQ
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')nickel(II)]-μ-acetamido-$\kappa^2O:N$]	Liu & Zhu (2007*g*)	10.1107/S1600536807056504	XIRGIP
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')copper(II)]-μ-acetamido-$\kappa^2O:N$]	Liu & Zhu (2007*h*)	10.1107/S1600536807059077	HIQROP
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')cobalt(II)]-μ-acetamidato-$\kappa^2O:N$]	Liu & Zhu (2007*i*)	10.1107/S1600536807060631	YIQMER
N′-Benzoyl-4-nitronicotinohydrazide	Liu & Zhu (2007*p*)	10.1107/S1600536807053068	CIPVON
N′-(3-Nitro-4-pyridylcarbonyl)pyridine-4-carbohydrazide	Liu & Zhu (2007*q*)	10.1107/S1600536807054876	RIRWEV

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Table 1 (continued)

Title	Reference	DOI	Refcode
Ethylenediammonium sulfate	Liu & Zhu (2007*r*)	10.1107/S1600536807056280	ETDAMS03
Ethylenediammonium perchlorate	Liu & Zhu (2007*s*)	10.1107/S1600536807059909	HIRYEN
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')manganese(II)]-μ-nitrato-$\kappa^2O:O'$]	Liu & Zhu (2008)	10.1107/S160053680706254X	MIRROV

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Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007*e*). *Acta Cryst.* E**63**, m2080–m2081.
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Bis(2,2′-bipyridine-κ*N*,*N*′)bis(thiocyanato-κ*N*)iron(II)

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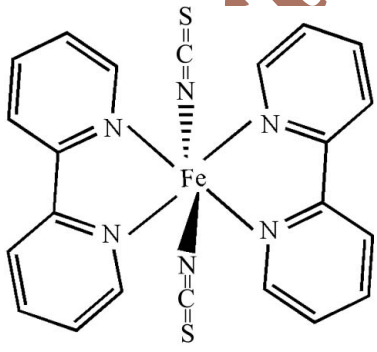
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.003 Å; R factor = 0.028; wR factor = 0.104; data-to-parameter ratio = 16.5.

The Fe^{II} atom in the title complex, $[Fe(NCS)_2(C_{10}H_8N_2)_2]$, is coordinated by four N atoms of two 2,2′-bipyridine ligands and two N atoms of two SCN^- ligands. This mononuclear complex is further extended into a supramolecular network structure *via* nonclassical hydrogen bonds between C—H groups of 2,2′-bipyridine and N and S atoms of neighbouring SCN^- ligands and π–π stacking interactions with a centroid-to-centroid distance of 3.619 (7) Å (symmetry code: 1 − *x*, 2 − *y*, 2 − *z*).

Related literature

For general background, see: Banglin *et al.* (2001); Ferey (2001); Hill (1998); Li *et al.* (2005); Liu *et al.* (2004); Pan & Xu (2004); Wu *et al.* (2003); Zhong *et al.* (2007*a*,*b*,*c*). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Fe(NCS)_2(C_{10}H_8N_2)_2]$
M_r = 484.38
Orthorhombic, *Pbca*
a = 16.087 (3) Å
b = 16.0117 (11) Å
c = 17.0781 (12) Å
V = 4399.1 (9) Å^3
Z = 8
Mo *Kα* radiation
μ = 0.90 mm^{-1}
T = 273 (2) K
0.36 × 0.34 × 0.22 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.738, T_{max} = 0.827
28231 measured reflections
4607 independent reflections
3440 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.104
S = 0.99
4607 reflections
280 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Fe1—N1	2.1762 (15)	Fe1—N4	2.1555 (15)
Fe1—N2	2.1452 (15)	Fe1—N5	2.0773 (18)
Fe1—N3	2.1847 (15)	Fe1—N6	2.0765 (17)
N1—Fe1—N2	75.72 (6)	N2—Fe1—N6	92.19 (6)
N1—Fe1—N3	80.97 (6)	N3—Fe1—N4	76.08 (6)
N1—Fe1—N4	98.73 (6)	N3—Fe1—N5	163.37 (7)
N1—Fe1—N5	91.50 (7)	N3—Fe1—N6	91.27 (6)
N1—Fe1—N6	164.50 (7)	N4—Fe1—N5	90.58 (6)
N2—Fe1—N3	97.66 (6)	N4—Fe1—N6	92.32 (6)
N2—Fe1—N4	172.35 (5)	N5—Fe1—N6	99.27 (7)
N2—Fe1—N5	94.78 (6)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···S1^{i}	0.93	2.85	3.736 (2)	159
C10—H10···N6	0.93	2.62	3.158 (3)	117
C20—H20···N5	0.93	2.60	3.146 (3)	118

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); 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: AT2391).

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Article retracted

supplementary materials

Article retracted

Acta Cryst. (2007). E**63**, m2506-m2507 [**doi:10.1107/S1600536807043486**]

Bis(2,2'-bipyridine-$\kappa N,N'$)bis(thiocyanato-κN)iron(II)

T. Liu and J. Y. Zhu

Comment

Research on organic-inorganic hybrid materials has attracted much attention owing to their applications in areas including catalysis, materials chemistry and biochemistry (Hill, 1998; Banglin *et al.*, 2001; Ferey, 2001). Weak interactions play an important role in these compounds and many frameworks are linked by different kinds of weak interactions, such as hydrogen bonds and π-π stacking. Several reported crystal structures of metal complexes incorporating the phenanthroline, quinoline and pyridyl ligand have shown the existence of π-π stacking between neighbouring aromatic rings in these structures (Wu *et al.*, 2003; Pan & Xu, 2004; Liu *et al.*, 2004; Li *et al.*, 2005). We report herein the crystal structure of the title compound, (I), and the crystal struture is similar with the structures recently reported (Zhong *et al.*, 2007*a*,b,c).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The six-coordinate environment of the Fe atom is completed by the four N atoms of two 2,2'-bipyridyl ligands and two N atoms of two SCN^- ligands (Table 1). The Fe—N bonds [average 2.1654 (15) Å] for the 2,2'-bipyridyl ligands are somewhat greater than the Fe—N bonds [average 2.0769 (18) Å] for the SCN^- ligands. The two 2,2'-bipyridyl ligands are nearly perpendicular to each other, with a dihedral angle of 105.4 (3)°.

In the crystal structure, C—H···S and C—H···N non-classical hydrogen bonds between C—H groups of 2,2'-bipyridyl and N and S atoms of neighbouring SCN^- ligands, with one C···S and two C···N distances of 3.736 (2), 3.146 (3) and 3.158 (3) Å, respectively, generate a layered hydrogen-bonded network (Table 2). The non-classical hydrogen-bonding interactions and π-π stacking interactions with centroid-centroid distance of 3.619 (7) Å [symmetry code: $1-x, 2-y, 2-z$] link the mononuclear complex into a supramolecular network structure (Fig. 2).

Experimental

Crystals of the title compound (I) were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb, which was then sealed. Potassium ferrocyanide trihydrate (84.5 mg, 0.2 mmol), 2,2'-bipyridyl (62.4 mg, 0.4 mmol), potassium thiocyanate (38.9 mg, 0.4 mmol) and distilled water (3 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure up to 423 K over the course of 7 d and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colourless solution was decanted from small colourless crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature.

Refinement

H atoms were positioned geometrically, with C—H = 0.93 Å, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Article retracted

Figures

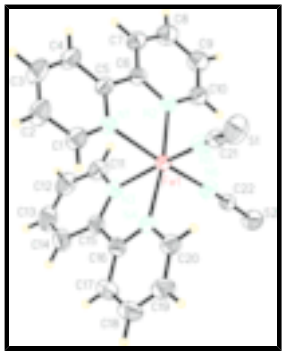

Fig. 1. View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

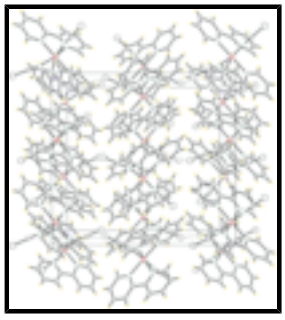

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

Article retracted

Bis(2,2'-bipyridine-κ*N*,*N*')bis(thiocyanato-κ*N*)iron(II)

Crystal data

$[Fe(NCS)_2(C_{10}H_8N_2)_2]$	F_{000} = 1984
M_r = 484.38	D_x = 1.463 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 11611 reflections
a = 16.087 (3) Å	θ = 2.4–27.5°
b = 16.0117 (11) Å	μ = 0.90 mm^{-1}
c = 17.0781 (12) Å	*T* = 273 (2) K
V = 4399.1 (9) Å^3	Block, colourless
Z = 8	0.36 × 0.34 × 0.22 mm

Data collection

Bruker APEXII area-detector diffractometer	4607 independent reflections
Radiation source: fine-focus sealed tube	3440 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.023
T = 273(2) K	θ_{max} = 26.6°
φ and ω scans	θ_{min} = 2.2°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −20→20

T_{min} = 0.738, T_{max} = 0.827
28231 measured reflections

k = −20→20
l = −20→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.104
S = 0.99
4607 reflections
280 parameters
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
$w = 1/[\sigma^2(F_o^2) + (0.0679P)^2 + 0.3898P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Extinction correction: none

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	0.702218 (14)	0.384015 (15)	−0.000737 (13)	0.04495 (11)
S1	0.57506 (4)	0.51147 (5)	−0.22505 (4)	0.0891 (2)
S2	0.51114 (4)	0.22577 (4)	0.15958 (4)	0.08023 (19)
N1	0.80962 (9)	0.46072 (9)	−0.02958 (10)	0.0536 (4)
N2	0.69900 (9)	0.48321 (9)	0.08364 (9)	0.0541 (4)
N3	0.79903 (8)	0.30887 (10)	0.05481 (9)	0.0542 (4)
N4	0.72299 (9)	0.28352 (9)	−0.08241 (9)	0.0513 (3)
N5	0.62928 (11)	0.44614 (11)	−0.08248 (11)	0.0705 (5)
N6	0.60985 (10)	0.31801 (10)	0.05743 (11)	0.0667 (4)
C1	0.86327 (13)	0.44587 (14)	−0.08809 (12)	0.0700 (5)
H1	0.8545	0.3992	−0.1194	0.084*
C2	0.93059 (14)	0.49603 (17)	−0.10431 (14)	0.0861 (7)
H2	0.9665	0.4837	−0.1454	0.103*
C3	0.94281 (14)	0.56411 (17)	−0.05820 (16)	0.0880 (7)
H3	0.9875	0.5996	−0.0678	0.106*
C4	0.88890 (15)	0.58084 (16)	0.00311 (13)	0.0759 (6)

Article retracted

H4	0.8968	0.6276	0.0346	0.091*
C5	0.82295 (12)	0.52690 (11)	0.01694 (11)	0.0544 (4)
C6	0.76284 (11)	0.53793 (11)	0.08202 (10)	0.0526 (4)
C7	0.77061 (13)	0.59913 (14)	0.13863 (12)	0.0693 (5)
H7	0.8158	0.6353	0.1379	0.083*
C8	0.71093 (15)	0.60623 (16)	0.19610 (14)	0.0821 (7)
H8	0.7162	0.6466	0.2349	0.098*
C9	0.64395 (15)	0.55372 (15)	0.19585 (13)	0.0786 (6)
H9	0.6019	0.5593	0.2329	0.094*
C10	0.64025 (13)	0.49220 (13)	0.13928 (12)	0.0653 (5)
H10	0.5954	0.4555	0.1396	0.078*
C11	0.83790 (13)	0.32758 (13)	0.12300 (12)	0.0674 (5)
H11	0.8168	0.3709	0.1533	0.081*
C12	0.90694 (15)	0.28565 (16)	0.14962 (15)	0.0832 (7)
H12	0.9317	0.2997	0.1970	0.100*
C13	0.93838 (14)	0.22198 (17)	0.10378 (18)	0.0909 (8)
H13	0.9854	0.1927	0.1197	0.109*
C14	0.89971 (13)	0.20211 (15)	0.03439 (16)	0.0756 (6)
H14	0.9207	0.1596	0.0029	0.091*
C15	0.82893 (11)	0.24598 (12)	0.01150 (11)	0.0550 (4)
C16	0.78122 (11)	0.22718 (11)	−0.06158 (12)	0.0545 (4)
C17	0.79405 (13)	0.15627 (14)	−0.10565 (14)	0.0735 (6)
H17	0.8349	0.1181	−0.0914	0.088*
C18	0.74578 (17)	0.14220 (15)	−0.17115 (14)	0.0812 (7)
H18	0.7537	0.0942	−0.2008	0.097*
C19	0.68650 (14)	0.19881 (14)	−0.19234 (14)	0.0723 (6)
H19	0.6534	0.1902	−0.2363	0.087*
C20	0.67727 (12)	0.26850 (12)	−0.14697 (12)	0.0607 (5)
H20	0.6374	0.3076	−0.1614	0.073*
C21	0.60591 (11)	0.47321 (11)	−0.14205 (13)	0.0589 (5)
C22	0.56819 (11)	0.28039 (11)	0.10015 (12)	0.0540 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.04535 (16)	0.04334 (17)	0.04615 (18)	−0.00323 (10)	0.00046 (9)	−0.00113 (10)
S1	0.0815 (4)	0.1094 (5)	0.0763 (4)	−0.0105 (3)	−0.0249 (3)	0.0132 (3)
S2	0.0866 (4)	0.0743 (4)	0.0797 (4)	−0.0121 (3)	0.0266 (3)	0.0007 (3)
N1	0.0555 (8)	0.0551 (9)	0.0501 (8)	−0.0065 (7)	0.0031 (7)	0.0005 (7)
N2	0.0557 (8)	0.0530 (8)	0.0535 (9)	−0.0036 (7)	0.0025 (7)	−0.0036 (7)
N3	0.0517 (8)	0.0587 (9)	0.0523 (9)	−0.0046 (6)	−0.0025 (7)	0.0072 (7)
N4	0.0515 (8)	0.0495 (8)	0.0528 (9)	−0.0019 (6)	0.0016 (7)	−0.0019 (6)
N5	0.0783 (11)	0.0576 (10)	0.0756 (12)	0.0020 (8)	−0.0177 (9)	0.0028 (9)
N6	0.0614 (9)	0.0605 (9)	0.0781 (11)	−0.0086 (8)	0.0105 (9)	−0.0036 (8)
C1	0.0714 (12)	0.0796 (14)	0.0588 (12)	−0.0141 (11)	0.0133 (10)	−0.0054 (10)
C2	0.0759 (14)	0.114 (2)	0.0682 (15)	−0.0253 (14)	0.0221 (12)	−0.0036 (14)
C3	0.0738 (14)	0.0989 (18)	0.0913 (17)	−0.0338 (13)	0.0144 (13)	0.0035 (14)
C4	0.0699 (14)	0.0731 (14)	0.0848 (17)	−0.0226 (12)	−0.0003 (11)	−0.0058 (11)

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C5	0.0526 (10)	0.0528 (10)	0.0578 (11)	−0.0057 (8)	−0.0061 (8)	0.0040 (8)
C6	0.0529 (9)	0.0526 (10)	0.0524 (10)	−0.0002 (8)	−0.0086 (8)	−0.0007 (8)
C7	0.0687 (12)	0.0690 (13)	0.0704 (14)	−0.0076 (10)	−0.0090 (11)	−0.0145 (11)
C8	0.0902 (17)	0.0883 (17)	0.0677 (15)	−0.0053 (13)	−0.0026 (12)	−0.0289 (13)
C9	0.0847 (15)	0.0872 (15)	0.0640 (13)	−0.0010 (13)	0.0134 (11)	−0.0174 (12)
C10	0.0684 (12)	0.0655 (12)	0.0620 (12)	−0.0058 (10)	0.0105 (10)	−0.0081 (9)
C11	0.0722 (12)	0.0690 (13)	0.0611 (12)	−0.0089 (10)	−0.0102 (10)	0.0084 (10)
C12	0.0768 (14)	0.0893 (17)	0.0836 (17)	−0.0152 (13)	−0.0283 (13)	0.0204 (14)
C13	0.0591 (13)	0.0988 (19)	0.115 (2)	0.0037 (12)	−0.0204 (14)	0.0276 (17)
C14	0.0565 (11)	0.0773 (14)	0.0929 (17)	0.0088 (10)	0.0021 (12)	0.0125 (13)
C15	0.0467 (9)	0.0546 (10)	0.0638 (12)	−0.0002 (8)	0.0078 (8)	0.0097 (8)
C16	0.0532 (9)	0.0533 (10)	0.0569 (11)	0.0000 (8)	0.0102 (8)	0.0007 (8)
C17	0.0804 (14)	0.0623 (12)	0.0779 (15)	0.0136 (10)	0.0085 (11)	−0.0067 (11)
C18	0.1001 (18)	0.0680 (14)	0.0754 (16)	0.0067 (13)	0.0120 (14)	−0.0194 (11)
C19	0.0844 (14)	0.0712 (13)	0.0613 (13)	−0.0083 (11)	0.0001 (11)	−0.0125 (10)
C20	0.0624 (10)	0.0608 (11)	0.0587 (12)	−0.0039 (9)	−0.0014 (9)	−0.0042 (9)
C21	0.0508 (9)	0.0505 (10)	0.0753 (14)	0.0006 (8)	−0.0090 (9)	−0.0096 (9)
C22	0.0496 (9)	0.0500 (9)	0.0623 (12)	0.0004 (8)	0.0022 (9)	−0.0094 (8)

Geometric parameters (Å, °)

Fe1—N1	2.1762 (15)	C5—C6	1.484 (3)
Fe1—N2	2.1452 (15)	C6—C7	1.382 (3)
Fe1—N3	2.1847 (15)	C7—C8	1.378 (3)
Fe1—N4	2.1555 (15)	C7—H7	0.9300
Fe1—N5	2.0773 (18)	C8—C9	1.367 (3)
Fe1—N6	2.0765 (17)	C8—H8	0.9300
S1—C21	1.622 (2)	C9—C10	1.381 (3)
S2—C22	1.624 (2)	C9—H9	0.9300
N1—C5	1.342 (2)	C10—H10	0.9300
N1—C1	1.342 (2)	C11—C12	1.375 (3)
N2—C10	1.348 (2)	C11—H11	0.9300
N2—C6	1.350 (2)	C12—C13	1.381 (4)
N3—C15	1.339 (2)	C12—H12	0.9300
N3—C11	1.355 (2)	C13—C14	1.376 (4)
N4—C20	1.347 (2)	C13—H13	0.9300
N4—C16	1.348 (2)	C14—C15	1.394 (3)
N5—C21	1.168 (2)	C14—H14	0.9300
N6—C22	1.159 (2)	C15—C16	1.496 (3)
C1—C2	1.376 (3)	C16—C17	1.378 (3)
C1—H1	0.9300	C17—C18	1.380 (3)
C2—C3	1.359 (3)	C17—H17	0.9300
C2—H2	0.9300	C18—C19	1.365 (3)
C3—C4	1.386 (3)	C18—H18	0.9300
C3—H3	0.9300	C19—C20	1.367 (3)
C4—C5	1.388 (3)	C19—H19	0.9300
C4—H4	0.9300	C20—H20	0.9300
N1—Fe1—N2	75.72 (6)	C7—C6—C5	123.32 (17)
N1—Fe1—N3	80.97 (6)	C8—C7—C6	119.59 (19)

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N1—Fe1—N4	98.73 (6)	C8—C7—H7	120.2
N1—Fe1—N5	91.50 (7)	C6—C7—H7	120.2
N1—Fe1—N6	164.50 (7)	C9—C8—C7	119.8 (2)
N2—Fe1—N3	97.66 (6)	C9—C8—H8	120.1
N2—Fe1—N4	172.35 (5)	C7—C8—H8	120.1
N2—Fe1—N5	94.78 (6)	C8—C9—C10	118.4 (2)
N2—Fe1—N6	92.19 (6)	C8—C9—H9	120.8
N3—Fe1—N4	76.08 (6)	C10—C9—H9	120.8
N3—Fe1—N5	163.37 (7)	N2—C10—C9	122.62 (19)
N3—Fe1—N6	91.27 (6)	N2—C10—H10	118.7
N4—Fe1—N5	90.58 (6)	C9—C10—H10	118.7
N4—Fe1—N6	92.32 (6)	N3—C11—C12	123.3 (2)
N5—Fe1—N6	99.27 (7)	N3—C11—H11	118.4
C5—N1—C1	118.56 (16)	C12—C11—H11	118.4
C5—N1—Fe1	116.02 (13)	C11—C12—C13	118.0 (2)
C1—N1—Fe1	125.40 (13)	C11—C12—H12	121.0
C10—N2—C6	118.59 (16)	C13—C12—H12	121.0
C10—N2—Fe1	124.72 (13)	C14—C13—C12	119.6 (2)
C6—N2—Fe1	116.63 (12)	C14—C13—H13	120.2
C15—N3—C11	118.37 (17)	C12—C13—H13	120.2
C15—N3—Fe1	115.50 (12)	C13—C14—C15	119.6 (2)
C11—N3—Fe1	125.47 (14)	C13—C14—H14	120.2
C20—N4—C16	118.42 (16)	C15—C14—H14	120.2
C20—N4—Fe1	125.33 (12)	N3—C15—C14	121.2 (2)
C16—N4—Fe1	115.87 (12)	N3—C15—C16	115.34 (16)
C21—N5—Fe1	160.89 (17)	C14—C15—C16	123.5 (2)
C22—N6—Fe1	168.26 (17)	N4—C16—C17	120.75 (19)
N1—C1—C2	123.5 (2)	N4—C16—C15	116.23 (16)
N1—C1—H1	118.2	C17—C16—C15	123.01 (18)
C2—C1—H1	118.2	C16—C17—C18	119.5 (2)
C3—C2—C1	117.7 (2)	C16—C17—H17	120.2
C3—C2—H2	121.1	C18—C17—H17	120.2
C1—C2—H2	121.1	C19—C18—C17	120.0 (2)
C2—C3—C4	120.2 (2)	C19—C18—H18	120.0
C2—C3—H3	119.9	C17—C18—H18	120.0
C4—C3—H3	119.9	C18—C19—C20	117.9 (2)
C3—C4—C5	119.1 (2)	C18—C19—H19	121.1
C3—C4—H4	120.4	C20—C19—H19	121.1
C5—C4—H4	120.4	N4—C20—C19	123.4 (2)
N1—C5—C4	120.85 (19)	N4—C20—H20	118.3
N1—C5—C6	115.68 (16)	C19—C20—H20	118.3
C4—C5—C6	123.47 (18)	N5—C21—S1	179.0 (2)
N2—C6—C7	120.96 (18)	N6—C22—S2	178.66 (18)
N2—C6—C5	115.71 (15)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···S1^{i}	0.93	2.85	3.736 (2)	159

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C10—H10···N6	0.93	2.62	3.158 (3)	117
C20—H20···N5	0.93	2.60	3.146 (3)	118

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

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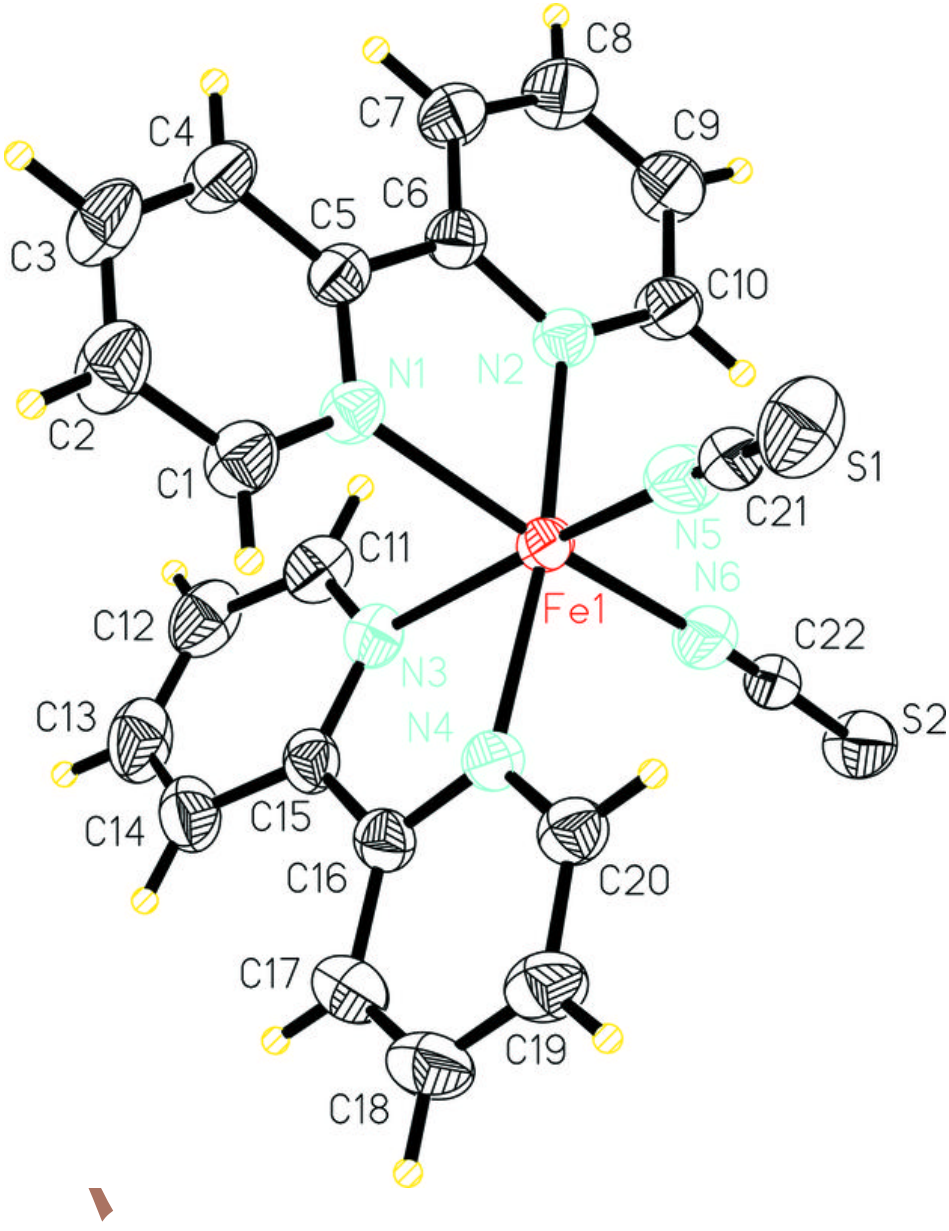
Fig. 1


C8
C7
C9
C4
C6
C5
C3
C10
N1
N2
C2
S1
C1
C21
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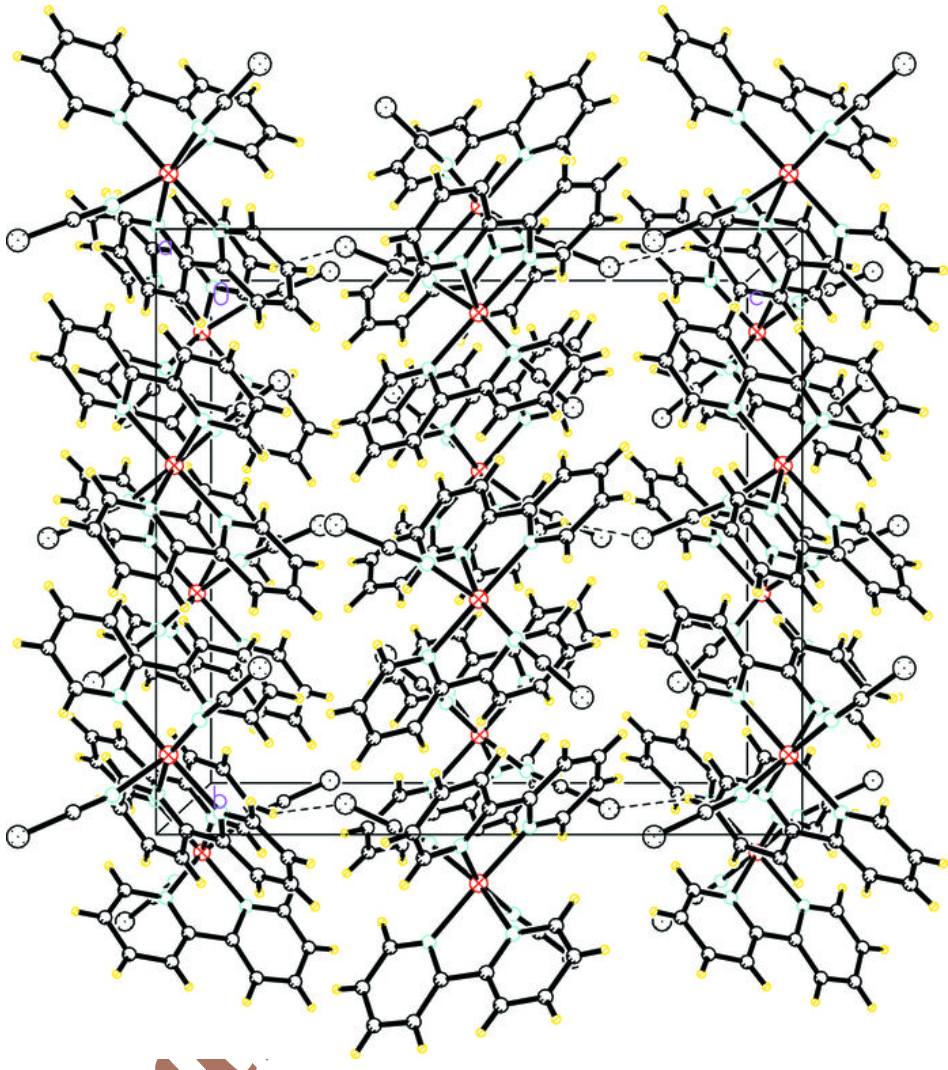
C11
N6
Fe1
C12
C22
N3
S2
C13
N4
C14
C15
C16
C20
C17
C19
C18

Fig. 2



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