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μ-Aqua-bis(μ-4-methylbenzoato-κ²O:O′)bis[(4-methylbenzoato-κO)-(1,10-phenanthroline-κ²N,N′)iron(II)]

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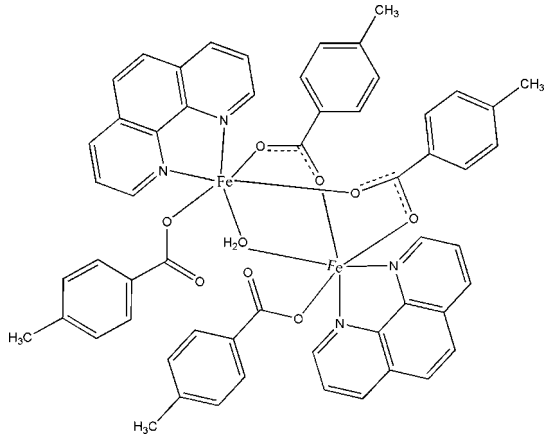
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.045; wR factor = 0.133; data-to-parameter ratio = 15.5.

In the title binuclear complex, $[Fe_2(C_8H_7O_2)_4(C_{12}H_8N_2)_2(H_2O)]$, the Fe^{II} ion is six-coordinated by three carboxylate O atoms from three 4-methylbenzoate ligands, two N atoms from two 1,10-phenanthroline ligands and one bridging aqua ligand in a distorted octahedral geometry. The coordinated water molecule acting as the bridging ligand is located on a twofold axes and the complex molecule displays C_2 molecular symmetry. The Fe···Fe separation in the binuclear complex is 3.490 (3) Å. The crystal structure is stabilized by hydrogen bonding and π–π stacking interactions [the centroid–centroid distance between adjacent 1,10-phenanthroline ring systems is 3.653 (2) Å, and that between the 1,10-phenanthroline ring system and the phenyl ring of the 4-methylbenzoate unit of a neighbouring complex is 3.622 (3) Å].

Related literature

For related literature, see: Song *et al.* (2007).



Experimental

Crystal data

$[Fe_2(C_8H_7O_2)_4(C_{12}H_8N_2)_2(H_2O)]$
M_r = 1030.67
Monoclinic, $C2/c$
a = 23.1987 (6) Å
b = 15.7222 (4) Å
c = 15.6464 (4) Å
β = 121.0170 (10)°
V = 4890.8 (2) Å³
Z = 4
Mo $K\alpha$ radiation
μ = 0.66 mm⁻¹
T = 296 (2) K
0.20 × 0.19 × 0.16 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.880, T_{max} = 0.902
31900 measured reflections
5066 independent reflections
3725 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.133
S = 1.05
5066 reflections
326 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.30 e Å⁻³
$\Delta\rho_{min}$ = −0.42 e Å⁻³

Table 1
Selected geometric parameters (Å, °).

Fe1—O3	2.1365 (18)	Fe1—N1	2.275 (2)
Fe1—O2^{i}	2.1369 (18)	Fe1—O1*W*	2.2970 (17)
Fe1—O1	2.1657 (18)	Fe1—N2	2.298 (2)
O3—Fe1—O2^{i}	93.91 (7)	O1—Fe1—O1*W*	83.73 (6)
O3—Fe1—O1	172.16 (8)	N1—Fe1—O1*W*	161.62 (6)
O2^{i}—Fe1—O1	89.79 (7)	O3—Fe1—N2	89.48 (8)
O3—Fe1—N1	100.73 (8)	O2^{i}—Fe1—N2	159.38 (8)
O2^{i}—Fe1—N1	86.60 (8)	O1—Fe1—N2	89.47 (7)
O1—Fe1—N1	86.37 (7)	N1—Fe1—N2	72.79 (8)
O3—Fe1—O1*W*	88.54 (6)	O1*W*—Fe1—N2	91.64 (7)
O2^{i}—Fe1—O1*W*	108.77 (7)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O4^{i}	0.938 (8)	1.80 (2)	2.578 (2)	138 (2)

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

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

The author acknowledges South China Normal University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2167).

References

Bruker (2004). *APEX2* and *SMART*. Bruker AXS Inc, Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Song, W.-D., Gu, C.-S., Hao, X.-M. & Liu, J.-W. (2007). *Acta Cryst.* E**63**, m1023–m1024.

supporting information

Acta Cryst. (2008). E**64**, m817–m818 [doi:10.1107/S1600536808014207]

μ-Aqua-bis(μ-4-methylbenzoato-κ^2O:O')bis[(4-methylbenzoato-κO)(1,10-phenanthroline-κ^2N,N')iron(II)]

Sun Feng

S1. Comment

In the structural investigation of 4-methylbenzoate complexes, it has been found that the 4-methylbenzoic acid functions as a multidentate ligand [Song *et al.* (2007)] with versatile binding and coordination modes. In this report, an iron(II) complex, (I) (Fig. 1) was obtained by the reaction of 4-methylbenzoic acid, 1,10-phenanthroline and ferrous chloride in alkaline aqueous solution.

A half of the binuclear complex is an asymmetric unit where Fe^{II} ion is in the distorted octahedral geometry with the six coordinating atoms: three carboxyl O atoms from two μ_2-bridging 4-methylbenzoate ligands and one 4-methylbenzoate ligand, two N atoms from one chelating 1,10-phenanthroline ligands, and one μ_2-bridging aqua ligand. The Fe···Fe separation is 3.490 (3) Å. The crystal packing is *via* O—H···O hydrogen bond (Table 1) and *via* two π-π stacking interactions (Fig. 2). The centroid to centroid distance between adjacent 1,10-phenanthroline rings (x, –y,-1/2 + z) is 3.653 (2) Å, whereas the centroid to centroid distance between 1,10-phenanthroline ring and phenyl ring of 4-methyl-benzoate of neighbouring complexes (1/2 - x, 1/2 - y, 1 - z) is 3.622 (3) Å.

S2. Experimental

A mixture of ferrous chloride (1 mmol), 4-methylbenzate (1 mmol), 1,10-phenanthroline (1 mmol), NaOH (1.5 mmol) and H_2O (12 mL) was placed in a 23 mL Teflon reactor, which was heated to 433 K for three days and then cooled to room temperature at a rate of 10 K h^{-1}. The crystals obtained were washed with water and dryed in air.

S3. Refinement

Carbon-bound H atoms were placed at calculated positions and were treated as riding on the parent C atoms with C—H = 0.93–0.97 Å, and with U_{iso}(H) = 1.2 U_{eq}(C). Water H atoms were tentatively located in difference Fourier maps and were refined with distance restraints of O–H = 0.82 Å, and with U_{iso}(H) = 1.5 U_{eq}(O).

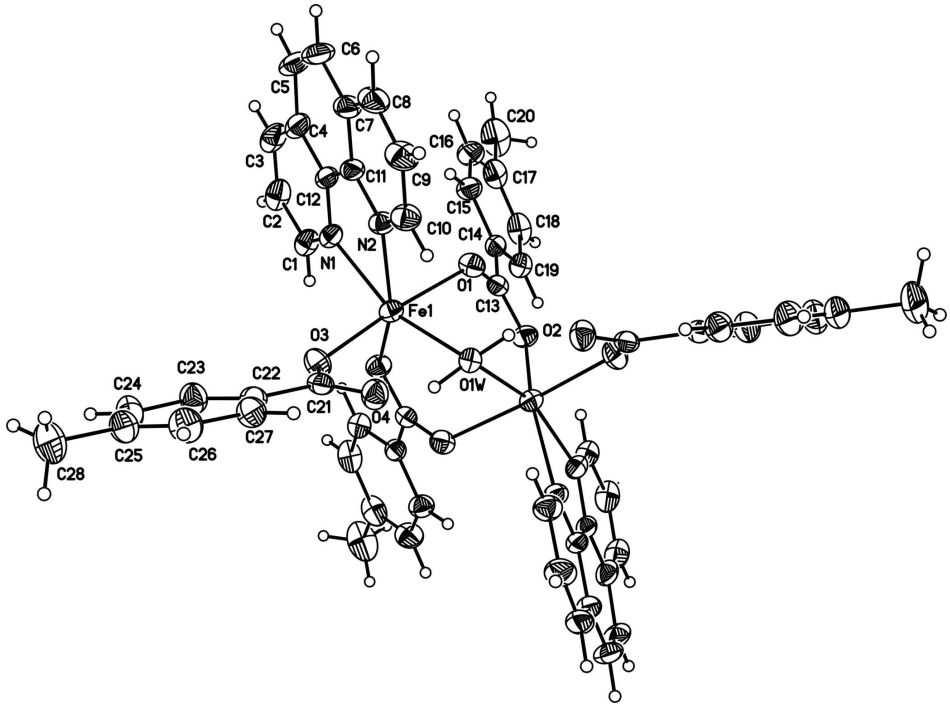


Figure 1

The structure of (I) showing the atomic numbering scheme. Non-H atoms are shown with the 30% probability displacement ellipsoids. Unlabelled atoms are related to the labelled atoms by the symmetry code (-*x*, *y*, 1/2 - *z*).

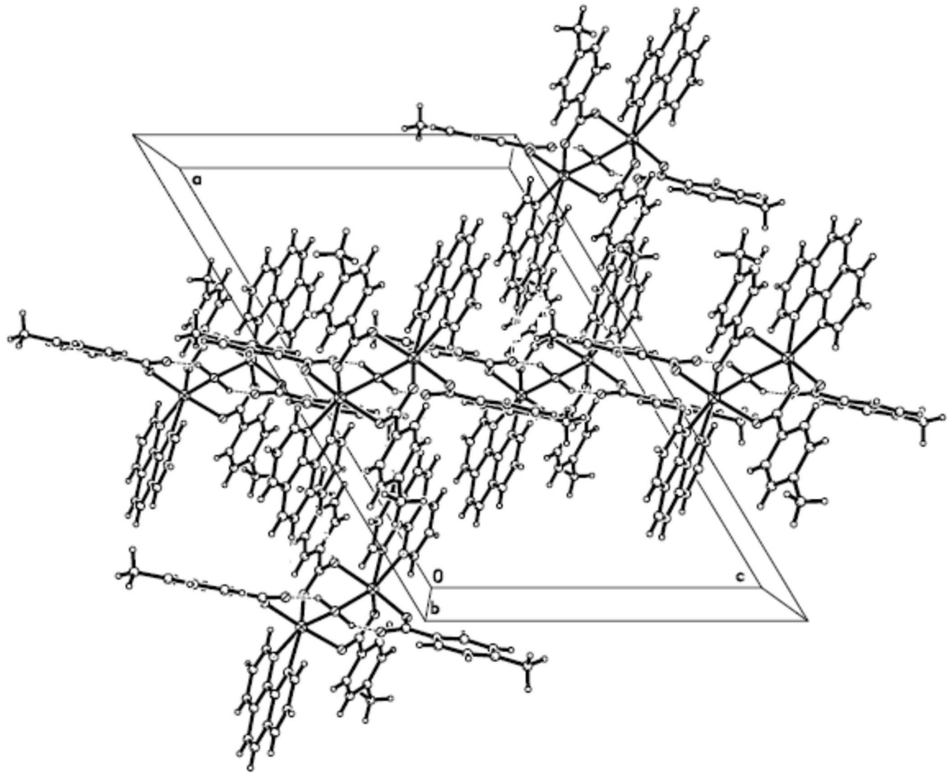


Figure 2

A packing view of the title compound.

μ-Aqua-bis(μ-4-methylbenzoato-κ²O:O′)bis[(4-methylbenzoato- κO)(1,10-phenanthroline-κ²N,N′)iron(II)]

Crystal data

$[Fe_2(C_8H_7O_2)_4(C_{12}H_8N_2)_2(H_2O)]$
$M_r = 1030.67$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 23.1987$ (6) Å
$b = 15.7222$ (4) Å
$c = 15.6464$ (4) Å
$\beta = 121.017$ (1)°
$V = 4890.8$ (2) Å^3
$Z = 4$
$F(000) = 2136$
$D_x = 1.400$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5300 reflections
$\theta = 1.3$–$28.0°$
$\mu = 0.66$ mm^{-1}
$T = 296$ K
Block, colourless
0.20 × 0.19 × 0.16 mm

Data collection

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.880$, $T_{max} = 0.902$
31900 measured reflections
5066 independent reflections
3725 reflections with $I > 2\sigma(I)$
$R_{int} = 0.053$
$\theta_{max} = 26.5°$, $\theta_{min} = 1.7°$
$h = -29 \rightarrow 29$
$k = -19 \rightarrow 19$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.133$
$S = 1.06$
5066 reflections
326 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0679P)^2 + 3.2244P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.041139 (18)	0.35596 (2)	0.37994 (3)	0.03908 (15)

C1	0.10393 (16)	0.51103 (18)	0.5379 (2)	0.0495 (7)
H1	0.0624	0.5365	0.4966	0.059*
C2	0.15332 (18)	0.5574 (2)	0.6182 (2)	0.0612 (9)
H2	0.1447	0.6126	0.6302	0.073*
C3	0.21397 (18)	0.5211 (2)	0.6784 (2)	0.0664 (10)
H3	0.2474	0.5515	0.7321	0.080*
C4	0.22666 (15)	0.4382 (2)	0.6603 (2)	0.0545 (8)
C5	0.28939 (16)	0.3946 (3)	0.7205 (2)	0.0717 (11)
H5	0.3250	0.4229	0.7738	0.086*
C6	0.29761 (16)	0.3135 (3)	0.7014 (2)	0.0691 (10)
H6	0.3389	0.2871	0.7417	0.083*
C7	0.24490 (14)	0.2671 (2)	0.6211 (2)	0.0543 (8)
C8	0.25042 (16)	0.1818 (2)	0.5991 (3)	0.0636 (9)
H8	0.2905	0.1524	0.6380	0.076*
C9	0.19760 (17)	0.1427 (2)	0.5217 (3)	0.0624 (9)
H9	0.2003	0.0855	0.5086	0.075*
C10	0.13890 (15)	0.18871 (19)	0.4614 (2)	0.0523 (7)
H10	0.1034	0.1616	0.4068	0.063*
C11	0.18322 (13)	0.30873 (18)	0.55822 (19)	0.0432 (6)
C12	0.17422 (13)	0.39593 (18)	0.57830 (19)	0.0414 (6)
C13	0.07480 (12)	0.46759 (16)	0.25133 (19)	0.0360 (6)
C14	0.11705 (13)	0.54627 (16)	0.28046 (19)	0.0384 (6)
C15	0.17772 (14)	0.54973 (19)	0.3703 (2)	0.0507 (7)
H15	0.1911	0.5041	0.4143	0.061*
C16	0.21825 (16)	0.6204 (2)	0.3949 (3)	0.0636 (9)
H16	0.2594	0.6209	0.4545	0.076*
C17	0.19931 (19)	0.6901 (2)	0.3334 (3)	0.0633 (9)
C18	0.13827 (19)	0.68755 (19)	0.2446 (3)	0.0609 (9)
H18	0.1245	0.7344	0.2023	0.073*
C19	0.09739 (15)	0.61659 (17)	0.2176 (2)	0.0462 (6)
H19	0.0567	0.6158	0.1572	0.055*
C20	0.2436 (2)	0.7685 (3)	0.3605 (4)	0.1012 (16)
H20A	0.2891	0.7538	0.4097	0.152*
H20B	0.2276	0.8114	0.3869	0.152*
H20C	0.2422	0.7900	0.3020	0.152*
C21	−0.03260 (13)	0.21381 (18)	0.4188 (2)	0.0419 (6)
C22	−0.04954 (13)	0.17394 (19)	0.4901 (2)	0.0441 (6)
C23	−0.05669 (16)	0.2209 (2)	0.5580 (2)	0.0582 (8)
H23	−0.0504	0.2795	0.5608	0.070*
C24	−0.07324 (18)	0.1821 (3)	0.6230 (3)	0.0715 (10)
H24	−0.0791	0.2152	0.6672	0.086*
C25	−0.08085 (18)	0.0948 (3)	0.6218 (3)	0.0680 (9)
C26	−0.07224 (18)	0.0482 (2)	0.5554 (3)	0.0677 (9)
H26	−0.0761	−0.0107	0.5550	0.081*
C27	−0.05788 (15)	0.08647 (19)	0.4887 (2)	0.0545 (8)
H27	−0.0538	0.0534	0.4428	0.065*
C28	−0.0974 (2)	0.0524 (3)	0.6938 (3)	0.1022 (15)
H28A	−0.0868	0.0904	0.7480	0.153*

H28B	−0.0714	0.0012	0.7194	0.153*
H28C	−0.1444	0.0387	0.6596	0.153*
N1	0.11349 (11)	0.43230 (14)	0.51775 (15)	0.0415 (5)
N2	0.13141 (10)	0.26953 (14)	0.47845 (16)	0.0411 (5)
O1	0.09509 (9)	0.40711 (12)	0.31245 (14)	0.0455 (5)
O2	0.02203 (9)	0.46592 (11)	0.16733 (14)	0.0449 (5)
O3	−0.01572 (10)	0.29140 (12)	0.43251 (15)	0.0517 (5)
O4	−0.03673 (11)	0.16889 (14)	0.35009 (15)	0.0555 (5)
O1W	0.0000	0.26095 (16)	0.2500	0.0398 (6)
H1W	0.0291 (12)	0.2479 (17)	0.227 (2)	0.060*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0366 (2)	0.0383 (2)	0.0366 (2)	0.00068 (15)	0.01482 (18)	0.00227 (16)
C1	0.0582 (18)	0.0447 (16)	0.0424 (15)	−0.0101 (14)	0.0236 (14)	−0.0025 (13)
C2	0.082 (2)	0.0510 (19)	0.0527 (18)	−0.0247 (17)	0.0359 (19)	−0.0115 (15)
C3	0.068 (2)	0.077 (2)	0.0430 (17)	−0.0399 (19)	0.0213 (17)	−0.0120 (17)
C4	0.0486 (17)	0.071 (2)	0.0358 (15)	−0.0213 (15)	0.0159 (14)	0.0032 (14)
C5	0.0423 (18)	0.105 (3)	0.0417 (18)	−0.0271 (19)	0.0026 (15)	0.0093 (19)
C6	0.0330 (16)	0.102 (3)	0.0511 (19)	−0.0008 (18)	0.0061 (15)	0.023 (2)
C7	0.0357 (15)	0.076 (2)	0.0480 (17)	0.0066 (14)	0.0190 (14)	0.0223 (15)
C8	0.0464 (18)	0.080 (2)	0.066 (2)	0.0248 (17)	0.0302 (18)	0.0348 (19)
C9	0.056 (2)	0.057 (2)	0.074 (2)	0.0179 (16)	0.0329 (19)	0.0174 (17)
C10	0.0472 (17)	0.0490 (17)	0.0554 (18)	0.0086 (13)	0.0226 (15)	0.0087 (14)
C11	0.0321 (13)	0.0574 (18)	0.0361 (14)	0.0012 (12)	0.0147 (12)	0.0144 (12)
C12	0.0354 (14)	0.0525 (16)	0.0314 (13)	−0.0105 (12)	0.0137 (12)	0.0046 (12)
C13	0.0333 (13)	0.0368 (14)	0.0404 (14)	−0.0016 (11)	0.0208 (12)	−0.0015 (11)
C14	0.0386 (14)	0.0401 (14)	0.0368 (14)	−0.0034 (11)	0.0197 (12)	−0.0051 (11)
C15	0.0429 (16)	0.0550 (18)	0.0469 (16)	−0.0032 (13)	0.0180 (14)	−0.0038 (14)
C16	0.0505 (19)	0.072 (2)	0.061 (2)	−0.0193 (17)	0.0235 (16)	−0.0280 (18)
C17	0.075 (2)	0.057 (2)	0.074 (2)	−0.0326 (17)	0.050 (2)	−0.0351 (18)
C18	0.093 (3)	0.0361 (16)	0.075 (2)	−0.0073 (16)	0.058 (2)	−0.0052 (15)
C19	0.0534 (17)	0.0385 (14)	0.0468 (16)	−0.0029 (13)	0.0259 (14)	−0.0041 (12)
C20	0.131 (4)	0.081 (3)	0.124 (4)	−0.067 (3)	0.089 (3)	−0.058 (3)
C21	0.0306 (13)	0.0470 (16)	0.0458 (15)	0.0021 (11)	0.0180 (12)	0.0079 (13)
C22	0.0338 (14)	0.0513 (16)	0.0443 (15)	−0.0009 (12)	0.0181 (13)	0.0071 (13)
C23	0.065 (2)	0.0578 (19)	0.0601 (19)	−0.0069 (16)	0.0380 (17)	0.0005 (16)
C24	0.079 (2)	0.087 (3)	0.066 (2)	−0.008 (2)	0.049 (2)	−0.0042 (19)
C25	0.065 (2)	0.085 (3)	0.061 (2)	−0.0109 (19)	0.0369 (18)	0.0139 (19)
C26	0.075 (2)	0.057 (2)	0.074 (2)	−0.0110 (17)	0.041 (2)	0.0135 (18)
C27	0.0579 (19)	0.0508 (18)	0.0568 (18)	−0.0047 (14)	0.0311 (16)	0.0045 (14)
C28	0.109 (3)	0.126 (4)	0.093 (3)	−0.022 (3)	0.068 (3)	0.025 (3)
N1	0.0429 (13)	0.0426 (13)	0.0329 (11)	−0.0052 (10)	0.0152 (10)	0.0019 (10)
N2	0.0356 (12)	0.0418 (12)	0.0402 (12)	0.0033 (10)	0.0155 (10)	0.0072 (10)
O1	0.0432 (11)	0.0407 (11)	0.0543 (12)	0.0012 (8)	0.0263 (9)	0.0097 (9)
O2	0.0400 (10)	0.0427 (11)	0.0442 (11)	−0.0085 (8)	0.0162 (9)	−0.0041 (8)
O3	0.0583 (12)	0.0442 (11)	0.0649 (13)	−0.0038 (9)	0.0406 (11)	0.0047 (9)

O4	0.0634 (13)	0.0565 (12)	0.0519 (12)	−0.0118 (10)	0.0334 (11)	−0.0035 (10)
O1W	0.0425 (15)	0.0403 (14)	0.0374 (14)	0.000	0.0211 (12)	0.000

Geometric parameters (Å, º)

Fe1—O3	2.1365 (18)	C14—C19	1.391 (4)
Fe1—O2^{i}	2.1369 (18)	C15—C16	1.376 (4)
Fe1—O1	2.1657 (18)	C15—H15	0.9300
Fe1—N1	2.275 (2)	C16—C17	1.373 (5)
Fe1—O1W	2.2970 (17)	C16—H16	0.9300
Fe1—N2	2.298 (2)	C17—C18	1.382 (5)
C1—N1	1.324 (4)	C17—C20	1.519 (4)
C1—C2	1.393 (4)	C18—C19	1.382 (4)
C1—H1	0.9300	C18—H18	0.9300
C2—C3	1.352 (5)	C19—H19	0.9300
C2—H2	0.9300	C20—H20A	0.9600
C3—C4	1.398 (5)	C20—H20B	0.9600
C3—H3	0.9300	C20—H20C	0.9600
C4—C12	1.400 (4)	C21—O4	1.248 (3)
C4—C5	1.436 (5)	C21—O3	1.265 (3)
C5—C6	1.346 (5)	C21—C22	1.499 (4)
C5—H5	0.9300	C22—C23	1.372 (4)
C6—C7	1.422 (5)	C22—C27	1.387 (4)
C6—H6	0.9300	C23—C24	1.398 (4)
C7—C8	1.406 (5)	C23—H23	0.9300
C7—C11	1.412 (4)	C24—C25	1.383 (5)
C8—C9	1.349 (5)	C24—H24	0.9300
C8—H8	0.9300	C25—C26	1.367 (5)
C9—C10	1.395 (4)	C25—C28	1.519 (5)
C9—H9	0.9300	C26—C27	1.387 (4)
C10—N2	1.328 (4)	C26—H26	0.9300
C10—H10	0.9300	C27—H27	0.9300
C11—N2	1.355 (3)	C28—H28A	0.9600
C11—C12	1.446 (4)	C28—H28B	0.9600
C12—N1	1.354 (3)	C28—H28C	0.9600
C13—O2	1.252 (3)	O2—Fe1^{i}	2.1369 (18)
C13—O1	1.256 (3)	O1W—Fe1^{i}	2.2970 (17)
C13—C14	1.496 (3)	O1W—H1W	0.938 (8)
C14—C15	1.386 (4)		
O3—Fe1—O2^{i}	93.91 (7)	C14—C15—H15	119.8
O3—Fe1—O1	172.16 (8)	C17—C16—C15	121.6 (3)
O2^{i}—Fe1—O1	89.79 (7)	C17—C16—H16	119.2
O3—Fe1—N1	100.73 (8)	C15—C16—H16	119.2
O2^{i}—Fe1—N1	86.60 (8)	C16—C17—C18	118.3 (3)
O1—Fe1—N1	86.37 (7)	C16—C17—C20	121.8 (4)
O3—Fe1—O1W	88.54 (6)	C18—C17—C20	120.0 (4)
O2^{i}—Fe1—O1W	108.77 (7)	C19—C18—C17	121.2 (3)

O1—Fe1—O1W	83.73 (6)	C19—C18—H18	119.4
N1—Fe1—O1W	161.62 (6)	C17—C18—H18	119.4
O3—Fe1—N2	89.48 (8)	C18—C19—C14	120.1 (3)
O2^{i}—Fe1—N2	159.38 (8)	C18—C19—H19	119.9
O1—Fe1—N2	89.47 (7)	C14—C19—H19	119.9
N1—Fe1—N2	72.79 (8)	C17—C20—H20A	109.5
O1W—Fe1—N2	91.64 (7)	C17—C20—H20B	109.5
N1—C1—C2	122.9 (3)	H20A—C20—H20B	109.5
N1—C1—H1	118.5	C17—C20—H20C	109.5
C2—C1—H1	118.5	H20A—C20—H20C	109.5
C3—C2—C1	119.0 (3)	H20B—C20—H20C	109.5
C3—C2—H2	120.5	O4—C21—O3	124.9 (3)
C1—C2—H2	120.5	O4—C21—C22	118.1 (3)
C2—C3—C4	120.3 (3)	O3—C21—C22	117.0 (3)
C2—C3—H3	119.8	C23—C22—C27	118.4 (3)
C4—C3—H3	119.8	C23—C22—C21	122.3 (3)
C3—C4—C12	117.0 (3)	C27—C22—C21	119.4 (3)
C3—C4—C5	124.1 (3)	C22—C23—C24	121.0 (3)
C12—C4—C5	118.9 (3)	C22—C23—H23	119.5
C6—C5—C4	121.2 (3)	C24—C23—H23	119.5
C6—C5—H5	119.4	C25—C24—C23	120.3 (3)
C4—C5—H5	119.4	C25—C24—H24	119.8
C5—C6—C7	121.8 (3)	C23—C24—H24	119.8
C5—C6—H6	119.1	C26—C25—C24	118.3 (3)
C7—C6—H6	119.1	C26—C25—C28	121.3 (4)
C8—C7—C11	117.3 (3)	C24—C25—C28	120.4 (4)
C8—C7—C6	124.0 (3)	C25—C26—C27	121.7 (3)
C11—C7—C6	118.6 (3)	C25—C26—H26	119.2
C9—C8—C7	120.0 (3)	C27—C26—H26	119.2
C9—C8—H8	120.0	C26—C27—C22	120.2 (3)
C7—C8—H8	120.0	C26—C27—H27	119.9
C8—C9—C10	119.3 (3)	C22—C27—H27	119.9
C8—C9—H9	120.4	C25—C28—H28A	109.5
C10—C9—H9	120.4	C25—C28—H28B	109.5
N2—C10—C9	123.0 (3)	H28A—C28—H28B	109.5
N2—C10—H10	118.5	C25—C28—H28C	109.5
C9—C10—H10	118.5	H28A—C28—H28C	109.5
N2—C11—C7	122.0 (3)	H28B—C28—H28C	109.5
N2—C11—C12	118.2 (2)	C1—N1—C12	118.0 (2)
C7—C11—C12	119.8 (3)	C1—N1—Fe1	125.91 (19)
N1—C12—C4	122.7 (3)	C12—N1—Fe1	115.70 (18)
N1—C12—C11	117.6 (2)	C10—N2—C11	118.3 (2)
C4—C12—C11	119.6 (3)	C10—N2—Fe1	126.82 (19)
O2—C13—O1	124.3 (2)	C11—N2—Fe1	114.71 (17)
O2—C13—C14	118.0 (2)	C13—O1—Fe1	124.66 (16)
O1—C13—C14	117.7 (2)	C13—O2—Fe1^{i}	120.36 (16)
C15—C14—C19	118.5 (3)	C21—O3—Fe1	126.24 (18)
C15—C14—C13	120.3 (2)	Fe1—O1W—Fe1^{i}	98.87 (10)

C19—C14—C13	121.1 (2)	Fe1—O1W—H1W	115.5 (18)
C16—C15—C14	120.3 (3)	Fe1^{i}—O1W—H1W	81.6 (18)
C16—C15—H15	119.8		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O4^{i}	0.94 (1)	1.80 (2)	2.578 (2)	138 (2)

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