Acta Crystallographica Section E
Structure Reports Online
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Retraction of articles

This article reports the retraction of five articles published in *Acta Crystallographica Section E* between 2004 and 2011.

After further thorough investigation (see Harrison *et al.*, 2010), five 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
Ammonium 2,6-dicarboxy-4-nitrophenolate	Sun & Nie (2004)	10.1107/S1600536804022135	PAHDUY
Triaqua(1,10-phenanthroline)sulfatocopper(II) monohydrate	An *et al.* (2007)	10.1107/S1600536807000591	HEWQUW
Diaqua-1κO,3κO-di-μ-cyanido-1:2κ^{2}N:C;2:3κ^{2}C:N-dicyanido-2κ^{2}C-bis{4,4′-dibromo-2,2′-[propane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-1κ^{4}O,N,N′,O′;3κ^{4}O,N,N′,O′-1,3-diiron(III)-2-nickel(II)	Zhang *et al.* (2008)	10.1107/S1600536808017893	SOGBOG
Bis(6-methoxy-2-{[tris(hydroxymethyl)methyl]iminomethyl}phenolato)copper(II) dihydrate	Zhang *et al.* (2009)	10.1107/S1600536808043948	ROLPAK
Oxonium picrate	Jin *et al.* (2011)	10.1107/S1600536811022574	EVILAX

References

An, Z., Wu, Y.-L., Lin, F. & Zhu, L. (2007). *Acta Cryst.* E**63**, m477–m478.
Harrison, W. T. A., Simpson, J. & Weil, M. (2010). *Acta Cryst.* E**66**, e1–e2.
Jin, S.-W., Chen, B.-X., Ge, Y.-S., Yin, H.-B. & Fang, Y.-P. (2011). *Acta Cryst.* E**67**, o1694.
Sun, Y.-X. & Nie, Y. (2004). *Acta Cryst.* E**60**, o1742–o1744.
Zhang, X., Wei, P., Dou, J., Li, B. & Hu, B. (2009). *Acta Cryst.* E**65**, m151–m152.
Zhang, X., Wei, P. & Li, B. (2008). *Acta Cryst.* E**64**, m926.

  doi:10.1107/S1600536811030649

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Diaqua-1κO,3κO-di-μ-cyanido-1:2$\kappa^2 N$:C;2:3$\kappa^2 C$:N-dicyanido-2$\kappa^2 C$-bis{4,4′-dibromo-2,2′-[propane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-1$\kappa^4 O$,N,N',O';3$\kappa^4 O$,N,N',O'-1,3-diiron(III)-2-nickel(II)

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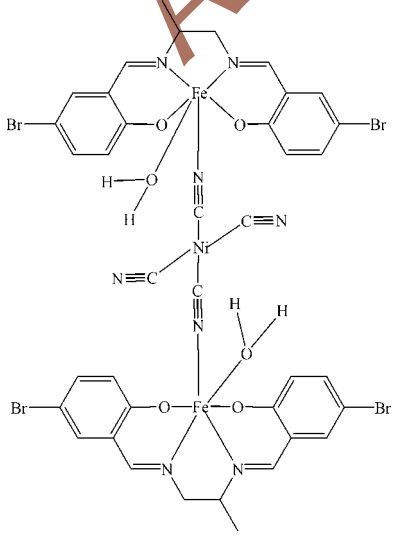
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.013 Å; R factor = 0.066; wR factor = 0.181; data-to-parameter ratio = 13.4.

The title compound, $[Fe_2Ni(C_{17}H_{14}Br_2N_2O_2)_2(CN)_4(H_2O)_2]$ or $[\{Fe(C_{17}H_{14}Br_2N_2O_2)(H_2O)\}_2(\mu\text{-}CN)_2\{Ni(CN)_2\}]$, is isostructural with its Mn^{III}-containing analogue. Each Fe^{III} atom is chelated by a Schiff base ligand *via* two N and two O atoms and is additionally coordinated by a water molecule, forming a slightly distorted octahedral geometry. The two Fe^{III} centres are bridged by a square-planar $Ni(CN)_4$ unit, which lies on an inversion centre. A two-dimensional network is formed *via* O—H···O and O—H···N hydrogen bonds.

Related literature

For related literature, see: Kuang *et al.* (2002); Kuchar *et al.* (2003); Yang *et al.* (2003). For the isostructural Mn^{III}-containing compound, see: Sun *et al.* (2008).



Experimental

Crystal data

$[Fe_2Ni(C_{17}H_{14}Br_2N_2O_2)_2(CN)_4(H_2O)_2]$
M_r = 1186.71
Monoclinic, $P2_1/n$
a = 11.599 (2) Å
b = 13.538 (3) Å
c = 14.715 (3) Å
β = 112.04 (3)°
V = 2141.8 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 4.89 mm^{-1}
T = 293 (2) K
0.10 × 0.10 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.449, T_{max} = 0.641
13404 measured reflections
3699 independent reflections
2263 reflections with $I > 2\sigma(I)$
R_{int} = 0.085

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.181
S = 1.00
3699 reflections
276 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.96 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H1W···O1^{i}	0.81 (2)	2.09 (4)	2.859 (7)	159 (8)
O3—H2W···N2^{ii}	0.81 (2)	2.02 (2)	2.813 (9)	167 (7)

Symmetry codes: (i) $-x+1, -y+2, -z+1$; (ii) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.

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: CF2205).

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Bruker (2004). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Kuang, S. M., Fanwick, P. E. & Walton, R. A. (2002). *Inorg. Chem.* **41**, 147–151.
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Sun, Z.-H., Yang, G.-B., Meng, L.-B. & Chen, S. (2008). *Acta Cryst.* E**64**, m783.
Yang, J. Y., Shores, M. P., Sokol, J. J. & Long, J. R. (2003). *Inorg. Chem.* **42**, 1403–1408.

supporting information

Acta Cryst. (2008). E**64**, m926 [doi:10.1107/S1600536808017893]

Diaqua-1κO,3κO-di-μ-cyanido-1:2$\kappa^2 N$:C;2:3$\kappa^2 C$:N-dicyanido-2$\kappa^2 C$-bis{4,4′-dibromo-2,2′-[propane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-1$\kappa^4 O$,N,N',O';3$\kappa^4 O$,N,N',O'-1,3-diiron(III)-2-nickel(II)

Xiutang Zhang, Peihai Wei and Bin Li

S1. Comment

Cyanide-bridged oligonuclear complexes with chain-like arrangements of metal ions and cyanide ligands have been studied for a long time due to the good electronic conductivity between the metallic groups (Kuang *et al.*, 2002; Kuchar *et al.*, 2003; Yang *et al.*, 2003). In this context, bulk properties such as magnetism, luminescence, electrical conductivity resulting from metal-metal charge transfer like multi-redox steps, mixed valence and long-range electronic interactions prompted us to report our research work on cyanide-bridged complexes. In this paper, we report the structure of the title compound, (I). It is isostructural with its Mn^{III}-containing analogue (Sun *et al.*, 2008).

As shown in Fig. 1, each Fe^{III} atom is chelated by a Schiff base ligand *via* two N and two O atoms and is additionally coordinated by a water molecule, forming a slightly distorted octahedral geometry. The Schiff base lies in the equatorial plane, and the cyanido and aqua ligands lie in the axial coordination sites. The Fe—N and Fe—O axial bond lengths are much longer than the equatorial ones. A centrosymmetric square-planar $Ni(CN)_4$ unit links two Fe^{III} centres. With O—H···O and O—H···N hydrogen bonds, a two-dimensional network is formed, as shown in Fig. 2.

S2. Experimental

A mixture of iron(III) acetylacetonate (1 mmol), *N*,*N*′-bis(2-hydroxy-5-bromobenzyl)-1,2-diaminopropane (1 mmol), and dipotassium tetracyanidonickelate(II) (1 mmol) in 20 ml methanol was refluxed for several hours. The cooled solution was filtered and the filtrate was kept in an ice box. One week later, brown blocks of (I) were obtained with a yield of 5%. Anal. Calc. for $C_{38}H_{32}Br_4Fe_2N_8NiO_6$: C 38.43, H 2.70, N 9.44%; Found: C 38.40, H 2.63, N 9.39.

S3. Refinement

All C-bound 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). H atoms on the aqua ligand were located in a difference density map and were refined with the distance restraint O—H = 0.82 (1) Å.

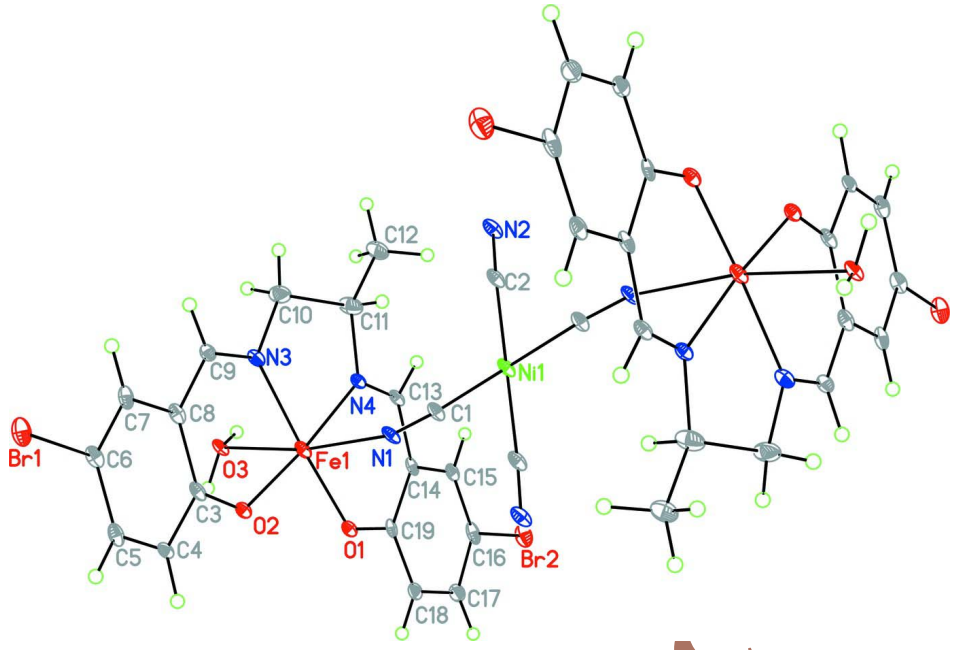

Figure 1

The molecular structure of (I), drawn with 30% probability displacement ellipsoids for the non-hydrogen atoms. [Symmetry code for unlabelled atoms: -x, 2-y, -z.]

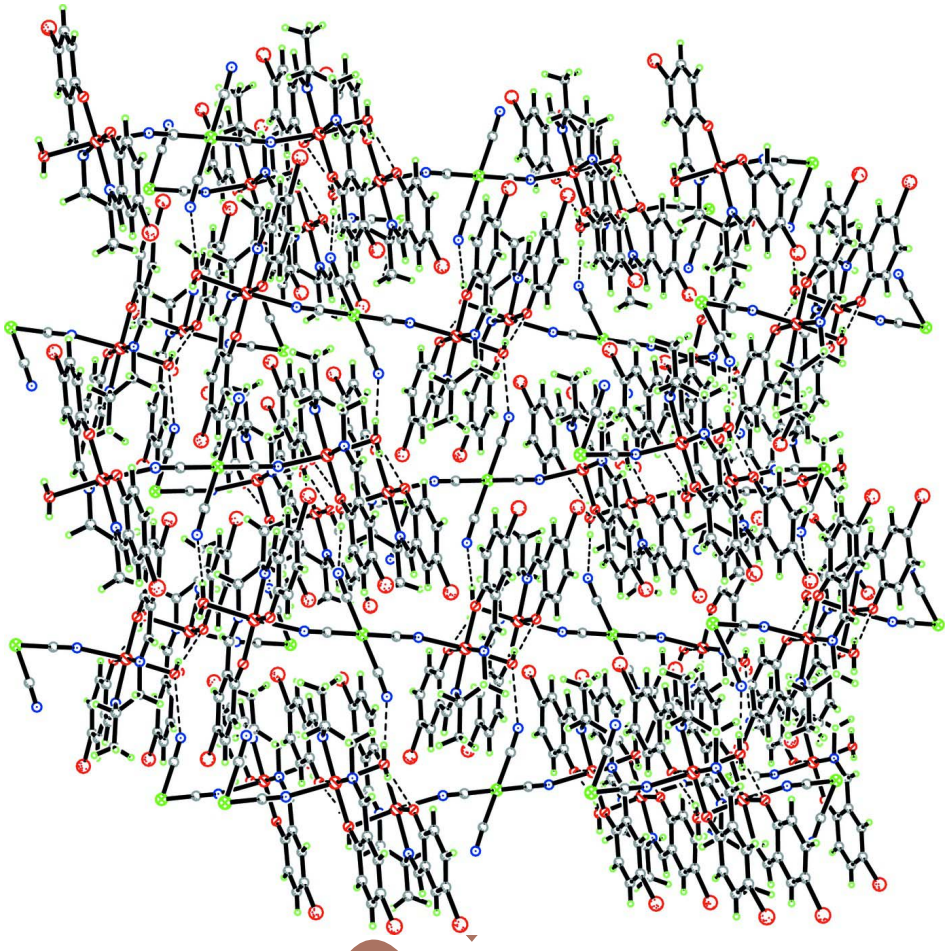

Figure 2

Two-dimensional network formed by hydrogen bonds (dashed lines).

Diaqua-1κO,3κO-di-μ-cyanido- 1:2$\kappa^2 N$:C;2:3$\kappa^2 C$:N-dicyanido-2$\kappa^2 C$- bis{4,4′-dibromo-2,2′-[propane-1,2-diylbis(nitrilomethylidyne)]diphenolato}- 1$\kappa^4 O,N,N',O'$;3$\kappa^4 O,N,N',O'$-1,3-diiron(III)-2-nickel(II)

Crystal data

$[Fe_2Ni(C_{17}H_{14}Br_2N_2O_2)_2(CN)_4(H_2O)_2]$
$M_r = 1186.71$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 11.599$ (2) Å
$b = 13.538$ (3) Å
$c = 14.715$ (3) Å
$\beta = 112.04$ (3)°
$V = 2141.8$ (7) Å^3
$Z = 2$
$F(000) = 1168$
$D_x = 1.840$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3699 reflections
$\theta = 3.0$–25.1°
$\mu = 4.89$ mm^{-1}
$T = 293$ K
Block, brown
0.10 × 0.10 × 0.10 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)
$T_{min} = 0.449$, $T_{max} = 0.641$

13404 measured reflections
3699 independent reflections
2263 reflections with $I > 2\sigma(I)$
$R_{int} = 0.085$
$\theta_{max} = 25.1°$, $\theta_{min} = 3.0°$
$h = -13 \rightarrow 12$
$k = -16 \rightarrow 15$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.066$
$wR(F^2) = 0.181$
$S = 1.00$
3699 reflections
276 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.09P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.96$ e Å^{-3}
$\Delta\rho_{min} = -0.64$ 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	0.29547 (11)	0.95323 (8)	0.36728 (8)	0.0341 (4)
Ni1	0.0000	1.0000	0.0000	0.0334 (4)
Br1	−0.07330 (10)	1.37221 (7)	0.43825 (7)	0.0569 (4)
Br2	0.75936 (10)	0.61244 (8)	0.30711 (8)	0.0621 (4)
C1	0.1210 (8)	0.9936 (5)	0.1261 (6)	0.035 (2)
C2	−0.0637 (8)	0.8804 (6)	0.0276 (6)	0.037 (2)
C3	0.2234 (8)	1.1459 (6)	0.4134 (6)	0.034 (2)
C4	0.2476 (8)	1.2492 (5)	0.4247 (5)	0.033 (2)
H4	0.3242	1.2728	0.4277	0.039*
C5	0.1608 (9)	1.3146 (6)	0.4311 (6)	0.042 (2)
H5	0.1780	1.3819	0.4362	0.050*
C6	0.0471 (9)	1.2807 (6)	0.4303 (6)	0.042 (2)
C7	0.0185 (9)	1.1818 (6)	0.4197 (6)	0.045 (2)
H7	−0.0581	1.1603	0.4187	0.054*
C8	0.1029 (8)	1.1136 (5)	0.4104 (6)	0.037 (2)
C9	0.0680 (8)	1.0105 (6)	0.3966 (6)	0.035 (2)
H9	−0.0079	0.9939	0.4004	0.042*
C10	0.0874 (10)	0.8350 (7)	0.3700 (9)	0.067 (3)
H10A	0.1154	0.8044	0.4343	0.080*
H10B	−0.0028	0.8331	0.3424	0.080*

C11	0.1355 (9)	0.7815 (7)	0.3082 (9)	0.067 (3)
H11	0.0893	0.8088	0.2429	0.080*
C12	0.1048 (10)	0.6739 (6)	0.2961 (8)	0.060 (3)
H12A	0.1567	0.6390	0.3537	0.091*
H12B	0.1188	0.6491	0.2400	0.091*
H12C	0.0191	0.6646	0.2869	0.091*
C13	0.3443 (8)	0.7546 (5)	0.3198 (5)	0.032 (2)
H13	0.3196	0.6893	0.3047	0.039*
C14	0.4688 (8)	0.7786 (6)	0.3302 (5)	0.033 (2)
C15	0.5437 (9)	0.7030 (6)	0.3193 (5)	0.038 (2)
H15	0.5141	0.6384	0.3116	0.046*
C16	0.6591 (9)	0.7209 (7)	0.3197 (6)	0.049 (3)
C17	0.7053 (9)	0.8158 (7)	0.3289 (6)	0.048 (2)
H17	0.7829	0.8280	0.3262	0.058*
C18	0.6337 (8)	0.8932 (6)	0.3422 (6)	0.039 (2)
H18	0.6657	0.9570	0.3509	0.047*
C19	0.5155 (8)	0.8770 (6)	0.3428 (5)	0.033 (2)
N1	0.1906 (7)	0.9903 (4)	0.2063 (5)	0.0368 (18)
N2	−0.0938 (7)	0.8039 (5)	0.0441 (5)	0.046 (2)
N3	0.1306 (6)	0.9396 (5)	0.3796 (5)	0.0400 (18)
N4	0.2649 (6)	0.8131 (4)	0.3289 (4)	0.0294 (16)
O1	0.4524 (5)	0.9530 (3)	0.3561 (4)	0.0309 (13)
O2	0.3095 (5)	1.0870 (4)	0.4047 (4)	0.0308 (13)
O3	0.3783 (5)	0.9024 (4)	0.5250 (4)	0.0352 (14)
H1W	0.433 (5)	0.942 (3)	0.547 (6)	0.042*
H2W	0.397 (6)	0.8444 (16)	0.530 (6)	0.042*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0365 (8)	0.0271 (7)	0.0247 (6)	0.0005 (5)	−0.0045 (5)	−0.0009 (5)
Ni1	0.0368 (9)	0.0254 (8)	0.0201 (7)	−0.0002 (6)	−0.0101 (6)	0.0006 (6)
Br1	0.0723 (8)	0.0473 (6)	0.0454 (6)	0.0242 (5)	0.0155 (5)	−0.0023 (5)
Br2	0.0537 (7)	0.0690 (8)	0.0549 (7)	0.0211 (5)	0.0105 (5)	−0.0137 (5)
C1	0.054 (6)	0.012 (4)	0.029 (5)	−0.002 (4)	0.003 (4)	0.000 (3)
C2	0.036 (5)	0.032 (5)	0.024 (4)	0.002 (4)	−0.010 (4)	0.000 (4)
C3	0.037 (5)	0.029 (4)	0.022 (4)	0.004 (4)	−0.007 (4)	−0.003 (3)
C4	0.039 (5)	0.031 (4)	0.018 (4)	−0.008 (4)	−0.001 (4)	0.001 (3)
C5	0.060 (7)	0.028 (5)	0.031 (5)	0.011 (5)	0.010 (5)	−0.004 (4)
C6	0.056 (6)	0.026 (5)	0.032 (5)	0.006 (4)	0.005 (4)	0.001 (4)
C7	0.052 (6)	0.054 (6)	0.022 (4)	0.011 (5)	0.005 (4)	−0.006 (4)
C8	0.044 (6)	0.030 (5)	0.024 (4)	0.009 (4)	−0.002 (4)	0.001 (3)
C9	0.031 (5)	0.038 (5)	0.030 (4)	0.001 (4)	0.004 (4)	−0.004 (4)
C10	0.064 (7)	0.043 (6)	0.104 (9)	−0.016 (5)	0.045 (7)	−0.025 (6)
C11	0.047 (7)	0.040 (6)	0.112 (10)	−0.004 (5)	0.030 (7)	−0.028 (6)
C12	0.059 (7)	0.039 (5)	0.076 (8)	−0.008 (5)	0.017 (6)	−0.008 (5)
C13	0.040 (5)	0.019 (4)	0.027 (4)	0.000 (4)	−0.001 (4)	−0.001 (3)
C14	0.034 (5)	0.034 (5)	0.020 (4)	0.009 (4)	−0.003 (4)	−0.008 (3)

C15	0.047 (6)	0.038 (5)	0.019 (4)	0.001 (4)	−0.001 (4)	0.000 (3)
C16	0.053 (6)	0.052 (6)	0.025 (5)	0.020 (5)	−0.004 (4)	−0.009 (4)
C17	0.043 (6)	0.054 (6)	0.043 (6)	−0.001 (5)	0.013 (5)	−0.011 (5)
C18	0.042 (6)	0.045 (5)	0.025 (4)	−0.003 (4)	0.006 (4)	−0.004 (4)
C19	0.035 (5)	0.043 (5)	0.010 (4)	0.010 (4)	−0.005 (3)	−0.003 (3)
N1	0.042 (4)	0.026 (4)	0.024 (4)	−0.007 (3)	−0.009 (3)	0.000 (3)
N2	0.055 (5)	0.029 (4)	0.037 (4)	−0.008 (4)	−0.001 (4)	−0.005 (3)
N3	0.038 (4)	0.033 (4)	0.043 (4)	−0.003 (3)	0.007 (4)	−0.011 (3)
N4	0.028 (4)	0.026 (4)	0.026 (4)	0.000 (3)	0.000 (3)	−0.001 (3)
O1	0.031 (3)	0.028 (3)	0.023 (3)	0.002 (2)	−0.001 (2)	0.001 (2)
O2	0.031 (3)	0.028 (3)	0.025 (3)	0.001 (2)	0.001 (2)	0.001 (2)
O3	0.040 (4)	0.025 (3)	0.025 (3)	−0.004 (3)	−0.004 (3)	−0.003 (3)

Geometric parameters (Å, º)

Fe1—O2	1.882 (5)	C9—H9	0.930
Fe1—O1	1.888 (6)	C10—C11	1.430 (13)
Fe1—N4	1.973 (6)	C10—N3	1.490 (11)
Fe1—N3	1.996 (7)	C10—H10A	0.970
Fe1—O3	2.261 (5)	C10—H10B	0.970
Fe1—N1	2.276 (6)	C11—N4	1.478 (11)
Ni1—C1^{i}	1.862 (8)	C11—C12	1.494 (11)
Ni1—C1	1.862 (8)	C11—H11	0.980
Ni1—C2	1.886 (9)	C12—H12A	0.960
Ni1—C2^{i}	1.886 (9)	C12—H12B	0.960
Br1—C6	1.903 (9)	C12—H12C	0.960
Br2—C16	1.924 (9)	C13—N4	1.260 (9)
C1—N1	1.154 (10)	C13—C14	1.431 (11)
C2—N2	1.148 (9)	C13—H13	0.930
C3—O2	1.322 (9)	C14—C15	1.390 (11)
C3—C4	1.423 (10)	C14—C19	1.424 (11)
C3—C8	1.449 (12)	C15—C16	1.359 (13)
C4—C5	1.371 (11)	C15—H15	0.930
C4—H4	0.930	C16—C17	1.378 (12)
C5—C6	1.393 (13)	C17—C18	1.396 (12)
C5—H5	0.930	C17—H17	0.930
C6—C7	1.374 (11)	C18—C19	1.392 (12)
C7—C8	1.389 (12)	C18—H18	0.930
C7—H7	0.930	C19—O1	1.318 (9)
C8—C9	1.445 (10)	O3—H1W	0.80 (6)
C9—N3	1.284 (10)	O3—H2W	0.81 (2)
O2—Fe1—O1	92.7 (2)	N3—C10—H10B	109.6
O2—Fe1—N4	174.5 (3)	H10A—C10—H10B	108.2
O1—Fe1—N4	92.8 (3)	C10—C11—N4	109.3 (8)
O2—Fe1—N3	92.5 (2)	C10—C11—C12	115.9 (10)
O1—Fe1—N3	174.6 (2)	N4—C11—C12	119.0 (8)
N4—Fe1—N3	82.0 (3)	C10—C11—H11	103.5

O2—Fe1—O3	92.1 (2)	N4—C11—H11	103.5
O1—Fe1—O3	92.1 (2)	C12—C11—H11	103.5
N4—Fe1—O3	87.8 (2)	C11—C12—H12A	109.5
N3—Fe1—O3	86.1 (3)	C11—C12—H12B	109.5
O2—Fe1—N1	92.7 (2)	H12A—C12—H12B	109.5
O1—Fe1—N1	93.8 (2)	C11—C12—H12C	109.5
N4—Fe1—N1	86.9 (2)	H12A—C12—H12C	109.5
N3—Fe1—N1	87.6 (3)	H12B—C12—H12C	109.5
O3—Fe1—N1	172.3 (2)	N4—C13—C14	126.5 (7)
C1^{i}—Ni1—C1	180.0 (4)	N4—C13—H13	116.8
C1^{i}—Ni1—C2	92.6 (3)	C14—C13—H13	116.8
C1—Ni1—C2	87.4 (3)	C15—C14—C19	118.8 (8)
C1^{i}—Ni1—C2^{i}	87.4 (3)	C15—C14—C13	118.0 (7)
C1—Ni1—C2^{i}	92.6 (3)	C19—C14—C13	123.0 (7)
C2—Ni1—C2^{i}	180.000 (1)	C16—C15—C14	121.7 (8)
N1—C1—Ni1	176.0 (9)	C16—C15—H15	119.2
N2—C2—Ni1	174.3 (8)	C14—C15—H15	119.2
O2—C3—C4	118.7 (8)	C15—C16—C17	120.9 (9)
O2—C3—C8	124.7 (7)	C15—C16—Br2	119.5 (7)
C4—C3—C8	116.5 (7)	C17—C16—Br2	119.6 (8)
C5—C4—C3	121.7 (8)	C16—C17—C18	118.9 (9)
C5—C4—H4	119.2	C16—C17—H17	120.5
C3—C4—H4	119.2	C18—C17—H17	120.5
C4—C5—C6	120.3 (8)	C19—C18—C17	121.5 (8)
C4—C5—H5	119.9	C19—C18—H18	119.2
C6—C5—H5	119.9	C17—C18—H18	119.2
C7—C6—C5	120.6 (8)	O1—C19—C18	118.8 (8)
C7—C6—Br1	119.4 (7)	O1—C19—C14	123.0 (8)
C5—C6—Br1	119.9 (6)	C18—C19—C14	118.2 (8)
C6—C7—C8	120.7 (9)	C1—N1—Fe1	165.6 (7)
C6—C7—H7	119.7	C9—N3—C10	122.3 (8)
C8—C7—H7	119.7	C9—N3—Fe1	125.4 (6)
C7—C8—C9	119.0 (9)	C10—N3—Fe1	112.3 (6)
C7—C8—C3	120.2 (8)	C13—N4—C11	121.5 (7)
C9—C8—C3	120.8 (7)	C13—N4—Fe1	125.1 (6)
N3—C9—C8	126.9 (8)	C11—N4—Fe1	113.4 (5)
N3—C9—H9	116.6	C19—O1—Fe1	128.4 (5)
C8—C9—H9	116.6	C3—O2—Fe1	128.5 (5)
C11—C10—N3	110.1 (8)	Fe1—O3—H1W	100 (6)
C11—C10—H10A	109.6	Fe1—O3—H2W	112 (6)
N3—C10—H10A	109.6	H1W—O3—H2W	118 (4)
C11—C10—H10B	109.6		

Symmetry code: (i) $-x, -y+2, -z$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H1*W*···O1^{ii}	0.81 (2)	2.09 (4)	2.859 (7)	159 (8)

O3—H2*W*···N2^{iii}	0.81 (2)	2.02 (2)	2.813 (9)	167 (7)

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