Acta Cryst E STRUCTURE REPORTS

ISSN 1600-5368

Received 30 September 2014
Accepted 7 October 2014

Edited by M. Weil, Vienna University of Technology, Austria

Keywords: crystal structure; tetradentate ligand; Fe^{III} high-spin complex

CCDC reference: 1027864
Supporting information: this article has supporting information at journals.iucr.org/e

Crystal structure of dichlorido{2-[(2-hydroxyethyl)(pyridin-2-ylmethyl)amino]ethanolato-κ^4N,N',O,O'}iron(III) dihydrate from synchrotron data

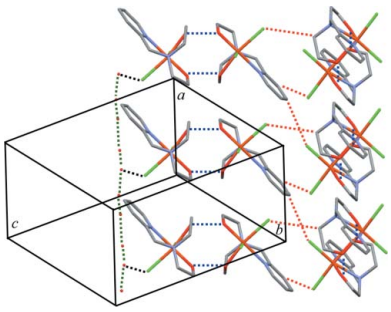
Jong Won Shin, Dae-Woong Kim and Dohyun Moon*

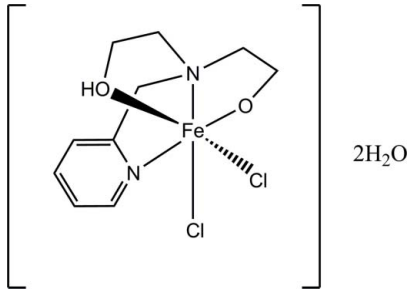
Beamline Department, Pohang Accelerator Laboratory/POSTECH 80, Pohang 790-784, Republic of Korea. *Correspondence e-mail: dmoon@postech.ac.kr

In the title compound, $[Fe(C_{10}H_{15}N_2O_2)Cl_2]\cdot 2H_2O$, the Fe^{III} ion is coordinated by two N and two O atoms of the tetradentate 2-{(2-hydroxyethyl)(pyridin-2-ylmethyl)amino}ethanolate ligand and by two chloride anions, resulting in a distorted octahedral coordination sphere. The average Fe—X (X = ligand N and O atoms) and Fe—Cl bond lengths are 2.10 and 2.32 Å, respectively. In the crystal, duplex O—H···O hydrogen bonds between the hydroxyl and ethoxy groups of two neighbouring complexes give rise to a dimeric unit. The dimers are connected to the lattice water molecules (one of which is equally disordered over two sets of sites) through O—H···Cl hydrogen bonds, forming undulating sheets parallel to (010). Weak C—H···Cl hydrogen bonds are also observed.

1. Chemical context

Tetradentate ligands including pyridine and hydroxyl groups have attracted considerable attention in chemistry and materials science (Paz *et al.*, 2012; Li *et al.*, 2007). These ligands are able to form multinuclear complexes with various transition metal ions, leading to dimeric, trimeric, tetrameric or polymeric structures through the deprotonation of hydroxyl groups (Shin *et al.*, 2010; Han *et al.*, 2009). Such multinuclear complexes have potential applications in catalysis and magnetic materials. For example, Fe^{III} and $Co^{II/III}$ complexes with aminoethanol moieties have been studied as oxidation catalysts of various olefins and investigated due to their magnetic properties (Shin *et al.*, 2011, 2014). Moreover, $Mn^{II/III}$ complexes containing hydroxyl substituents exhibit excellent single-molecular magnetic properties due to magnetic spin-orbit anisotropy (Wu *et al.*, 2010).





Here, we report the synthesis and crystal structure of a complex with six-coordinate Fe^{III} constructed from the tetradentate ligand 2-[(2-hydroxyethyl)(pyridin-2-ylmethyl)-amino]ethanol (H_2pmide; $C_{10}H_{17}N_2O_2$) and chloride anions, $[Fe(Hpmide)Cl_2]\cdot 2H_2O$, (I).

OPEN ACCESS

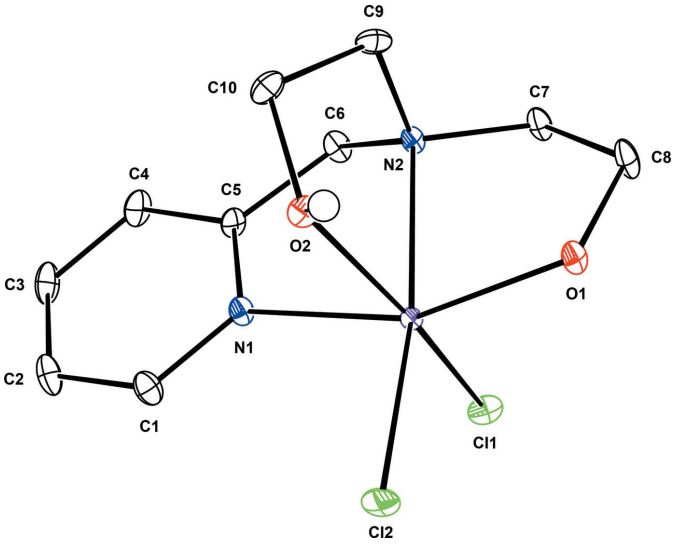


Figure 1
View of the molecular structure of the title compound, showing the atom-labelling scheme, with displacement ellipsoids drawn at the 50% probability level. H atoms and lattice water molecules are omitted for clarity except for the H atom of the hydroxyl group.

2. Structural commentary

A view of the molecular structure of compound (I) is shown in Fig. 1. The coordination sphere of the Fe^{III} ion can be described as distorted octahedral, consisting of the two N atoms and two O atoms from the Hpmide ligand, and two chloride anions. The chloride anions are *trans* to the deprotonated ethoxy O atom and the N atom of the pyridine group of the Hpmide ligand, respectively, and coordinate in *cis* position to each other. The average $Fe-X_{Hpmide}$ (X = N, O) bond length is 2.10 Å and the Fe—Cl bond lengths are 2.2773 (5) (equatorial) and 2.3581 (7) (axial) Å. Both the average Fe—N (2.182 Å) and Fe—O (2.010 Å) distances in (I) are comparable to those found in related N_2O_2-chelated high-spin Fe^{III} complexes (Shin *et al.*, 2014; Cappillino *et al.*, 2012). The bite angles of the five-membered chelate rings in (I) range from 76.59 (5) to 81.45 (4)°.

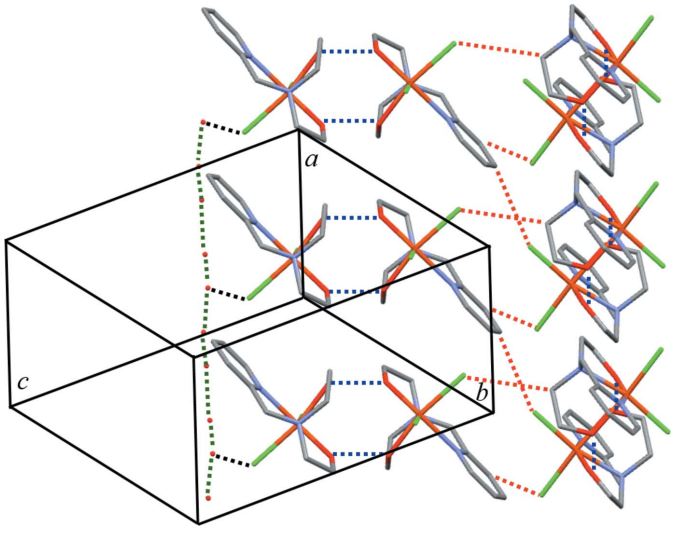


Figure 2
View of the crystal packing of the title compound, with intermolecular O—H···O hydrogen bonds between Fe^{III} complex molecules drawn as blue dashed lines. C—H···Cl hydrogen bonds are indicated as red dashed lines; water molecules and chloride anions are also connected through O—H···O hydrogen bonds (black dashed lines).

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

D—H···A	D—H	H···A	D···A	D—H···A
O1*W*1—H1*W*1···Cl1	0.84 (1)	2.51 (3)	3.279 (4)	152 (5)
O1*W*2—H2*W*2···Cl1	0.84 (1)	2.91 (5)	3.470 (4)	125 (5)
O2—H1O2···O1^{i}	0.83 (2)	1.69 (2)	2.5196 (14)	177 (2)
O1*W*1—H2*W*1···O2*W*^{ii}	0.84 (1)	2.15 (4)	2.876 (7)	144 (7)
O1*W*2—H1*W*2···O2*W*^{ii}	0.84 (1)	2.06 (5)	2.647 (8)	126 (5)
O1*W*2—H1*W*2···O2*W*^{iii}	0.84 (1)	2.06 (3)	2.836 (8)	153 (6)
C4—H4···Cl1^{iv}	0.95	2.76	3.5962 (16)	147
C9—H9*A*···Cl1^{v}	0.99	2.78	3.6371 (15)	145
C3—H3···Cl2^{vi}	0.95	2.80	3.5721 (16)	139

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

3. Supramolecular features

The hydroxyl substituent of the Hpmide ligand forms a strong hydrogen bond with the O atom of the deprotonated ethoxy group of a neighbouring molecule. These duplex interactions lead to a dinuclear dimeric unit. The dimers are linked through O—H···Cl interactions to the lattice water molecules, that are likewise connected to each other through O—H···O hydrogen bonds. All these hydrogen-bonding interactions (Steed & Atwood, 2009) lead to the formation of undulating sheets parallel to (010). Further weak hydrogen bonding between pyridine and methyl H atoms and chloride anions stabilizes this arrangement (Fig. 2 and Table 1).

4. Database survey

A search of the Cambridge Structural Database (Version 5.35, November 2013 with three updates; Groom & Allen, 2014) indicated that five complexes derived from the H_2pmide ligand have been reported. These include Ni^{II} and $Mn^{II/III}$; Fe^{III} complexes have been studied for their magnetic properties and catalytic effects (Saalfrank *et al.*, 2001; Wu *et al.*, 2010; Shin *et al.*, 2014).

5. Synthesis and crystallization

The H_2pmide ligand was prepared following a previously reported method (Wu *et al.*, 2010). Compound (I) was prepared as follows: to a MeOH solution (4 ml) of $FeCl_2{\cdot}4H_2O$ (81 mg, 0.408 mmol) was added dropwise a MeOH solution (3 ml) of H_2pmide (80 mg, 0.408 mmol). The colour became yellow, and then the solution was stirred for 30 min at room temperature. Yellow crystals of (I) were obtained by diffusion of diethyl ether into the yellow solution for several days, and were collected by filtration and washed with diethyl ether and

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Fe(C_{10}H_{15}N_2O_2)Cl_2]\cdot 2H_2O$
M_r	358.02
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	7.2690 (15), 14.497 (3), 14.094 (3)
β (°)	95.86 (3)
V (Å^3)	1477.4 (5)
Z	4
Radiation type	Synchrotron, λ = 0.62998 Å
μ (mm^{-1})	0.99
Crystal size (mm)	0.10 × 0.10 × 0.08
Data collection	
Diffractometer	ADSC Q210 CCD area-detector
Absorption correction	Empirical (using intensity measurements) (*HKL3000sm SCALEPACK*; Otwinowski & Minor, 1997)
T_{min}, T_{max}	0.907, 0.925
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14975, 4056, 3866
R_{int}	0.021
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.696
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.027, 0.073, 1.04
No. of reflections	4056
No. of parameters	197
No. of restraints	7
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.51, −0.84

Computer programs: *PAL ADSC Quantum-210 ADX* (Arvai & Nielsen, 1983), *HKL3000sm* (Otwinowski & Minor, 1997), *SHELXS2013/1* and *SHELXL2014/7* (Sheldrick, 2008), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012).

dried in air. Yield: 67 mg (46%). Elemental analysis calculated for $C_{10}H_{15}Cl_2FeN_2O_2$: C 37.30, H 4.70, N 8.70%; found: C 37.19, H 4.58, N 8.78%.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms attached to C atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.95 (aromatic H atoms) and 0.99 Å (open-chain H atoms) and with U_{iso}(H) values of 1.2U_{eq}(C) of the parent atoms. One lattice water molecule (O*W*1) was found to be equally disordered over two positions. The H atoms of this disordered water molecule (H1*W*1 and H1*W*2) were located from difference Fourier maps and refined with restraints and a fixed O—H distances of 0.84 Å, with U_{iso}(H) values of 1.2U_{eq}(O). Moreover, the second water molecule (O2*W*) was modelled without hydrogen atoms because difference Fourier maps did not suggest suitable H atoms.

Acknowledgements

This work was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (NRF-2012R1A1A2002507) and supported by the Institute for Basic Science (IBS, IBS-R007-D1-2014-a01). X-ray crystallography at the PLS-II 2D-SMC beamline was supported in part by MSIP and POSTECH.

References

Arvai, A. J. & Nielsen, C. (1983). *ADSC Quantum-210 ADX*. Area Detector System Corporation, Poway, CA, USA.
Cappillino, P. J., Miecznikowski, J. R., Tyler, L. A., Tarves, P. C., McNally, J. S., Lo, W., Kasibhatla, B. S. T., Krzyaniak, M. D., McCracken, J., Wang, F., Armstrong, W. H. & Caradonna, J. P. (2012). *Dalton Trans.* **41**, 5662–5677.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Groom, C. R. & Allen, F. H. (2014). *Angew. Chem. Int. Ed. Engl.* **53**, 662–671.
Han, J. H., Shin, J. W. & Min, K. S. (2009). *Bull. Korean Chem. Soc.* **30**, 1113–1117.
Li, F., Wang, M., Li, P., Zhang, T. & Sun, L. (2007). *Inorg. Chem.* **46**, 9364–9371.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Paz, F. A. A., Klinowski, J., Vilela, S. M. F., Tomé, J. P. C., Cavaleiro, J. A. S. & Rocha, J. (2012). *Chem. Soc. Rev.* **41**, 1088–1110.
Saalfrank, R. W., Bernt, I. & Hampel, F. (2001). *Chem. Eur. J.* **13**, 2770–2774.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Shin, J. W., Bae, J. M., Kim, C. & Min, K. S. (2014). *Dalton Trans.* **43**, 3999–4008.
Shin, J. W., Rowthu, S. R., Hyun, M. Y., Song, Y. J., Kim, C., Kim, B. G. & Min, K. S. (2011). *Dalton Trans.* **40**, 5762–5773.
Shin, J. W., Rowthu, S. R., Kim, B. G. & Min, K. S. (2010). *Dalton Trans.* **39**, 2765–2767.
Steed, J. W. & Atwood, J. L. (2009). *Supramolecular Chemistry*, 2nd ed. Chichester: John Wiley & Sons Ltd.
Wu, C.-C., Datta, S., Wernsdorfer, W., Lee, G.-H., Hill, S. & Yang, E.-C. (2010). *Dalton Trans.* **39**, 10160–10168.

supporting information

Acta Cryst. (2014). E**70**, 334-336 [doi:10.1107/S1600536814022089]

Crystal structure of dichlorido{2-[(2-hydroxyethyl)(pyridin-2-ylmethyl)amino]-ethanolato-κ^4N,N',O,O'}iron(III) dihydrate from synchrotron data

Jong Won Shin, Dae-Woong Kim and Dohyun Moon

Computing details

Data collection: *PAL ADSC Quantum-210 ADX* (Arvai & Nielsen, 1983); cell refinement: *HKL3000sm* (Otwinowski & Minor, 1997); data reduction: *HKL3000sm* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS2013*/1 (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014*/7 (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

Dichlorido{2-[(2-hydroxyethyl)(pyridin-2-ylmethyl)amino]ethanolato-κ^4N,N',O,O'}iron(III) dihydrate

Crystal data

$[Fe(C_{10}H_{15}N_2O_2)Cl_2]\cdot 2H_2O$
M_r = 358.02
Monoclinic, $P2_1/c$
a = 7.2690 (15) Å
b = 14.497 (3) Å
c = 14.094 (3) Å
β = 95.86 (3)°
V = 1477.4 (5) Å^3
Z = 4
$F(000)$ = 740
D_x = 1.610 Mg m^{-3}
Synchrotron radiation, λ = 0.62998 Å
Cell parameters from 47717 reflections
θ = 0.4–33.6°
μ = 0.99 mm^{-1}
T = 100 K
Block, yellow
0.10 × 0.10 × 0.08 mm

Data collection

ADSC Q210 CCD area-detector diffractometer
Radiation source: PLSII 2D bending magnet
ω scan
Absorption correction: empirical (using intensity measurements) (*HKL3000sm SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.907, T_{max} = 0.925
14975 measured reflections
4056 independent reflections
3866 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 26.0°, θ_{min} = 2.5°
h = −10→10
k = −19→19
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.073
S = 1.04
4056 reflections
197 parameters
7 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0354P)^2 + 1.6679P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.84 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Fe1	0.49921 (2)	0.59458 (2)	0.35450 (2)	0.00581 (6)	
Cl1	0.66209 (5)	0.61966 (2)	0.22045 (2)	0.01181 (8)	
Cl2	0.32215 (5)	0.47400 (2)	0.29547 (2)	0.01270 (8)	
O1	0.70234 (13)	0.53542 (7)	0.42787 (7)	0.00933 (18)	
O2	0.33434 (14)	0.60360 (7)	0.46844 (7)	0.00925 (18)	
H1O2	0.322 (3)	0.5590 (12)	0.5041 (13)	0.011*	
N1	0.32550 (15)	0.70945 (8)	0.30279 (8)	0.0085 (2)	
N2	0.62789 (15)	0.71338 (8)	0.43157 (8)	0.0075 (2)	
C1	0.15712 (19)	0.70132 (10)	0.25359 (10)	0.0117 (2)	
H1	0.1099	0.6415	0.2383	0.014*	
C2	0.05082 (19)	0.77769 (11)	0.22469 (10)	0.0143 (3)	
H2	−0.0669	0.7703	0.1896	0.017*	
C3	0.1193 (2)	0.86521 (11)	0.24795 (11)	0.0156 (3)	
H3	0.0492	0.9185	0.2288	0.019*	
C4	0.2913 (2)	0.87365 (10)	0.29950 (11)	0.0130 (3)	
H4	0.3401	0.9328	0.3169	0.016*	
C5	0.39138 (18)	0.79407 (9)	0.32537 (10)	0.0089 (2)	
C6	0.58321 (19)	0.79876 (9)	0.37700 (10)	0.0107 (2)	
H6A	0.6743	0.8079	0.3302	0.013*	
H6B	0.5917	0.8522	0.4210	0.013*	
C7	0.82796 (18)	0.69147 (9)	0.43890 (10)	0.0102 (2)	
H7A	0.8958	0.7310	0.4879	0.012*	
H7B	0.8770	0.7035	0.3771	0.012*	
C8	0.85570 (19)	0.58946 (9)	0.46615 (11)	0.0125 (3)	
H8A	0.9699	0.5663	0.4416	0.015*	
H8B	0.8706	0.5835	0.5365	0.015*	
C9	0.56136 (19)	0.71512 (10)	0.52794 (10)	0.0113 (2)	
H9A	0.5759	0.7781	0.5548	0.014*	
H9B	0.6373	0.6726	0.5708	0.014*	
C10	0.35997 (19)	0.68663 (10)	0.52331 (10)	0.0117 (2)	
H10A	0.3250	0.6762	0.5885	0.014*	
H10B	0.2804	0.7362	0.4932	0.014*	
O1W1	0.4145 (8)	0.5368 (3)	0.0321 (3)	0.0527 (11)	0.5
H1W1	0.444 (8)	0.551 (5)	0.0896 (16)	0.063*	0.5
H2W1	0.300 (3)	0.526 (6)	0.025 (4)	0.063*	0.5
O1W2	0.3007 (7)	0.5629 (4)	0.0504 (3)	0.0549 (11)	0.5
H1W2	0.190 (3)	0.546 (5)	0.041 (4)	0.066*	0.5
H2W2	0.314 (8)	0.593 (4)	0.101 (3)	0.066*	0.5
O2W	0.0911 (9)	0.4335 (4)	0.9619 (4)	0.182 (2)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.00713 (10)	0.00133 (10)	0.00853 (10)	−0.00039 (6)	−0.00140 (6)	0.00067 (6)
Cl1	0.01740 (15)	0.00679 (15)	0.01158 (14)	−0.00204 (11)	0.00321 (11)	0.00141 (10)
Cl2	0.01370 (15)	0.00686 (15)	0.01705 (15)	−0.00509 (10)	−0.00075 (11)	−0.00279 (11)
O1	0.0089 (4)	0.0039 (4)	0.0146 (4)	−0.0005 (3)	−0.0017 (3)	0.0029 (3)
O2	0.0115 (4)	0.0047 (4)	0.0117 (4)	−0.0016 (3)	0.0018 (3)	0.0014 (3)
N1	0.0085 (5)	0.0051 (5)	0.0115 (5)	0.0001 (4)	−0.0005 (4)	0.0023 (4)
N2	0.0082 (5)	0.0031 (5)	0.0105 (5)	−0.0002 (4)	−0.0016 (4)	0.0019 (4)
C1	0.0100 (6)	0.0114 (6)	0.0132 (6)	−0.0008 (5)	−0.0009 (5)	0.0036 (5)
C2	0.0083 (5)	0.0179 (7)	0.0165 (6)	0.0022 (5)	−0.0004 (5)	0.0072 (5)
C3	0.0129 (6)	0.0134 (7)	0.0206 (7)	0.0072 (5)	0.0025 (5)	0.0074 (5)
C4	0.0144 (6)	0.0056 (6)	0.0191 (6)	0.0035 (5)	0.0025 (5)	0.0040 (5)
C5	0.0102 (5)	0.0045 (6)	0.0121 (6)	0.0012 (4)	0.0010 (4)	0.0023 (4)
C6	0.0120 (6)	0.0019 (5)	0.0172 (6)	−0.0010 (4)	−0.0033 (5)	0.0028 (4)
C7	0.0072 (5)	0.0068 (6)	0.0161 (6)	−0.0016 (4)	−0.0022 (4)	0.0025 (4)
C8	0.0079 (5)	0.0077 (6)	0.0207 (7)	−0.0005 (4)	−0.0041 (5)	0.0046 (5)
C9	0.0156 (6)	0.0083 (6)	0.0099 (6)	−0.0024 (5)	0.0001 (5)	−0.0024 (4)
C10	0.0147 (6)	0.0070 (6)	0.0140 (6)	0.0008 (5)	0.0041 (5)	−0.0012 (5)
O1W1	0.095 (4)	0.035 (2)	0.0249 (16)	−0.019 (2)	−0.0105 (19)	0.0025 (14)
O1W2	0.066 (3)	0.069 (3)	0.0270 (18)	−0.008 (2)	−0.0078 (18)	−0.0038 (18)
O2W	0.229 (6)	0.182 (5)	0.138 (4)	−0.037 (5)	0.023 (4)	0.009 (4)

Geometric parameters (Å, º)

Fe1—O1	1.9165 (11)	C4—C5	1.3925 (18)
Fe1—O2	2.1036 (12)	C4—H4	0.9500
Fe1—N1	2.1704 (12)	C5—C6	1.5071 (19)
Fe1—N2	2.1939 (12)	C6—H6A	0.9900
Fe1—Cl2	2.2773 (5)	C6—H6B	0.9900
Fe1—Cl1	2.3581 (7)	C7—C8	1.5360 (19)
O1—C8	1.4229 (16)	C7—H7A	0.9900
O2—C10	1.4326 (17)	C7—H7B	0.9900
O2—H1O2	0.829 (15)	C8—H8A	0.9900
N1—C5	1.3433 (17)	C8—H8B	0.9900
N1—C1	1.3488 (17)	C9—C10	1.516 (2)
N2—C6	1.4759 (17)	C9—H9A	0.9900
N2—C7	1.4818 (17)	C9—H9B	0.9900
N2—C9	1.4878 (18)	C10—H10A	0.9900
C1—C2	1.387 (2)	C10—H10B	0.9900
C1—H1	0.9500	O1W1—H1W1	0.842 (10)
C2—C3	1.390 (2)	O1W1—H2W1	0.842 (10)
C2—H2	0.9500	O1W2—H1W2	0.842 (10)
C3—C4	1.386 (2)	O1W2—H2W2	0.839 (10)
C3—H3	0.9500		
O1—Fe1—O2	94.79 (4)	C3—C4—H4	120.6

O1—Fe1—N1	156.10 (4)	C5—C4—H4	120.6
O2—Fe1—N1	81.45 (4)	N1—C5—C4	122.05 (13)
O1—Fe1—N2	79.52 (5)	N1—C5—C6	116.46 (11)
O2—Fe1—N2	79.66 (4)	C4—C5—C6	121.45 (12)
N1—Fe1—N2	76.59 (5)	N2—C6—C5	110.93 (10)
O1—Fe1—Cl2	103.25 (4)	N2—C6—H6A	109.5
O2—Fe1—Cl2	88.96 (3)	C5—C6—H6A	109.5
N1—Fe1—Cl2	100.28 (4)	N2—C6—H6B	109.5
N2—Fe1—Cl2	168.51 (3)	C5—C6—H6B	109.5
O1—Fe1—Cl1	94.54 (4)	H6A—C6—H6B	108.0
O2—Fe1—Cl1	166.87 (3)	N2—C7—C8	109.06 (11)
N1—Fe1—Cl1	86.28 (3)	N2—C7—H7A	109.9
N2—Fe1—Cl1	92.98 (3)	C8—C7—H7A	109.9
Cl2—Fe1—Cl1	97.869 (19)	N2—C7—H7B	109.9
C8—O1—Fe1	119.26 (8)	C8—C7—H7B	109.9
C10—O2—Fe1	114.30 (8)	H7A—C7—H7B	108.3
C10—O2—H1O2	110.1 (14)	O1—C8—C7	110.95 (11)
Fe1—O2—H1O2	121.2 (14)	O1—C8—H8A	109.4
C5—N1—C1	118.97 (12)	C7—C8—H8A	109.4
C5—N1—Fe1	116.11 (9)	O1—C8—H8B	109.4
C1—N1—Fe1	124.88 (9)	C7—C8—H8B	109.4
C6—N2—C7	112.22 (11)	H8A—C8—H8B	108.0
C6—N2—C9	112.75 (11)	N2—C9—C10	111.01 (11)
C7—N2—C9	110.38 (11)	N2—C9—H9A	109.4
C6—N2—Fe1	109.90 (8)	C10—C9—H9A	109.4
C7—N2—Fe1	103.42 (8)	N2—C9—H9B	109.4
C9—N2—Fe1	107.66 (8)	C10—C9—H9B	109.4
N1—C1—C2	122.02 (13)	H9A—C9—H9B	108.0
N1—C1—H1	119.0	O2—C10—C9	108.90 (11)
C2—C1—H1	119.0	O2—C10—H10A	109.9
C1—C2—C3	118.93 (13)	C9—C10—H10A	109.9
C1—C2—H2	120.5	O2—C10—H10B	109.9
C3—C2—H2	120.5	C9—C10—H10B	109.9
C4—C3—C2	119.12 (13)	H10A—C10—H10B	108.3
C4—C3—H3	120.4	H1W1—O1W1—H2W1	108 (3)
C2—C3—H3	120.4	H1W2—O1W2—H2W2	109 (3)
C3—C4—C5	118.90 (14)		

C5—N1—C1—C2	0.7 (2)	Fe1—N2—C6—C5	34.62 (13)
Fe1—N1—C1—C2	178.26 (10)	N1—C5—C6—N2	−26.63 (17)
N1—C1—C2—C3	−0.6 (2)	C4—C5—C6—N2	155.71 (13)
C1—C2—C3—C4	−0.2 (2)	C6—N2—C7—C8	−161.67 (11)
C2—C3—C4—C5	0.8 (2)	C9—N2—C7—C8	71.64 (14)
C1—N1—C5—C4	−0.1 (2)	Fe1—N2—C7—C8	−43.28 (12)
Fe1—N1—C5—C4	−177.80 (10)	Fe1—O1—C8—C7	−0.47 (15)
C1—N1—C5—C6	−177.70 (12)	N2—C7—C8—O1	31.76 (16)
Fe1—N1—C5—C6	4.56 (16)	C6—N2—C9—C10	83.81 (14)
C3—C4—C5—N1	−0.7 (2)	C7—N2—C9—C10	−149.79 (11)

C3—C4—C5—C6	176.80 (13)	Fe1—N2—C9—C10	−37.58 (12)
C7—N2—C6—C5	149.11 (12)	Fe1—O2—C10—C9	−35.00 (13)
C9—N2—C6—C5	−85.49 (14)	N2—C9—C10—O2	48.37 (15)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*1—H1*W*1···Cl1	0.84 (1)	2.51 (3)	3.279 (4)	152 (5)
O1*W*2—H2*W*2···Cl1	0.84 (1)	2.91 (5)	3.470 (4)	125 (5)
O2—H1*O*2···O1^{i}	0.83 (2)	1.69 (2)	2.5196 (14)	177 (2)
O1*W*1—H2*W*1···O2*W*^{ii}	0.84 (1)	2.15 (4)	2.876 (7)	144 (7)
O1*W*2—H1*W*2···O2*W*^{ii}	0.84 (1)	2.06 (5)	2.647 (8)	126 (5)
O1*W*2—H1*W*2···O2*W*^{iii}	0.84 (1)	2.06 (3)	2.836 (8)	153 (6)
C4—H4···Cl1^{iv}	0.95	2.76	3.5962 (16)	147
C9—H9*A*···Cl1^{v}	0.99	2.78	3.6371 (15)	145
C3—H3···Cl2^{vi}	0.95	2.80	3.5721 (16)	139

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