Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Di-$\mu$-hydroxido-bis[aqua(pyridine-2,6-dicarboxylato)iron(III)] monohydrate

**Hossein Eshtiagh-Hosseini,[a]* Nafiseh Alfi,[a] Masoud Mirzaei,[a] Philip Fanwick[b] and Phillip E. Fanwick[b]***

[a]Department of Chemistry, School of Sciences, Ferdowsi University of Mashhad, Mashhad, Iran, and [b]Department of Chemistry, Purdue University, W. Lafayette, IN 47907, USA
Correspondence e-mail: heshtiagh@um.ac.ir, pfanwick@purdue.edu

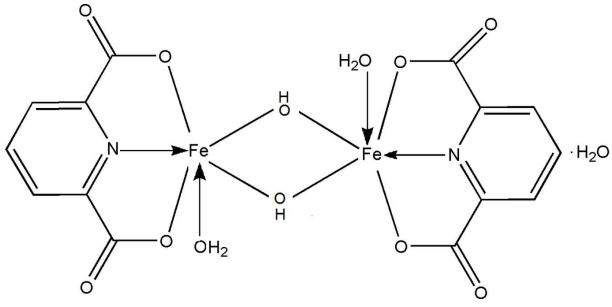
Received 5 September 2010; accepted 16 October 2010

Key indicators: single-crystal X-ray study; $T$ = 150 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.057; $wR$ factor = 0.153; data-to-parameter ratio = 9.1.

In the dinuclear title complex, $[Fe_2(OH)_2(C_7H_3NO_4)_2(H_2O)_2]\cdot H_2O$, the two Fe atoms are separated by 3.063 (1) Å. Intermolecular O—H···O hydrogen bonds form an extensive three-dimensional hydrogen-bonding network, which consolidates the crystal packing.

## Related literature

The crystal structure of the anhydrous form of the title dinuclear complex has been reported by Thich *et al.* (1976). For related structures, see: Aghabozorg *et al.* (2008); Eshtiagh-Hosseini *et al.* (2010).




## Experimental

### Crystal data

$[Fe_2(OH)_2(C_7H_3NO_4)_2(H_2O_2)_2]\cdot H_2O$
$M_r$ = 529.97
Monoclinic, $P2_1/c$
$a$ = 11.4786 (11) Å
$b$ = 21.7080 (16) Å
$c$ = 7.3291 (6) Å
$\beta$ = 90.099 (7)°
$V$ = 1826.2 (3) Å$^3$
$Z$ = 4
Cu $K\alpha$ radiation
$\mu$ = 13.53 mm$^{-1}$
$T$ = 150 K
0.20 × 0.20 × 0.14 mm

### Data collection

Rigaku Rapid II diffractometer
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
$T_{min}$ = 0.120, $T_{max}$ = 0.150
14275 measured reflections
2831 independent reflections
2695 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.048

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.153
$S$ = 1.07
2831 reflections
311 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.97 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.76 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···O1W | 0.70 (5) | 2.34 (5) | 2.966 (3) | 151 (5) |
| O2—H2···O1W$^{i}$ | 0.72 (5) | 2.28 (5) | 2.936 (3) | 151 (5) |
| O15—H151···O12$^{ii}$ | 0.83 (5) | 1.78 (5) | 2.611 (5) | 173 (5) |
| O15—H152···O14$^{iii}$ | 0.80 (4) | 1.79 (4) | 2.577 (4) | 171 (5) |
| O25—H251···O24$^{iv}$ | 0.78 (4) | 1.80 (4) | 2.577 (4) | 176 (5) |
| O25—H252···O22$^{v}$ | 0.71 (5) | 1.87 (5) | 2.576 (5) | 173 (6) |
| O1W—H1W1···O23$^{iii}$ | 0.87 (4) | 2.10 (4) | 2.962 (4) | 176 (4) |
| O1W—H1W2···O13$^{iii}$ | 0.87 (5) | 2.22 (4) | 3.072 (4) | 169 (4) |

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

Data collection: *CrystalClear* (Rigaku, 2001); cell refinement: *DENZO*/*SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO*/*SCALEPACK*; method used to solve structure: charge flipping (Oszlányi & Sütő, 2004) implemented in *PLATON* (Spek, 2009); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976) and *PLATON*; software used to prepare material for publication: *SHELXL97*.

Financial support as well as provision of X-ray facilities from the Ferdowsi University of Mashhad and Purdue University, W. Lafayette, are gratefully acknowledged by the authors.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2763).

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# supplementary materials

*Acta Cryst.* (2010). E**66**, m1450 [ **doi:10.1107/S1600536810041966** ]

# Di-$\mu$-hydroxido-bis[aqua(pyridine-2,6-dicarboxylato)iron(III)] monohydrate

**H. Eshtiagh-Hosseini, N. Alfi, M. Mirzaei, P. Fanwick and P. E. Fanwick**

## Comment

In continuation of our structural study of coordination compounds bearing different dicaroxylic acid and amine base fragments *via* proton transfer methodology (Aghabozorg *et al.*, 2008 and references therein; Eshtiagh-Hosseini *et al.* 2010), we present here the title compound, (**I**). The crystal structure of anhydrous form of **I** already has been reported by Thich *et al.* (1976); $[(pydc)H_2OFeOH]_2$ (**II**). The considerable feature of the title compound, is that the basic properties of $(pydc)^{2-}$ did not allow 5-bromo-6-methyl-2-(4-methylpiperazine-1-yl)pyrimidine-4-amine (bmpa) participitate in the crystalline network. The other interesting point is that two $Fe^{III}$ ions have different chemical environment making them non equivalent but with similar coordination geometry, that is, each $Fe^{III}$ ion is hexa-coordinated by one tridentate $(pydc)^{2-}$, two µ-hydroxo, and one coordinated water molecule (Fig. 1).

The above-mentioned complexes are very similar in terms of molecular structure but with different crystal structures. Both structures consist of $[(pydc)H_2OFe(OH)]_2$ dimeric units but the only difference between them is the peresence of a crystalline water molecule in the **I**.

In **I** (Fig. 1), all bond lengths and angles are normal and comparable with those observed in anhydrous form of the title dinuclear complex (Thich *et al.*, 1976). In the crystal structure, intermolecular O—H···O hydrogen bonds (Table 1) form an extensive three-dimensional hydrogen-bonding network, which consolidate the crystal packing. Indeed, firstly, covalent bonds cause to constructe dinuclear skeleton, and then the classical hydrogen bond interactions caused by O—H···O, lead to the self-aggregation process.

## Experimental

A solution of $FeCl_3.6H_2O$ was added to a mixture of $pydcH_2$ and bmpa in molar ratios of 1:2:2, respectively. The obtained solution was refluxed for 6 hrs in the 343 K. Suitable orange chunk $[(\mu\text{-}OH)_2Fe_2(pydc)_2(H_2O)_2].H_2O$ crystals for single crystal X-ray structure determination were obtained after slow evaporation of solvent in R.T.

## Refinement

C-bound H atoms were geometrically positioned (C—H 0.93 Å) and refined as riding, with $U_{iso}(H)=1.2U_{eq}(C)$. O-bound H atoms were located on a difference map and isotropically refined.

## Figures

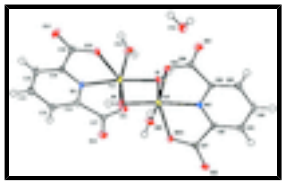

Fig. 1. The molecular structure of **I** showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

## Di-μ-hydroxido-bis[aqua(pyridine-2,6-dicarboxylato)iron(III)] monohydrate

### *Crystal data*

| | |
|---|---|
| $[Fe_2(OH)_2(C_7H_3NO_4)_2(H_2O_2)_2]\cdot H_2O$ | $F(000) = 1072$ |
| $M_r = 529.97$ | $D_x = 1.927$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Cu - $K\alpha$ radiation, $\lambda = 1.54184$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 2932 reflections |
| $a = 11.4786$ (11) Å | $\theta = 2$–$63°$ |
| $b = 21.7080$ (16) Å | $\mu = 13.53$ mm$^{-1}$ |
| $c = 7.3291$ (6) Å | $T = 150$ K |
| $\beta = 90.099$ (7)° | Chunk, orange |
| $V = 1826.2$ (3) Å$^3$ | 0.20 × 0.20 × 0.14 mm |
| $Z = 4$ | |

### *Data collection*

| | |
|---|---|
| Rigaku Rapid II diffractometer | 2695 reflections with $I > 2\sigma(I)$ |
| confocal optics | $R_{int} = 0.048$ |
| ω scans | $\theta_{max} = 63.3°$, $\theta_{min} = 2.0°$ |
| Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997) | $h = -11\rightarrow12$ |
| $T_{min} = 0.120$, $T_{max} = 0.150$ | $k = -25\rightarrow0$ |
| 14275 measured reflections | $l = 0\rightarrow8$ |
| 2831 independent reflections | |

### *Refinement*

| | |
|---|---|
| Refinement on $F^2$ | 0 restraints |
| Least-squares matrix: full | H atoms treated by a mixture of independent and constrained refinement |
| $R[F^2 > 2\sigma(F^2)] = 0.057$ | $w = 1/[\sigma^2(F_o^2) + (0.1304P)^2 + 0.6186P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.153$ | $(\Delta/\sigma)_{max} < 0.001$ |
| $S = 1.07$ | $\Delta\rho_{max} = 0.97$ e Å$^{-3}$ |
| 2831 reflections | $\Delta\rho_{min} = -0.76$ e Å$^{-3}$ |
| 311 parameters | |

*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**. Outlier data were removed using a local program based on the method of Prince and Nicholson [Prince, E. & Nicholson, W. L. (1983). *Acta Cryst.* A**39**, 407–410.]

Refinement on $F^2$ for ALL reflections except for 0 with very negative $F^2$ or flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating R_factor_obs *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 | 0.63100 (5) | 0.12044 (2) | 0.72067 (7) | 0.0080 (3) |
| Fe2 | 0.89320 (5) | 0.11910 (2) | 0.79919 (7) | 0.0082 (3) |
| O1 | 0.7813 (3) | 0.11982 (10) | 0.5976 (4) | 0.0131 (7) |
| O2 | 0.7419 (3) | 0.11662 (10) | 0.9247 (4) | 0.0111 (6) |
| O11 | 0.6011 (2) | 0.02831 (10) | 0.6877 (3) | 0.0135 (6) |
| O12 | 0.4819 (2) | −0.05113 (9) | 0.7494 (3) | 0.0161 (6) |
| O13 | 0.57708 (19) | 0.20747 (9) | 0.8073 (3) | 0.0115 (5) |
| O14 | 0.4320 (2) | 0.26115 (10) | 0.9362 (3) | 0.0186 (6) |
| O15 | 0.5550 (2) | 0.14072 (12) | 0.4813 (3) | 0.0159 (6) |
| O1W | 0.7628 (2) | 0.19217 (14) | 0.2554 (3) | 0.0220 (7) |
| O22 | 1.0531 (2) | −0.04764 (10) | 0.7153 (3) | 0.0163 (6) |
| O23 | 0.9419 (2) | 0.20979 (9) | 0.7383 (3) | 0.0133 (5) |
| O24 | 1.0833 (2) | 0.26950 (10) | 0.6214 (3) | 0.0191 (6) |
| O25 | 0.9767 (2) | 0.13003 (13) | 1.0362 (4) | 0.0150 (6) |
| O221 | 0.9281 (2) | 0.02666 (10) | 0.8040 (3) | 0.0118 (5) |
| N11 | 0.4717 (2) | 0.10535 (13) | 0.8448 (4) | 0.0076 (6) |
| N21 | 1.0478 (3) | 0.11096 (12) | 0.6582 (4) | 0.0091 (7) |
| C12 | 0.4279 (3) | 0.04863 (14) | 0.8479 (4) | 0.0109 (7) |
| C13 | 0.3222 (3) | 0.03599 (14) | 0.9274 (4) | 0.0123 (7) |
| C14 | 0.2600 (3) | 0.08500 (16) | 1.0037 (4) | 0.0164 (8) |
| C15 | 0.3062 (3) | 0.14464 (15) | 0.9951 (4) | 0.0154 (8) |
| C16 | 0.4128 (3) | 0.15301 (15) | 0.9138 (4) | 0.0111 (7) |
| C17 | 0.5088 (3) | 0.00355 (14) | 0.7540 (4) | 0.0110 (7) |
| C18 | 0.4780 (3) | 0.21304 (14) | 0.8853 (4) | 0.0116 (7) |
| C22 | 1.0924 (3) | 0.05521 (14) | 0.6318 (4) | 0.0100 (7) |
| C23 | 1.1952 (3) | 0.04648 (15) | 0.5364 (4) | 0.0131 (7) |
| C24 | 1.2517 (3) | 0.09854 (16) | 0.4704 (4) | 0.0156 (8) |
| C25 | 1.2059 (3) | 0.15709 (15) | 0.5038 (4) | 0.0149 (7) |
| C26 | 1.1027 (3) | 0.16140 (14) | 0.5996 (4) | 0.0100 (7) |

| | | | | |
|---|---|---|---|---|
| C27 | 1.0193 (3) | 0.00617 (14) | 0.7233 (4) | 0.0110 (7) |
| C28 | 1.0388 (3) | 0.21935 (14) | 0.6557 (4) | 0.0125 (7) |
| H1 | 0.799 (5) | 0.132 (2) | 0.514 (8) | 0.026 (14)* |
| H2 | 0.724 (5) | 0.132 (2) | 1.007 (8) | 0.032 (15)* |
| H13 | 0.2930 | −0.0039 | 0.9304 | 0.015* |
| H14 | 0.1886 | 0.0780 | 1.0597 | 0.020* |
| H15 | 0.2656 | 0.1779 | 1.0435 | 0.019* |
| H23 | 1.2253 | 0.0072 | 0.5172 | 0.016* |
| H24 | 1.3201 | 0.0944 | 0.4037 | 0.019* |
| H25 | 1.2440 | 0.1923 | 0.4627 | 0.018* |
| H151 | 0.539 (4) | 0.111 (2) | 0.414 (7) | 0.028 (12)* |
| H152 | 0.522 (4) | 0.173 (2) | 0.474 (6) | 0.041 (14)* |
| H1W1 | 0.817 (4) | 0.2200 (19) | 0.255 (6) | 0.025 (11)* |
| H1W2 | 0.704 (4) | 0.217 (2) | 0.262 (6) | 0.042 (15)* |
| H251 | 1.006 (4) | 0.161 (2) | 1.063 (6) | 0.039 (14)* |
| H252 | 0.973 (5) | 0.106 (2) | 1.101 (8) | 0.047* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Fe1 | 0.0075 (4) | 0.0056 (4) | 0.0109 (4) | 0.00088 (17) | 0.0042 (2) | −0.00093 (16) |
| Fe2 | 0.0078 (4) | 0.0058 (4) | 0.0108 (4) | −0.00005 (17) | 0.0047 (2) | 0.00054 (16) |
| O1 | 0.0074 (17) | 0.0223 (15) | 0.0096 (14) | −0.0017 (9) | 0.0030 (11) | 0.0039 (9) |
| O2 | 0.0066 (16) | 0.0154 (14) | 0.0114 (14) | 0.0015 (9) | 0.0032 (11) | −0.0035 (9) |
| O11 | 0.0179 (15) | 0.0068 (11) | 0.0158 (12) | 0.0024 (9) | 0.0035 (10) | −0.0009 (8) |
| O12 | 0.0242 (15) | 0.0072 (12) | 0.0170 (11) | −0.0010 (9) | −0.0031 (10) | −0.0016 (8) |
| O13 | 0.0120 (14) | 0.0062 (11) | 0.0164 (11) | −0.0011 (9) | 0.0047 (9) | −0.0019 (8) |
| O14 | 0.0146 (14) | 0.0089 (11) | 0.0323 (14) | 0.0016 (9) | 0.0049 (10) | −0.0058 (9) |
| O15 | 0.0231 (16) | 0.0076 (13) | 0.0169 (13) | 0.0073 (11) | −0.0031 (10) | −0.0043 (10) |
| O1W | 0.0215 (18) | 0.0158 (15) | 0.0288 (16) | −0.0023 (11) | 0.0084 (12) | −0.0012 (9) |
| O22 | 0.0270 (16) | 0.0077 (12) | 0.0141 (11) | 0.0037 (9) | 0.0041 (10) | 0.0003 (8) |
| O23 | 0.0142 (14) | 0.0062 (11) | 0.0195 (12) | 0.0031 (9) | 0.0070 (10) | 0.0022 (8) |
| O24 | 0.0188 (15) | 0.0076 (11) | 0.0309 (13) | −0.0019 (10) | 0.0039 (10) | 0.0052 (10) |
| O25 | 0.0210 (16) | 0.0102 (12) | 0.0138 (13) | −0.0068 (11) | 0.0003 (11) | 0.0020 (9) |
| O221 | 0.0129 (14) | 0.0061 (11) | 0.0164 (11) | −0.0010 (9) | 0.0046 (9) | −0.0012 (8) |
| N11 | 0.0020 (16) | 0.0097 (13) | 0.0111 (14) | 0.0001 (11) | 0.0014 (11) | −0.0024 (11) |
| N21 | 0.0082 (18) | 0.0089 (14) | 0.0103 (14) | −0.0002 (11) | 0.0013 (12) | 0.0023 (10) |
| C12 | 0.0107 (19) | 0.0116 (16) | 0.0104 (15) | −0.0015 (13) | −0.0023 (13) | −0.0011 (12) |
| C13 | 0.0108 (19) | 0.0107 (15) | 0.0155 (15) | −0.0052 (13) | −0.0020 (13) | 0.0038 (12) |
| C14 | 0.011 (2) | 0.0233 (18) | 0.0154 (16) | −0.0001 (14) | 0.0020 (13) | 0.0030 (13) |
| C15 | 0.016 (2) | 0.0147 (17) | 0.0157 (16) | 0.0010 (14) | 0.0053 (14) | −0.0016 (13) |
| C16 | 0.012 (2) | 0.0105 (16) | 0.0104 (15) | 0.0042 (13) | 0.0022 (13) | −0.0016 (12) |
| C17 | 0.0147 (19) | 0.0079 (16) | 0.0106 (13) | 0.0013 (13) | −0.0023 (13) | 0.0018 (12) |
| C18 | 0.011 (2) | 0.0104 (16) | 0.0135 (15) | −0.0002 (13) | 0.0005 (13) | −0.0014 (12) |
| C22 | 0.010 (2) | 0.0086 (15) | 0.0114 (15) | 0.0008 (13) | 0.0015 (12) | −0.0025 (12) |
| C23 | 0.014 (2) | 0.0128 (16) | 0.0123 (16) | 0.0013 (13) | −0.0007 (13) | −0.0026 (12) |
| C24 | 0.010 (2) | 0.0244 (18) | 0.0128 (15) | −0.0009 (15) | 0.0055 (13) | −0.0027 (14) |
| C25 | 0.015 (2) | 0.0134 (16) | 0.0163 (16) | −0.0044 (14) | 0.0041 (14) | 0.0026 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C26 | 0.0128 (19) | 0.0079 (15) | 0.0093 (14) | 0.0006 (13) | 0.0013 (13) | 0.0021 (12) |
| C27 | 0.015 (2) | 0.0106 (16) | 0.0078 (15) | 0.0011 (13) | 0.0004 (12) | 0.0014 (12) |
| C28 | 0.015 (2) | 0.0090 (16) | 0.0141 (15) | −0.0010 (13) | 0.0028 (14) | 0.0011 (12) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Fe1—O1 | 1.948 (3) | O25—H251 | 0.77 (5) |
| Fe1—O2 | 1.964 (3) | O25—H252 | 0.71 (5) |
| Fe1—O15 | 2.007 (2) | O221—C27 | 1.283 (4) |
| Fe1—O11 | 2.043 (2) | N11—C12 | 1.330 (4) |
| Fe1—N11 | 2.070 (3) | N11—C16 | 1.336 (4) |
| Fe1—O13 | 2.087 (2) | N21—C22 | 1.328 (4) |
| Fe2—O1 | 1.956 (3) | N21—C26 | 1.335 (4) |
| Fe2—O2 | 1.967 (3) | C12—C13 | 1.375 (5) |
| Fe2—O25 | 1.997 (3) | C12—C17 | 1.515 (4) |
| Fe2—O221 | 2.047 (2) | C13—C14 | 1.398 (5) |
| Fe2—N21 | 2.063 (3) | C13—H13 | 0.9300 |
| Fe2—O23 | 2.095 (2) | C14—C15 | 1.400 (5) |
| O1—H1 | 0.70 (5) | C14—H14 | 0.9300 |
| O2—H2 | 0.72 (5) | C15—C16 | 1.374 (5) |
| O11—C17 | 1.285 (4) | C15—H15 | 0.9300 |
| O12—C17 | 1.227 (4) | C16—C18 | 1.517 (4) |
| O13—C18 | 1.280 (4) | C22—C23 | 1.385 (5) |
| O14—C18 | 1.229 (4) | C22—C27 | 1.513 (4) |
| O15—H151 | 0.82 (5) | C23—C24 | 1.390 (5) |
| O15—H152 | 0.80 (5) | C23—H23 | 0.9300 |
| O1W—H1W1 | 0.87 (4) | C24—C25 | 1.397 (5) |
| O1W—H1W2 | 0.87 (5) | C24—H24 | 0.9300 |
| O22—C27 | 1.232 (4) | C25—C26 | 1.382 (5) |
| O23—C28 | 1.284 (4) | C25—H25 | 0.9300 |
| O24—C28 | 1.229 (4) | C26—C28 | 1.514 (4) |
| O1—Fe1—O2 | 77.23 (13) | C12—N11—Fe1 | 119.2 (2) |
| O1—Fe1—O15 | 88.89 (11) | C16—N11—Fe1 | 119.5 (2) |
| O2—Fe1—O15 | 162.77 (11) | C22—N21—C26 | 121.2 (3) |
| O1—Fe1—O11 | 94.99 (9) | C22—N21—Fe2 | 118.9 (2) |
| O2—Fe1—O11 | 99.04 (9) | C26—N21—Fe2 | 119.8 (2) |
| O15—Fe1—O11 | 92.22 (10) | N11—C12—C13 | 121.7 (3) |
| O1—Fe1—N11 | 170.43 (11) | N11—C12—C17 | 111.0 (3) |
| O2—Fe1—N11 | 103.34 (12) | C13—C12—C17 | 127.3 (3) |
| O15—Fe1—N11 | 92.06 (11) | C12—C13—C14 | 118.0 (3) |
| O11—Fe1—N11 | 75.46 (10) | C12—C13—H13 | 121.00 |
| O1—Fe1—O13 | 114.22 (9) | C14—C13—H13 | 121.00 |
| O2—Fe1—O13 | 89.93 (9) | C13—C14—C15 | 119.5 (3) |
| O15—Fe1—O13 | 86.48 (9) | C13—C14—H14 | 120.30 |
| O11—Fe1—O13 | 150.70 (9) | C15—C14—H14 | 120.30 |
| N11—Fe1—O13 | 75.34 (10) | C16—C15—C14 | 118.6 (3) |
| O1—Fe2—O2 | 76.95 (14) | C16—C15—H15 | 120.70 |
| O1—Fe2—O25 | 165.85 (12) | C14—C15—H15 | 120.70 |
| O2—Fe2—O25 | 91.08 (12) | N11—C16—C15 | 120.9 (3) |

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| O1—Fe2—O221 | 98.57 (9) | N11—C16—C18 | 111.3 (3) |
| O2—Fe2—O221 | 97.93 (9) | C15—C16—C18 | 127.8 (3) |
| O25—Fe2—O221 | 90.46 (10) | O12—C17—O11 | 127.0 (3) |
| O1—Fe2—N21 | 100.77 (12) | O12—C17—C12 | 118.9 (3) |
| O2—Fe2—N21 | 173.12 (11) | O11—C17—C12 | 114.1 (3) |
| O25—Fe2—N21 | 91.96 (11) | O14—C18—O13 | 126.8 (3) |
| O221—Fe2—N21 | 75.88 (10) | O14—C18—C16 | 118.4 (3) |
| O1—Fe2—O23 | 90.39 (10) | O13—C18—C16 | 114.8 (3) |
| O2—Fe2—O23 | 111.18 (9) | N21—C22—C23 | 121.8 (3) |
| O25—Fe2—O23 | 86.90 (10) | N21—C22—C27 | 111.2 (3) |
| O221—Fe2—O23 | 150.80 (10) | C23—C22—C27 | 126.9 (3) |
| N21—Fe2—O23 | 75.16 (10) | C22—C23—C24 | 117.5 (3) |
| Fe1—O1—Fe2 | 103.38 (14) | C22—C23—H23 | 121.20 |
| Fe1—O1—H1 | 132 (4) | C24—C23—H23 | 121.20 |
| Fe2—O1—H1 | 118 (4) | C23—C24—C25 | 120.2 (3) |
| Fe1—O2—Fe2 | 102.37 (13) | C23—C24—H24 | 119.90 |
| Fe1—O2—H2 | 116 (4) | C25—C24—H24 | 119.90 |
| Fe2—O2—H2 | 129 (4) | C26—C25—C24 | 118.3 (3) |
| C17—O11—Fe1 | 120.21 (19) | C26—C25—H25 | 120.90 |
| C18—O13—Fe1 | 119.0 (2) | C24—C25—H25 | 120.90 |
| Fe1—O15—H151 | 117 (3) | N21—C26—C25 | 120.9 (3) |
| Fe1—O15—H152 | 117 (3) | N21—C26—C28 | 111.4 (3) |
| H151—O15—H152 | 123 (5) | C25—C26—C28 | 127.7 (3) |
| H1W1—O1W—H1W2 | 97 (5) | O22—C27—O221 | 127.4 (3) |
| C28—O23—Fe2 | 118.9 (2) | O22—C27—C22 | 118.1 (3) |
| Fe2—O25—H251 | 122 (3) | O221—C27—C22 | 114.5 (3) |
| Fe2—O25—H252 | 118 (5) | O24—C28—O23 | 126.9 (3) |
| H251—O25—H252 | 120 (6) | O24—C28—C26 | 118.6 (3) |
| C27—O221—Fe2 | 119.46 (19) | O23—C28—C26 | 114.5 (3) |
| C12—N11—C16 | 121.3 (3) | | |
| O2—Fe1—O1—Fe2 | −2.02 (11) | O2—Fe2—N21—C26 | 157.8 (8) |
| O15—Fe1—O1—Fe2 | 167.69 (12) | O25—Fe2—N21—C26 | −86.0 (3) |
| O11—Fe1—O1—Fe2 | −100.17 (11) | O221—Fe2—N21—C26 | −176.0 (3) |
| N11—Fe1—O1—Fe2 | −96.5 (6) | O23—Fe2—N21—C26 | 0.3 (2) |
| O13—Fe1—O1—Fe2 | 82.06 (12) | C16—N11—C12—C13 | −2.2 (5) |
| O2—Fe2—O1—Fe1 | 2.02 (11) | Fe1—N11—C12—C13 | −179.6 (2) |
| O25—Fe2—O1—Fe1 | −30.9 (5) | C16—N11—C12—C17 | 177.4 (3) |
| O221—Fe2—O1—Fe1 | 98.23 (11) | Fe1—N11—C12—C17 | 0.1 (3) |
| N21—Fe2—O1—Fe1 | 175.38 (10) | N11—C12—C13—C14 | 0.9 (5) |
| O23—Fe2—O1—Fe1 | −109.66 (10) | C17—C12—C13—C14 | −178.7 (3) |
| O1—Fe1—O2—Fe2 | 2.00 (11) | C12—C13—C14—C15 | 0.6 (5) |
| O15—Fe1—O2—Fe2 | −35.1 (4) | C13—C14—C15—C16 | −1.0 (5) |
| O11—Fe1—O2—Fe2 | 95.11 (10) | C12—N11—C16—C15 | 1.9 (5) |
| N11—Fe1—O2—Fe2 | 172.19 (10) | Fe1—N11—C16—C15 | 179.2 (2) |
| O13—Fe1—O2—Fe2 | −112.90 (10) | C12—N11—C16—C18 | −177.1 (3) |
| O1—Fe2—O2—Fe1 | −1.99 (11) | Fe1—N11—C16—C18 | 0.3 (3) |
| O25—Fe2—O2—Fe1 | 170.38 (11) | C14—C15—C16—N11 | −0.2 (5) |
| O221—Fe2—O2—Fe1 | −99.01 (10) | C14—C15—C16—C18 | 178.5 (3) |
| N21—Fe2—O2—Fe1 | −73.4 (9) | Fe1—O11—C17—O12 | −177.6 (2) |

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| O23—Fe2—O2—Fe1 | 83.29 (12) | Fe1—O11—C17—C12 | 1.9 (3) |
| O1—Fe1—O11—C17 | 177.9 (2) | N11—C12—C17—O12 | 178.3 (3) |
| O2—Fe1—O11—C17 | 100.1 (2) | C13—C12—C17—O12 | −2.1 (5) |
| O15—Fe1—O11—C17 | −93.0 (2) | N11—C12—C17—O11 | −1.2 (4) |
| N11—Fe1—O11—C17 | −1.5 (2) | C13—C12—C17—O11 | 178.4 (3) |
| O13—Fe1—O11—C17 | −6.3 (3) | Fe1—O13—C18—O14 | −176.5 (3) |
| O1—Fe1—O13—C18 | 178.2 (2) | Fe1—O13—C18—C16 | 2.9 (3) |
| O2—Fe1—O13—C18 | −105.9 (2) | N11—C16—C18—O14 | 177.4 (3) |
| O15—Fe1—O13—C18 | 91.0 (2) | C15—C16—C18—O14 | −1.4 (5) |
| O11—Fe1—O13—C18 | 2.7 (3) | N11—C16—C18—O13 | −2.0 (4) |
| N11—Fe1—O13—C18 | −2.1 (2) | C15—C16—C18—O13 | 179.1 (3) |
| O1—Fe2—O23—C28 | −103.7 (2) | C26—N21—C22—C23 | −2.6 (5) |
| O2—Fe2—O23—C28 | −179.9 (2) | Fe2—N21—C22—C23 | 179.2 (2) |
| O25—Fe2—O23—C28 | 90.2 (2) | C26—N21—C22—C27 | 175.4 (3) |
| O221—Fe2—O23—C28 | 4.8 (3) | Fe2—N21—C22—C27 | −2.7 (4) |
| N21—Fe2—O23—C28 | −2.7 (2) | N21—C22—C23—C24 | 0.8 (5) |
| O1—Fe2—O221—C27 | 97.8 (2) | C27—C22—C23—C24 | −176.9 (3) |
| O2—Fe2—O221—C27 | 175.7 (2) | C22—C23—C24—C25 | 1.2 (5) |
| O25—Fe2—O221—C27 | −93.1 (2) | C23—C24—C25—C26 | −1.5 (5) |
| N21—Fe2—O221—C27 | −1.2 (2) | C22—N21—C26—C25 | 2.3 (5) |
| O23—Fe2—O221—C27 | −8.6 (3) | Fe2—N21—C26—C25 | −179.5 (2) |
| O1—Fe1—N11—C12 | −3.1 (8) | C22—N21—C26—C28 | −176.5 (3) |
| O2—Fe1—N11—C12 | −95.4 (2) | Fe2—N21—C26—C28 | 1.7 (4) |
| O15—Fe1—N11—C12 | 92.4 (2) | C24—C25—C26—N21 | −0.2 (5) |
| O11—Fe1—N11—C12 | 0.7 (2) | C24—C25—C26—C28 | 178.3 (3) |
| O13—Fe1—N11—C12 | 178.2 (3) | Fe2—O221—C27—O22 | 179.1 (2) |
| O1—Fe1—N11—C16 | 179.5 (6) | Fe2—O221—C27—C22 | 0.1 (3) |
| O2—Fe1—N11—C16 | 87.2 (2) | N21—C22—C27—O22 | −177.4 (3) |
| O15—Fe1—N11—C16 | −85.0 (2) | C23—C22—C27—O22 | 0.5 (5) |
| O11—Fe1—N11—C16 | −176.8 (3) | N21—C22—C27—O221 | 1.7 (4) |
| O13—Fe1—N11—C16 | 0.8 (2) | C23—C22—C27—O221 | 179.6 (3) |
| O1—Fe2—N21—C22 | −94.0 (2) | Fe2—O23—C28—O24 | −174.8 (3) |
| O2—Fe2—N21—C22 | −24.0 (10) | Fe2—O23—C28—C26 | 4.3 (3) |
| O25—Fe2—N21—C22 | 92.2 (3) | N21—C26—C28—O24 | 175.3 (3) |
| O221—Fe2—N21—C22 | 2.2 (2) | C25—C26—C28—O24 | −3.4 (5) |
| O23—Fe2—N21—C22 | 178.5 (3) | N21—C26—C28—O23 | −3.8 (4) |
| O1—Fe2—N21—C26 | 87.8 (3) | C25—C26—C28—O23 | 177.5 (3) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···O1W | 0.70 (5) | 2.34 (5) | 2.966 (3) | 151 (5) |
| O2—H2···O1W$^{i}$ | 0.72 (5) | 2.28 (5) | 2.936 (3) | 151 (5) |
| O15—H151···O12$^{ii}$ | 0.83 (5) | 1.78 (5) | 2.611 (5) | 173 (5) |
| O15—H152···O14$^{iii}$ | 0.80 (4) | 1.79 (4) | 2.577 (4) | 171 (5) |
| O25—H251···O24$^{iv}$ | 0.78 (4) | 1.80 (4) | 2.577 (4) | 176 (5) |
| O25—H252···O22$^{v}$ | 0.71 (5) | 1.87 (5) | 2.576 (5) | 173 (6) |
| O1W—H1W1···O23$^{iii}$ | 0.87 (4) | 2.10 (4) | 2.962 (4) | 176 (4) |

| | | | | |
|---|---|---|---|---|
| O1W—H1W2···O13$^{iii}$ | 0.87 (5) | 2.22 (4) | 3.072 (4) | 169 (4) |

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

**Fig. 1**