

## Retraction of articles

This article reports the retraction of articles published in *Acta Crystallographica Section E* between 2005 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            |
|---|--|--|--------------------|
| <i>Poly[diuaquadi-<math>\mu_3</math>-malonato-<math>\mu</math>-pyrazine-dinickel(II)] catena-Poly[[[diaqua(6-carboxypyridine-2-carboxylato)samarium(II)]-<math>\mu</math>-pyridine-2,6-dicarboxylato] tetrahydrate]</i> | Liu <i>et al.</i> (2005)<br>Liu <i>et al.</i> (2006) | 10.1107/S1600536805026358<br>10.1107/S1600536806038141 | GATWAA<br>FONCUH03 |
| <i>Poly[[[<math>\mu_4</math>-4,4'-carbonylbis(benzene-3,4-dicarboxylato)]tetrakis(1,10-phenanthroline)-dipalladium(II)] dihydrate]</i>  | Li, Wang, Zhang & Yu (2007e)                         | 10.1107/S1600536807039050                              | AFELAZ             |
| <i>Poly[diuaqua-<math>\mu_3</math>-malonato-<math>\mu</math>-pyrazine-diiron(II)]</i>   | Li, Liu <i>et al.</i> (2007)                         | 10.1107/S1600536807038743                              | AFELON             |
| <i>Poly[diuaqua-di-<math>\mu_3</math>-malonato-<math>\mu</math>-pyrazine-dimanganese(II)]</i>   | Li, Wang, Zhang & Yu (2007f)                         | 10.1107/S1600536807039773                              | VIJZAO             |
| <i>Poly[[aqua(2,2-bipyridine)(<math>\mu_3</math>-pyridine-3,4-dicarboxylato)cobalt(II)] monohydrate]</i>  | Li, Wang, Zhang & Yu (2007g)                         | 10.1107/S1600536807040275                              | VIKIC              |
| <i>catena-Poly[[[diaqua(6-carboxypyridine-2-carboxylato)holmium(III)]-<math>\mu</math>-pyridine-2,6-dicarboxylato] tetrahydrate]</i>  | Li, Wang, Zhang & Yu (2007a)                         | 10.1107/S1600536807041657                              | DILGEL             |
| <i>catena-Poly[[[2,2'-bipyridine-<math>\kappa^2</math>N,N']iron(II)]-<math>\mu</math>-5-carboxy-4-carboxylatoimidazol-1-ido-<math>\kappa^4</math>N<sup>3</sup>,O<sup>4</sup>:N<sup>1</sup>,O<sup>2</sup>]</i>           | Li, Wang, Zhang & Yu (2007h)                         | 10.1107/S1600536807042122                              | XIKWAO             |
| <i>Poly[[aqua(2,2'-bipyridine)(<math>\mu_3</math>-pyridine-3,4-dicarboxylato)nickel(II)] monohydrate]</i>   | Li, Wang, Zhang & Yu (2007b)                         | 10.1107/S1600536807046466                              | LEVZAO01           |
| <i>2-(Benzyliminomethyl)-6-methoxyphenol</i>  | Li, Wang, Zhang & Yu (2007i)                         | 10.1107/S1600536807042134                              | SILDEX             |
| <i>Poly[aqua(2,2'-bipyridine)(<math>\mu_3</math>-pyridine-2,4-dicarboxylato)palladium(II)]</i>  | Li, Wang, Zhang & Yu (2007c)                         | 10.1107/S1600536807047575                              | SILXAN             |
| <i><math>\mu</math>-Oxido-bis[chlorido[tris(2-pyridylmethyl)amine]iron(III)] bis(hexafluoridophosphate)</i>   | Liu, Dou, Li & Zhang (2007)                          | 10.1107/S1600536807049665                              | TINRIS             |
| <i><math>\mu</math>-Oxido-bis[(4,4'-dibromo-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato)-manganese(III)]</i>   | Liu, Dou, Niu & Zhang (2007a)                        | 10.1107/S1600536807051008                              | GIMZAE             |
| <i>Bis[N-(8-quinolyl)pyridine-2-carboxamidato]iron(III) perchlorate monohydrate</i>   | Li, Wang, Zhang & Yu (2007d)                         | 10.1107/S1600536807048556                              | WIMZIC             |
| <i><math>\mu</math>-Oxido-bis[(4,4'-dibromo-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato)-chromium(III)]</i>  | Liu, Dou, Niu & Zhang (2007b)                        | 10.1107/S1600536807057996                              | HIOFIX             |
| <i><math>\mu</math>-Oxido-bis[chlorido[tris(2-pyridylmethyl)amine]chromium(III)] bis(hexafluoridophosphate)</i>   | Li, Wang <i>et al.</i> (2008)                        | 10.1107/S1600536807061296                              | MIRNAD             |
| <i><math>\mu</math>-Oxido-bis[(4,4'-dibromo-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato)-iron(III)]</i>  | Meng <i>et al.</i> (2008a)                           | 10.1107/S1600536807063143                              | MIRWUG             |
| <i>catena-Poly[[bis(1H-benzimidazole-<math>\kappa</math>N<sup>3</sup>)palladium(II)]-<math>\mu</math>-benzene-1,4-dicarboxylato-<math>\kappa^2</math>O<sup>1</sup>:O<sup>2</sup>]</i>                                   | Meng <i>et al.</i> (2008b)                           | 10.1107/S1600536807065051                              | XISCAE             |
| <i>Oxalato-bis(propene-1,3-diamine)manganese(II) chloride monohydrate</i>   | Meng <i>et al.</i> (2008e)                           | 10.1107/S1600536807065361                              | SISWIB             |
| <i><math>\mu</math>-Oxido-bis[chlorido[tris(2-pyridylmethyl)amine]manganese(III)] bis(hexafluoridophosphate)</i>  | Meng <i>et al.</i> (2008c)                           | 10.1107/S1600536807066512                              | RISRIV             |
| <i>Bis[N-(8-quinolyl)pyridine-2-carboxamidato-<math>\kappa^3</math>N,N',N''manganese(III) perchlorate monohydrate</i>   | Meng <i>et al.</i> (2008d)                           | 10.1107/S1600536808000287                              | GISLEA             |
| <i>Diaquabis(pyridine-2-carboxylato-<math>\kappa^2</math>N,O)cobalt(II)</i>   | Huang (2008)   | 10.1107/S1600536808010507                              | WIZPOL             |
| <i>Tetra-<math>\mu</math>-2,5-difluorobenzoato-bis[(2,2'-bipyridine)(2,5-difluorobenzoato)gadolinium(III)]</i>  | Li, Zhang <i>et al.</i> (2008)                       | 10.1107/S1600536808023507                              | BOFQIX             |
| <i>catena-Poly[[[2,2'-bipyridine-<math>\kappa^2</math>N,N']nickel(II)]-<math>\mu</math>-oxalato-<math>\kappa^4</math>O<sup>1</sup>,O<sup>2</sup>:O<sup>1</sup>,O<sup>2</sup>]</i>                                       | Li, Yan <i>et al.</i> (2008)                         | 10.1107/S1600536808028389                              | NOHYUF             |
| <i>catena-Poly[[aqua(2,2'-bipyridyl)cobalt(II)]-<math>\mu</math>-5-nitrosophthalalato]</i>  | Liu <i>et al.</i> (2008)                             | 10.1107/S1600536808038178                              | AFIREN             |
| <i>Diaquabis(pyridine-2-carboxylato-<math>\kappa^2</math>N,O)iron(II)</i>   | Xia & Sun (2009)                                     | 10.1107/S1600536809005765                              | RONFEG             |
| <i>catena-Poly[[[diaquathulium(III)]-<math>\mu</math>-6-carboxynicotinato-<math>\mu</math>-pyridine-2,5-dicarboxylato] dihydrate]</i>   | Li <i>et al.</i> (2009)                              | 10.1107/S1600536809008836                              | NOQNIR             |
| <i>1-Phenyl-3-(2,4,6-trimethoxyphenyl)prop-2-en-1-one</i>   | Liu <i>et al.</i> (2009)                             | 10.1107/S1600536809040227                              | PUGLOT             |

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## $\mu$ -Oxido-bis({4,4'-dibromo-2,2'-ethane-1,2-diylbis(nitrilomethylidene)}-diphenolato}iron(III))

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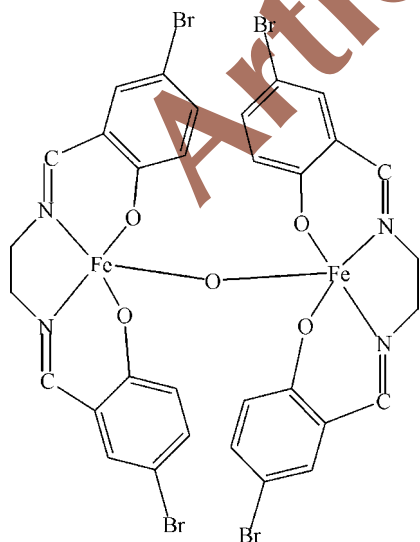
Received 8 November 2007; accepted 25 November 2007

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.008$  Å;  $R$  factor = 0.059;  $wR$  factor = 0.147; data-to-parameter ratio = 14.9.

In the title compound,  $[\text{Fe}_2(\text{C}_{16}\text{H}_{12}\text{Br}_2\text{N}_2\text{O}_2)_2\text{O}]$ , the complete molecule is generated by twofold symmetry, with the bridging O atom, which links the iron centres, lying on the rotation axis. The Fe(III) ion is chelated by the  $N,N,O,O$ -tetradentate Schiff base dianion, resulting in an  $\text{FeN}_2\text{O}_3$  square-based pyramid, with the two N atoms in the basal plane.

### Related literature

For related literature, see: Karacan & Somer (2004); Chen *et al.* (2006).



### Experimental

#### Crystal data

|  |                                   |
|--|-----------------------------------|
| $[\text{Fe}_2(\text{C}_{16}\text{H}_{12}\text{Br}_2\text{N}_2\text{O}_2)_2\text{O}]$ | $V = 3486.3$ (7) Å <sup>3</sup>   |
| $M_r = 975.89$   | $Z = 4$                           |
| Orthorhombic, $Pcca$   | Mo $K\alpha$ radiation            |
| $a = 21.094$ (2) Å   | $\mu = 5.46$ mm <sup>-1</sup>     |
| $b = 13.8168$ (18) Å   | $T = 293$ (2) K                   |
| $c = 11.9619$ (12) Å   | $0.43 \times 0.28 \times 0.22$ mm |

#### Data collection

|  |  |
|--|--|
| Bruker APEXII CCD diffractometer                         | 11548 measured reflections             |
| Absorption correction: multi-scan (SADABS; Bruker, 2001) | 3182 independent reflections           |
| $T_{\min} = 0.202$ , $T_{\max} = 0.380$                  | 2257 reflections with $I > 2\sigma(I)$ |
| (expected range = 0.160–0.301)                           | $R_{\text{int}} = 0.049$               |

#### Refinement

|                                 |   |
|---------------------------------|---|
| $R[F^2 > 2\sigma(F^2)] = 0.059$ | 213 parameters                                |
| $wR(F^2) = 0.147$               | H atom parameters constrained                 |
| $S = 1.00$                      | $\Delta\rho_{\max} = 1.05$ e Å <sup>-3</sup>  |
| 3182 reflections                | $\Delta\rho_{\min} = -0.70$ e Å <sup>-3</sup> |

**Table 1**

Selected geometric parameters (Å, °).

|                          |             |        |           |
|--------------------------|-------------|--------|-----------|
| Fe1—O3                   | 1.8162 (18) | Fe1—N2 | 2.116 (4) |
| Fe1—O2                   | 1.926 (4)   | Fe1—N1 | 2.141 (4) |
| Fe1—O1                   | 1.930 (4)   |        |           |
| Fe1 <sup>i</sup> —O3—Fe1 | 139.4 (3)   |        |           |

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); 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: HB2647).

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## supporting information

*Acta Cryst.* (2008). E64, m63 [https://doi.org/10.1107/S1600536807063143]

**$\mu$ -Oxido-bis({4,4'-dibromo-2,2'-ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}iron(III))**

**Qingguo Meng, Lintong Wang, Yanzhen Liu and Yan Pang**

### S1. Comment

Recently, Schiff base ligands, especially flexible symmetrical or unsymmetrical Schiff base ligands and their hydrogenated derivatives have been widely employed to assembly alkoxo- or phenoxo-bridged manganese clusters and polymers with novel topological structures and interesting magnetic, catalysis and photochemical properties. (Karacan & Somer, 2004; Chen *et al.*, 2006). In this paper, we report the structure of the title compound, (I).

As shown in Fig. 1, the Fe(III) ion in (I) is chelated by the dianionic Schiff base ligand in a tetradentate N,N,O,O coordination in an approximately square planar arrangement. An oxo ligand (site symmetry 2) caps the FeN<sub>2</sub>O<sub>2</sub> grouping to result in a square based pyramid. The oxo ligand also bridges to a second, crystallographically generated Fe atom. The Fe—O capping distance is much shorter than the other bonds (Table 1). The Fe $\cdots$ Fe<sup>i</sup> (i = -x, y, 1/2 - z) distance is 3.4066 (12) Å.

### S2. Experimental

A mixture of iron(III) chloride (1 mmol) and N,N'-bis(2-hydroxy-5-bromobenzyl)ethylenediamine (1 mmol) in 20 ml methanol was refluxed for two hours. The above cooled solution was filtered and the filtrate was evaporated naturally at room temperature. Two days later, brown blocks of (I) were obtained with a yield of 32%. Anal. Calc. for C<sub>32</sub>H<sub>24</sub>Br<sub>4</sub>Fe<sub>2</sub>N<sub>4</sub>O<sub>5</sub>: C 39.34, H 2.46, N 5.74%; Found: C 39.32, H 2.48, N 5.69%.

### S3. Refinement

The H atoms were included in calculated positions (C—H = 0.93–0.97 Å) and refined as riding with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{methyl C})$ .

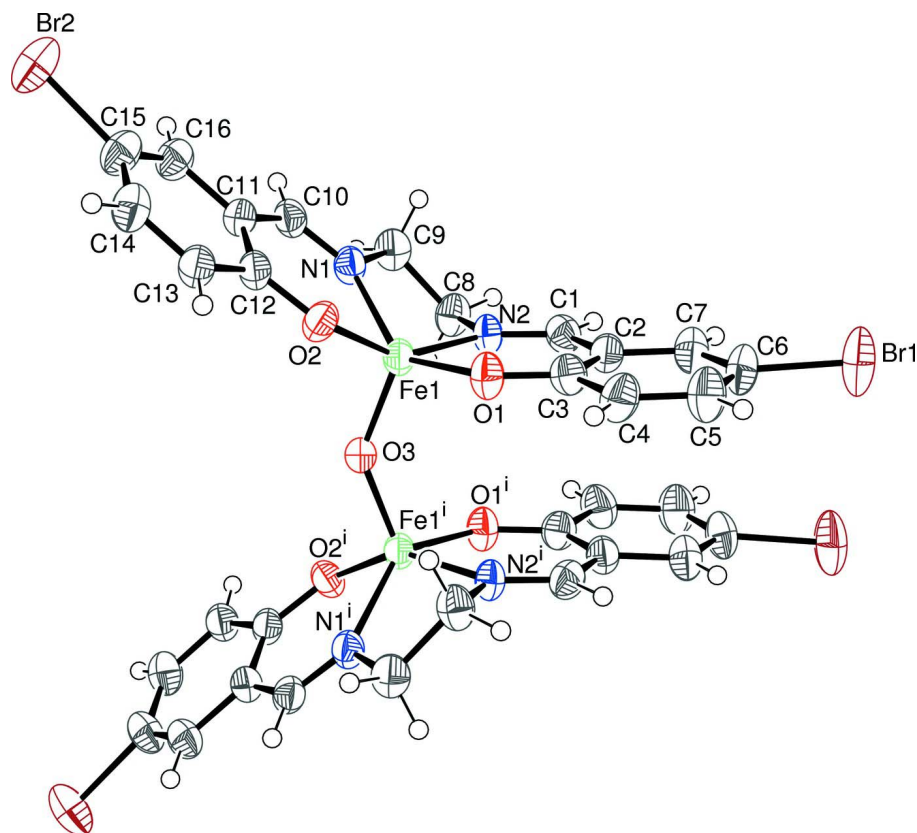


Figure 1

The molecular structure of (I), drawn with 50% probability displacement ellipsoids for the non-hydrogen atoms. Symmetry code: (i)  $-x, y, 1/2 - z$ .

**$\mu$ -Oxido-bis({4,4'-dibromo-2,2'-ethane-1,2-diylnitrilomethylidene}diphenolato)iron(III))**

*Crystal data*

[Fe<sub>2</sub>(C<sub>16</sub>H<sub>12</sub>Br<sub>2</sub>N<sub>2</sub>O<sub>2</sub>)<sub>2</sub>O]

$M_r = 975.89$

Orthorhombic, *Pcca*

Hall symbol:  $-P\ 2a\ 2ac$

$a = 21.094\ (2)\ \text{\AA}$

$b = 13.8168\ (18)\ \text{\AA}$

$c = 11.9619\ (12)\ \text{\AA}$

$V = 3486.3\ (7)\ \text{\AA}^3$

$Z = 4$

$F(000) = 1904$

$D_x = 1.859\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3182 reflections

$\theta = 3.0\text{--}25.4^\circ$

$\mu = 5.46\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Block, brown

$0.43 \times 0.28 \times 0.22\ \text{mm}$

*Data collection*

Bruker APEX II CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2001)

$T_{\min} = 0.202, T_{\max} = 0.380$

11548 measured reflections

3182 independent reflections

2257 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.049$

$\theta_{\max} = 25.4^\circ, \theta_{\min} = 3.0^\circ$

$h = -25 \rightarrow 25$

$k = -16 \rightarrow 16$

$l = 0 \rightarrow 14$

*Refinement*Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.059$  $wR(F^2) = 0.147$  $S = 1.00$ 

3182 reflections

213 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methodsSecondary atom site location: difference Fourier  
mapHydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.077P)^2]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} = 0.018$  $\Delta\rho_{\max} = 1.05 \text{ e } \text{\AA}^{-3}$  $\Delta\rho_{\min} = -0.70 \text{ e } \text{\AA}^{-3}$ *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 ( $\text{\AA}^2$ )*

|     | <i>x</i>    | <i>y</i>     | <i>z</i>    | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|--------------|-------------|----------------------------------|
| Fe1 | 0.07194 (4) | 0.12987 (5)  | 0.31467 (6) | 0.0342 (2)                       |
| Br1 | 0.10796 (4) | 0.66034 (5)  | 0.24478 (7) | 0.0776 (3)                       |
| Br2 | 0.28253 (3) | -0.28115 (5) | 0.48690 (6) | 0.0663 (3)                       |
| C1  | 0.0405 (3)  | 0.3280 (4)   | 0.4134 (4)  | 0.0404 (13)                      |
| H1  | 0.0230      | 0.3670       | 0.4687      | 0.048*                           |
| C2  | 0.0734 (3)  | 0.3750 (4)   | 0.3197 (5)  | 0.0392 (12)                      |
| C3  | 0.1029 (3)  | 0.3259 (4)   | 0.2294 (5)  | 0.0405 (13)                      |
| C4  | 0.1303 (3)  | 0.3799 (4)   | 0.1413 (5)  | 0.0514 (15)                      |
| H4  | 0.1477      | 0.3477       | 0.0803      | 0.062*                           |
| C5  | 0.1316 (3)  | 0.4776 (4)   | 0.1447 (6)  | 0.0574 (17)                      |
| H5  | 0.1504      | 0.5126       | 0.0872      | 0.069*                           |
| C6  | 0.1039 (3)  | 0.5260 (4)   | 0.2367 (5)  | 0.0519 (16)                      |
| C7  | 0.0744 (3)  | 0.4748 (4)   | 0.3235 (5)  | 0.0476 (14)                      |
| H7  | 0.0557      | 0.5077       | 0.3829      | 0.057*                           |
| C8  | 0.0009 (3)  | 0.1958 (4)   | 0.5204 (5)  | 0.0432 (14)                      |
| H8A | -0.0382     | 0.1650       | 0.4970      | 0.052*                           |
| H8B | -0.0091     | 0.2462       | 0.5741      | 0.052*                           |
| C9  | 0.0461 (3)  | 0.1213 (4)   | 0.5721 (4)  | 0.0423 (13)                      |
| H9A | 0.0765      | 0.1534       | 0.6202      | 0.051*                           |
| H9B | 0.0224      | 0.0751       | 0.6166      | 0.051*                           |
| C10 | 0.1146 (3)  | -0.0002 (4)  | 0.5091 (4)  | 0.0385 (13)                      |
| H10 | 0.1140      | -0.0181      | 0.5840      | 0.046*                           |
| C11 | 0.1561 (3)  | -0.0556 (4)  | 0.4331 (4)  | 0.0370 (12)                      |
| C12 | 0.1643 (3)  | -0.0340 (3)  | 0.3168 (4)  | 0.0356 (11)                      |
| C13 | 0.2041 (3)  | -0.0949 (4)  | 0.2516 (5)  | 0.0410 (13)                      |

|     |              |             |            |             |
|-----|--------------|-------------|------------|-------------|
| H13 | 0.2075       | -0.0849     | 0.1749     | 0.049*      |
| C14 | 0.2370 (3)   | -0.1675 (4) | 0.3005 (5) | 0.0474 (14) |
| H14 | 0.2640       | -0.2058     | 0.2576     | 0.057*      |
| C15 | 0.2308 (3)   | -0.1858 (4) | 0.4169 (5) | 0.0463 (14) |
| C16 | 0.1901 (3)   | -0.1313 (4) | 0.4831 (5) | 0.0428 (14) |
| H16 | 0.1856       | -0.1448     | 0.5589     | 0.051*      |
| N1  | 0.0797 (2)   | 0.0703 (3)  | 0.4793 (4) | 0.0363 (10) |
| N2  | 0.0348 (2)   | 0.2370 (3)  | 0.4227 (4) | 0.0360 (10) |
| O1  | 0.10571 (18) | 0.2321 (3)  | 0.2223 (3) | 0.0435 (9)  |
| O2  | 0.13721 (19) | 0.0409 (3)  | 0.2686 (3) | 0.0414 (9)  |
| O3  | 0.0000       | 0.0842 (4)  | 0.2500     | 0.0388 (12) |

*Atomic displacement parameters (Å<sup>2</sup>)*

|     | $U^{11}$   | $U^{22}$   | $U^{33}$    | $U^{12}$     | $U^{13}$     | $U^{23}$     |
|-----|------------|------------|-------------|--------------|--------------|--------------|
| Fe1 | 0.0433 (5) | 0.0267 (4) | 0.0327 (4)  | 0.0006 (3)   | 0.0003 (3)   | -0.0002 (3)  |
| Br1 | 0.1084 (7) | 0.0293 (4) | 0.0950 (6)  | -0.0024 (3)  | 0.0277 (5)   | 0.0093 (4)   |
| Br2 | 0.0660 (5) | 0.0586 (5) | 0.0744 (5)  | 0.0225 (3)   | 0.0087 (4)   | 0.0251 (4)   |
| C1  | 0.044 (3)  | 0.036 (3)  | 0.041 (3)   | 0.001 (2)    | 0.001 (3)    | -0.007 (2)   |
| C2  | 0.042 (3)  | 0.031 (3)  | 0.045 (3)   | 0.000 (2)    | -0.001 (3)   | 0.002 (2)    |
| C3  | 0.042 (3)  | 0.037 (3)  | 0.043 (3)   | -0.003 (2)   | 0.003 (3)    | 0.001 (3)    |
| C4  | 0.062 (4)  | 0.042 (3)  | 0.050 (3)   | 0.001 (3)    | 0.007 (3)    | 0.011 (3)    |
| C5  | 0.067 (4)  | 0.040 (3)  | 0.066 (4)   | -0.007 (3)   | 0.013 (3)    | 0.009 (3)    |
| C6  | 0.064 (4)  | 0.029 (3)  | 0.064 (4)   | -0.004 (3)   | 0.005 (3)    | 0.012 (3)    |
| C7  | 0.051 (4)  | 0.032 (3)  | 0.060 (4)   | 0.001 (3)    | 0.004 (3)    | 0.002 (3)    |
| C8  | 0.050 (4)  | 0.038 (3)  | 0.042 (3)   | 0.001 (3)    | 0.011 (3)    | 0.004 (3)    |
| C9  | 0.052 (3)  | 0.041 (3)  | 0.034 (3)   | -0.001 (3)   | 0.010 (3)    | 0.001 (2)    |
| C10 | 0.051 (4)  | 0.030 (3)  | 0.035 (3)   | -0.006 (2)   | -0.001 (3)   | 0.001 (2)    |
| C11 | 0.041 (3)  | 0.030 (3)  | 0.041 (3)   | -0.001 (2)   | -0.003 (2)   | 0.003 (2)    |
| C12 | 0.043 (3)  | 0.027 (2)  | 0.037 (3)   | -0.001 (2)   | 0.001 (2)    | -0.001 (2)   |
| C13 | 0.049 (3)  | 0.034 (3)  | 0.041 (3)   | 0.003 (2)    | 0.001 (3)    | 0.001 (2)    |
| C14 | 0.048 (3)  | 0.038 (3)  | 0.057 (4)   | 0.005 (3)    | 0.008 (3)    | 0.002 (3)    |
| C15 | 0.044 (3)  | 0.043 (3)  | 0.052 (3)   | 0.003 (3)    | 0.005 (3)    | 0.016 (3)    |
| C16 | 0.047 (3)  | 0.038 (3)  | 0.043 (3)   | -0.001 (3)   | 0.002 (3)    | 0.010 (3)    |
| N1  | 0.045 (3)  | 0.029 (2)  | 0.035 (2)   | 0.0013 (19)  | 0.002 (2)    | -0.0019 (19) |
| N2  | 0.042 (3)  | 0.025 (2)  | 0.041 (2)   | -0.0042 (18) | 0.005 (2)    | 0.0019 (19)  |
| O1  | 0.055 (3)  | 0.030 (2)  | 0.045 (2)   | -0.0026 (17) | 0.0101 (19)  | 0.0019 (17)  |
| O2  | 0.056 (2)  | 0.034 (2)  | 0.0346 (18) | 0.0113 (17)  | -0.0020 (18) | 0.0024 (16)  |
| O3  | 0.045 (3)  | 0.028 (3)  | 0.043 (3)   | 0.000        | -0.009 (2)   | 0.000        |

*Geometric parameters (Å, °)*

|        |             |        |           |
|--------|-------------|--------|-----------|
| Fe1—O3 | 1.8162 (18) | C8—C9  | 1.533 (8) |
| Fe1—O2 | 1.926 (4)   | C8—H8A | 0.9700    |
| Fe1—O1 | 1.930 (4)   | C8—H8B | 0.9700    |
| Fe1—N2 | 2.116 (4)   | C9—N1  | 1.493 (7) |
| Fe1—N1 | 2.141 (4)   | C9—H9A | 0.9700    |
| Br1—C6 | 1.861 (6)   | C9—H9B | 0.9700    |

|           |             |                     |             |
|-----------|-------------|---------------------|-------------|
| Br2—C15   | 1.905 (6)   | C10—N1              | 1.272 (7)   |
| C1—N2     | 1.268 (6)   | C10—C11             | 1.474 (7)   |
| C1—C2     | 1.470 (7)   | C10—H10             | 0.9300      |
| C1—H1     | 0.9300      | C11—C16             | 1.404 (7)   |
| C2—C7     | 1.380 (7)   | C11—C12             | 1.434 (7)   |
| C2—C3     | 1.419 (8)   | C12—O2              | 1.314 (6)   |
| C3—O1     | 1.299 (6)   | C12—C13             | 1.422 (7)   |
| C3—C4     | 1.414 (8)   | C13—C14             | 1.354 (8)   |
| C4—C5     | 1.351 (8)   | C13—H13             | 0.9300      |
| C4—H4     | 0.9300      | C14—C15             | 1.421 (8)   |
| C5—C6     | 1.414 (9)   | C14—H14             | 0.9300      |
| C5—H5     | 0.9300      | C15—C16             | 1.388 (8)   |
| C6—C7     | 1.402 (8)   | C16—H16             | 0.9300      |
| C7—H7     | 0.9300      | O3—Fe1 <sup>i</sup> | 1.8162 (18) |
| C8—N2     | 1.483 (7)   |                     |             |
| O3—Fe1—O2 | 104.71 (16) | N1—C9—C8            | 108.2 (4)   |
| O3—Fe1—O1 | 108.58 (16) | N1—C9—H9A           | 110.1       |
| O2—Fe1—O1 | 92.29 (16)  | C8—C9—H9A           | 110.1       |
| O3—Fe1—N2 | 101.14 (16) | N1—C9—H9B           | 110.1       |
| O2—Fe1—N2 | 152.39 (17) | C8—C9—H9B           | 110.1       |
| O1—Fe1—N2 | 88.51 (16)  | H9A—C9—H9B          | 108.4       |
| O3—Fe1—N1 | 108.78 (15) | N1—C10—C11          | 124.6 (5)   |
| O2—Fe1—N1 | 87.89 (16)  | N1—C10—H10          | 117.7       |
| O1—Fe1—N1 | 141.27 (17) | C11—C10—H10         | 117.7       |
| N2—Fe1—N1 | 74.66 (16)  | C16—C11—C12         | 120.4 (5)   |
| N2—C1—C2  | 123.4 (5)   | C16—C11—C10         | 115.4 (5)   |
| N2—C1—H1  | 118.3       | C12—C11—C10         | 124.2 (5)   |
| C2—C1—H1  | 118.3       | O2—C12—C13          | 118.8 (4)   |
| C7—C2—C3  | 119.8 (5)   | O2—C12—C11          | 122.4 (5)   |
| C7—C2—C1  | 115.0 (5)   | C13—C12—C11         | 118.7 (5)   |
| C3—C2—C1  | 125.1 (5)   | C14—C13—C12         | 120.3 (5)   |
| O1—C3—C2  | 123.1 (5)   | C14—C13—H13         | 119.8       |
| O1—C3—C4  | 117.3 (5)   | C12—C13—H13         | 119.8       |
| C2—C3—C4  | 119.6 (5)   | C13—C14—C15         | 120.5 (5)   |
| C5—C4—C3  | 120.9 (6)   | C13—C14—H14         | 119.8       |
| C5—C4—H4  | 119.6       | C15—C14—H14         | 119.8       |
| C3—C4—H4  | 119.6       | C16—C15—C14         | 121.3 (5)   |
| C4—C5—C6  | 119.2 (6)   | C16—C15—Br2         | 118.6 (4)   |
| C4—C5—H5  | 120.4       | C14—C15—Br2         | 120.0 (4)   |
| C6—C5—H5  | 120.4       | C15—C16—C11         | 118.5 (5)   |
| C7—C6—C5  | 121.4 (5)   | C15—C16—H16         | 120.7       |
| C7—C6—Br1 | 119.0 (5)   | C11—C16—H16         | 120.7       |
| C5—C6—Br1 | 119.5 (4)   | C10—N1—C9           | 115.4 (4)   |
| C2—C7—C6  | 119.1 (6)   | C10—N1—Fe1          | 126.6 (4)   |
| C2—C7—H7  | 120.5       | C9—N1—Fe1           | 117.8 (3)   |
| C6—C7—H7  | 120.5       | C1—N2—C8            | 119.7 (5)   |
| N2—C8—C9  | 106.0 (4)   | C1—N2—Fe1           | 127.2 (4)   |



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|            |       |                          |           |
|------------|-------|--------------------------|-----------|
| N2—C8—H8A  | 110.5 | C8—N2—Fe1                | 113.0 (3) |
| C9—C8—H8A  | 110.5 | C3—O1—Fe1                | 132.5 (3) |
| N2—C8—H8B  | 110.5 | C12—O2—Fe1               | 133.4 (3) |
| C9—C8—H8B  | 110.5 | Fe1 <sup>i</sup> —O3—Fe1 | 139.4 (3) |
| H8A—C8—H8B | 108.7 |                          |           |

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Symmetry code: (i)  $-x, y, -z+1/2$ .

Article retracted