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Crystal structure of hexakis(N,N-dimethylformamide-κO)iron(III) μ-chlorido-bis(trichloridocadmium)

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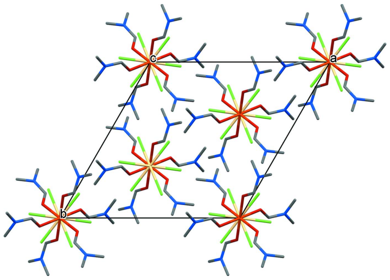
The title compound, $[Fe(C_3H_7NO)_6][Cd_2Cl_7]$, crystallizes in the trigonal space group $R\overline{3}$ and is assembled from discrete $[Fe(DMF)_6]^{3+}$ cations (DMF = *N*,*N*-dimethylformamide) and $[Cd_2Cl_7]^{3-}$ anions. In the cation, the iron(III) atom, located on a special position of $\overline{3}$ site symmetry, is coordinated by six oxygen atoms from DMF ligands with all Fe—O distances being equal [2.0072 (16) Å]. A slight distortion of the octahedral environment of the metal comes from the *cis* O—Fe—O angles deviating from the ideal value of 90° [86.85 (7) and 93.16 (7)°] whilst all the *trans* angles are strictly 180°. The central Cl atom of the $[Cd_2Cl_7]^{3-}$ anion is also located on a special position of $\overline{3}$ site symmetry and bridges two corner sharing, tetrahedrally coordinated Cd^{II} atoms. The two Cd atoms and the central Cl atom are colinear. The two sets of terminal chloride ligands on either side of the dumbbell-like anion are rotated relative to each other by 30°. In the crystal, the cations and anions, stacked one above the other along the *c*-axis direction, are held in place principally by electrostatic interactions. There are also C—H···Cl and C—H···O interactions, but these are rather weak. Of the six crystal structures reported to date for ionic salts of $[Fe(DMF)_6]^{n+}$ cations ($n = 2, 3$), five contain Fe^{II} ions. The title compound is the second example of a stable compound containing the $[Fe(DMF)_6]^{3+}$ cation. The existence of both $[Fe(DMF)_6]^{2+}$ and $[Fe(DMF)_6]^{3+}$ cations shows that the DMF ligand coordination sphere can accommodate changes in the charge and spin states of the metal centre.

1. Chemical context

In our ongoing research into the new functions and applications of coordination compounds with Schiff-base ligands, we have utilized a synthetic scheme involving a zerovalent metal as the source of metal ions, together with another metal salt, in order to prepare new heterometallic complexes (Kokozay *et al.*, 2018; Vassilyeva *et al.*, 2018, 2021). In a typical procedure, the metal powder undergoes oxidative dissolution in air to generate metal ions that then interact with the second metal salt and pre-formed ligand. The condensation reaction between the Schiff-base precursors occurs *in situ* without isolation of the imine. Dioxygen from the air is reduced to form a water molecule with participation of protons donated by the imine, which is capable of deprotonation.

By using the above scheme, new homo- and heterometallic Co^{III}, Co^{III}/Zn^{II} and Co^{III}/Cd^{II} complexes with a Schiff-base ligand derived from 2-hydroxy-3-methoxybenzaldehyde (*o*-vanillin) and the simple amine methylamine have been prepared (Nesterova *et al.*, 2018, 2019). Comparative studies



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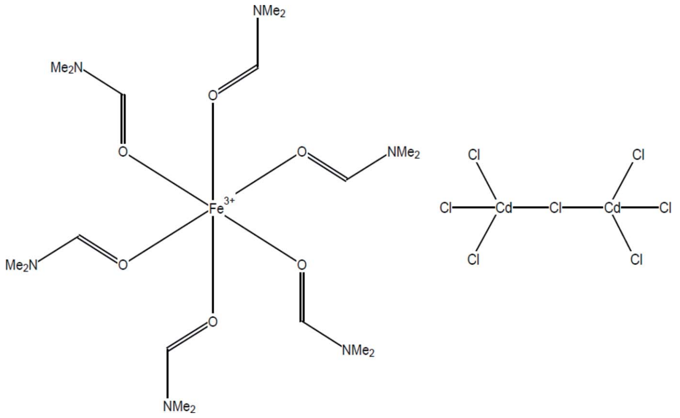
of their catalytic behaviours in oxidation reactions of alkanes with H_2O_2 and *m*-chloroperoxybenzoic acid were undertaken to elucidate the role of the second (inactive) metal centre (Cd) in the catalytic performance of the heterometallic compounds. Given the remarkable catalytic activity of the Schiff base Fe^{III} metal complexes mimicking the Fe-containing enzymes that oxidize alkanes in nature (Nesterov *et al.*, 2015), we decided to extend our work and replace the cobalt centre with iron in a heterometallic core supported by the above Schiff-base ligand.

To facilitate formation of the desired compound, an additional basic agent, *N*-phenyldiethanolamine, was introduced following the previous successful participation of diethanolamine in the formation of a mixed-ligand Schiff base Ni^{II}/Zn^{II} dimer (Vassilyeva *et al.*, 2021). In the latter compound, the deprotonated aminoalcohol molecules provide additional alkoxo-bridges between the metal centres. The use of aminoalcohol deprotonation in reactions employing zero-valent metals in the synthesis of heterometallics was established by a number of us several years ago (Vassilyeva *et al.*, 1997; Buvaylo *et al.*, 2005, 2012).



In the present work, the treatment of cadmium powder and $FeCl_3·6H_2O$ with a solution of the *in situ*-formed Schiff base in open air worked a different way than expected and led to the isolation of the title compound, the mixed-metal ionic salt $[Fe^{III}(DMF)_6][Cd_2Cl_7]$, (**1**), the identity of which was established by X-ray crystallography and confirmed by chemical analysis.

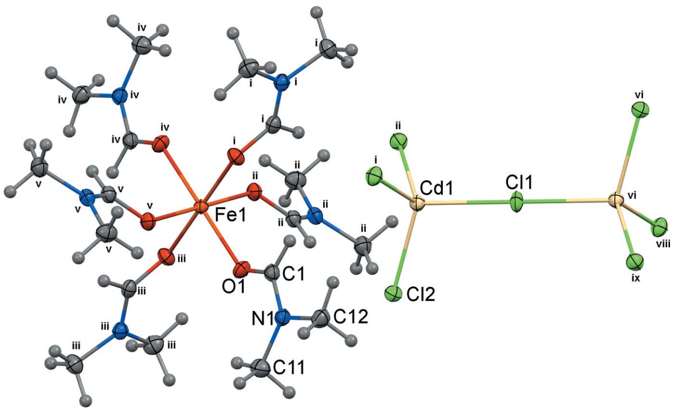


Figure 1
Molecular structure and labelling of $[Fe^{III}(DMF)_6][Cd_2Cl_7]$ (**1**) with displacement ellipsoids at the 50% probability level. [Symmetry codes: (i) $-y+1, x-y+1, z$; (ii) $-x+y, -x+1, z$; (iii) $y-\frac{1}{3}, -x+y+\frac{1}{3}, -z+\frac{4}{3}$; (iv) $-x+\frac{2}{3}, -y+\frac{4}{3}, -z+\frac{4}{3}$; (v) $x-y+\frac{2}{3}, x+\frac{1}{3}, -z+\frac{4}{3}$; (vi) $-x+\frac{2}{3}, -y+\frac{4}{3}, -z+\frac{1}{3}$; (viii) $y-\frac{1}{3}, -x+y+\frac{1}{3}, -z+\frac{1}{3}$; (ix) $x-y+\frac{2}{3}, x+\frac{1}{3}, -z+\frac{1}{3}$.]

Table 1
Selected geometric parameters (Å, °).

Cd1—Cl2	2.4358 (5)	Fe1—O1	2.0072 (16)
Cd1—Cl1	2.5377 (3)		
$Cl2^i$—Cd1—Cl2	111.325 (13)	$O1^{ii}$—Fe1—O1	93.15 (7)
Cl2—Cd1—Cl1	107.547 (14)	$O1^{iii}$—Fe1—O1	86.84 (7)

Symmetry codes: (i) $-y+1, x-y+1, z$; (ii) $-x+y, -x+1, z$; (iii) $y-\frac{1}{3}, -x+y+\frac{1}{3}, -z+\frac{4}{3}$.

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C12—H123$\cdots Cl2^{vii}$	0.98	2.82	3.783 (3)	167
C1—H1$\cdots Cl2^i$	0.97 (3)	2.86 (3)	3.772 (3)	158 (2)
C1—H1$\cdots O1^i$	0.97 (3)	2.62 (3)	3.097 (3)	111 (2)
C12—H122$\cdots Cl2^i$	0.98	2.94	3.861 (3)	157

Symmetry codes: (i) $-y+1, x-y+1, z$; (vii) $-x+\frac{4}{3}, -y+\frac{5}{3}, -z+\frac{2}{3}$.

2. Structural commentary

Compound (**1**), $[Fe(C_3H_7NO)_6][Cd_2Cl_7]$, crystallizes in the trigonal space group $R\overline{3}$ and is assembled from discrete $[Fe(DMF)_6]^{3+}$ cations (DMF = *N*,*N*-dimethylformamide) and $[Cd_2Cl_7]^{3-}$ anions. In the cation, the iron(III) atom sits on a special position of $\overline{3}$ site symmetry and is coordinated by six oxygen atoms from the DMF ligands with all the Fe—O bond lengths being equal at 2.0072 (16) Å (Fig. 1, Table 1). The octahedral environment of the metal is slightly distorted as a result of the *cis* O1—Fe1—O1 angles deviating from the ideal value of 90° [86.85 (7) and 93.16 (7)°] while all the *trans* angles are strictly 180°. The central Cl atom of the $[Cd_2Cl_7]^{3-}$ anion, Cl1, is also located on a special position of $\overline{3}$ site symmetry and bridges two corner-sharing, tetrahedrally coordinated Cd^{II} atoms. The two Cd atoms and the central Cl atom are colinear (Cd1—Cl1—$Cd1^{vi}$ angle = 180°) and the bridging Cd1$\cdots Cd1^{vi}$ distance is 5.0752 (3) Å (Fig. 1). The two sets of terminal chloride ligands, Cl2, on either side of the dumbbell–like anion are rotated relative to each other by 30°. Around each Cd atom, the bridging Cd—Cl1 distance at 2.5377 (3) Å is 0.1 Å longer than that of the terminal Cd—Cl2 distance (2.4358 (5) Å) and the Cl2—Cd1—Cl1 and Cl2—Cd1—$Cl2^i$ angles are 107.547 (14) and 111.325 (13)°, respectively, which are very close to the ideal value of 109°. The bond lengths and angles of the DMF ligands are similar to those found in $[Fe(DMF)_6](ClO_4)_3$ (Houlton *et al.*, 2015).

3. Supramolecular features

In the crystal, the cations and anions are stacked one above the other along the *c*-axis direction (Fig. 2). Although classical

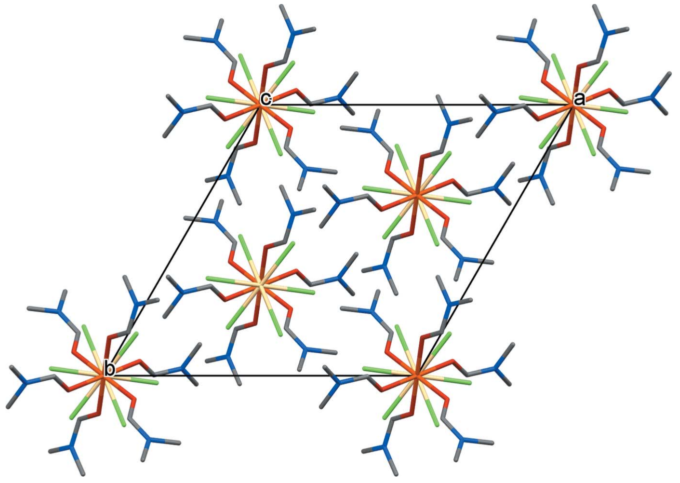


Figure 2
Crystal packing of (**1**) along the *c* axis showing stacks of cations and anions alternating in the *c*-axis direction. Hydrogen atoms are not shown.

hydrogen bonds are absent, several weak C—H···O and C—H···Cl interactions are detected in the structure [C1—H1···Cl2^{i}, 3.772 (3) Å; C12—H123···Cl12^{vii}, 3.783 (3) Å and C1—H1···O1^{i}, 3.097 (3) Å]. The minimum H···O distance (H1···O^{i}) between DMF molecules within the same cation is 2.62 (3) Å and the shortest distance between Cl atoms of the anions and adjacent H atoms of DMF methyl groups (H123···Cl2^{vii}) is 2.82 Å (Table 2), implying that the halide ions act as weak hydrogen-bond acceptors.

4. Database survey

A survey of the Cambridge Structural Database (CSD, Version 5.42, update May 2021; Groom *et al.*, 2016) reveals six ionic salts containing octahedral $[Fe(DMF)_6]^{n+}$ (n = 2, 3) cations. Five of the structures contain Fe^{II} ions, which crystallize in the presence of the counter-anions $[FeCl_4]^{2-}$ (CALMOS01; Cheaib *et al.*, 2013), $[FeCl_2S_4W]^{2-}$(CUSNOT; Coucouvanis *et al.*, 1984), $[Mo_2S_6]^{2-}$ (DEZMIF; Li *et al.*, 2007), $[Fe_2Cl_4S_2]^{2-}$ (VAMFIY; Müller *et al.*, 1989) and ClO_4^- (GAZGET; Baumgartner, 1986). The only example to date containing the Fe^{III} cation, $[Fe(DMF)_6]^{3+}$, is found as the perchlorate salt (DMFAFE01; Houlton *et al.*, 2015).

In the pair of perchlorate salts, the Fe^{II} and Fe^{III} ions are easily distinguishable by their dissimilar Fe—O bond distances that vary in the ranges 2.08–2.11 and 1.9869 (15)–1.9985 (14) Å for $[Fe(DMF)_6](ClO_4)_2$ (GAZGET) and $[Fe(DMF)_6](ClO_4)_3$ (DMFAFE01), respectively. Both Fe-based octahedra are only slightly distorted with *cis* bond angles in the ranges 86.3–93.7° (GAZGET) and 88.57 (6)–91.43 (6)° (DMFAFE01), while all the *trans* angles are equal to the ideal value of 180°. The geometric parameters of the $[Fe(DMF)_6]^{3+}$ cation in the title compound, (**1**), are very close to those found in $[Fe(DMF)_6](ClO_4)_3$ (DMFAFE01) with slight differences arising due to the different counter-anions present. The existence of both $[Fe(DMF)_6]^{2+}$ and $[Fe(DMF)_6]^{3+}$ cations shows that the DMF ligand coordination sphere can accommodate changes in the charge and spin states of the metal centre.

Considering the anion found in (**1**), there are six more examples of $[Cd_2Cl_7]^{3-}$ anions in the CSD [LOVLUF (Chen *et al.*, 2014); MANBIP and MANCAI (Shen *et al.*, 2017); NIZXUR (Zhou *et al.*, 2014); WEYLUJ (Sharma *et al.*, 2012) and YAYFIQ (Cui *et al.*, 2017)] with different degrees of distorted tetrahedral geometry around the Cd atoms and a Cd—Cl—Cd angle ranging from 103.92 (4)° in $[Co(phen)_3][Cd_2Cl_7]\cdot 3H_2O$ (WEYLUJ) to 180° in (**1**). The Cd···Cd distance of 3.9983 (5) Å in the 'bent' structure is significantly lower than that found in (**1**) [5.0752 (3) Å], showing conformational flexibility of the polychloride dicadmium anion to achieve shape complementarity to the countercation.

5. Synthesis and crystallization

2-Hydroxy-3-methoxy-benzaldehyde (0.3 g, 2 mmol) was stirred magnetically with $CH_3NH_2\cdot HCl$ (0.14 g, 2 mmol) and *N*-phenyldiethanolamine (0.36 g, 2 mmol) in methanol (20 mL) in a 50 mL conical flask at 303 K for 20 min. A fine Cd powder (0.11 g, 1 mmol) and dry $FeCl_3\cdot 6H_2O$ (0.27 g, 1 mmol) were introduced to the flask, and the mixture was kept stirring at 333 K to achieve dissolution of the zerovalent metal (1 h). The resulting dark blue–green solution was then filtered and allowed to evaporate at room temperature. After a week, the solution was diluted with DMF (7 mL) since it was thickening and filtered again. Dark-green octahedral crystals of (**1**) formed over two months after successive addition of Pr^{i}OH (4 mL) and diethyl ether (4 mL) in several portions. The crystals were filtered off, washed with diethyl ether and finally dried in air. Yield (based on Fe): 0.13 g (64%). Analysis calculated for $C_{18}H_{42}FeN_6O_6Cd_2Cl_7$ (967.37): C 22.35, H 4.38, N 8.69%. Found: C 22.86, H 4.30, C 8.36%.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Anisotropic displacement parameters were refined for all non-hydrogen atoms. All the carbon-bound hydrogen atoms were placed in calculated positions and refined using a riding model with isotropic displacement parameters based on those of the parent atom [C—H = 0.95 Å, $U_{iso}(H) = 1.2U_{eq}(C)$ for CH and C—H = 0.98 Å, $U_{iso}(H) = 1.5U_{eq}(C)$ for CH_3].

Acknowledgements

The authors acknowledge use of the facilities and the scientific and technical assistance at the Australian Microscopy & Microanalysis Research Facility at the Centre for Microscopy, Characterization & Analysis, The University of Western Australia. This facility is funded by the University, State and Commonwealth Governments.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Fe(C_3H_7NO)_6][Cd_2Cl_7]$
M_r	967.37
Crystal system, space group	Trigonal, $R\overline{3}$
Temperature (K)	100
a, c (Å)	13.7143 (2), 16.1312 (2)
V (Å^3)	2627.51 (5)
Z	3
Radiation type	Cu $K\alpha$
μ (mm^{-1})	18.18
Crystal size (mm)	0.06 × 0.05 × 0.05
Data collection	
Diffractometer	Oxford Diffraction Gemini-R Ultra, Ruby CCD
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.760, 1.0
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	16143, 1051, 980
R_{int}	0.038
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.598
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.020, 0.057, 1.00
No. of reflections	1051
No. of parameters	67
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.79, −0.33

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014/7* (Sheldrick, 2015*b*) and *Mercury* (Macrae *et al.*, 2020).

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supporting information

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Crystal structure of hexakis(*N*,*N*-dimethylformamide-*κO*)iron(III) *μ*-chlorido-bis(trichloridocadmium)

Olga Yu. Vassilyeva, Vladimir N. Kokozay, Svitlana Petrusenko and Alexandre N. Sobolev

Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2015); cell refinement: *CrysAlis PRO* (Rigaku OD, 2015); data reduction: *CrysAlis PRO* (Rigaku OD, 2015); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014/7* (Sheldrick, 2015b); molecular graphics: *Mercury* (Macrae *et al.*, 2020); software used to prepare material for publication: *SHELXL2014/7* (Sheldrick, 2015b).

Hexakis(*N*,*N*-dimethylformamide-*κO*)iron(III) *μ*-chlorido-bis(trichloridocadmium)

Crystal data

$[Fe(C_3H_7NO)_6][Cd_2Cl_7]$
$M_r = 967.37$
Trigonal, $R\bar{3}$
$a = 13.7143\ (2)$ Å
$c = 16.1312\ (2)$ Å
$V = 2627.51\ (5)$ Å^3
$Z = 3$
$F(000) = 1443$
$D_x = 1.834$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 9616 reflections
$\theta = 4.6$–$67.0°$
$\mu = 18.18$ mm^{-1}
$T = 100$ K
Octahedral, dark green
0.06 × 0.05 × 0.05 mm

Data collection

Oxford Diffraction Gemini-R Ultra, Ruby CCD diffractometer
Radiation source: Enhance (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.4738 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2015)
$T_{min} = 0.760$, $T_{max} = 1.0$
16143 measured reflections
1051 independent reflections
980 reflections with $I > 2\sigma(I)$
$R_{int} = 0.038$
$\theta_{max} = 67.2°$, $\theta_{min} = 4.6°$
$h = -16 \rightarrow 15$
$k = -16 \rightarrow 16$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.020$
$wR(F^2) = 0.057$
$S = 1.00$
1051 reflections
67 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0422P)^2 + 4.220P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.79$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	*y*	*z*	$U_{\rm iso}$*/$U_{\rm eq}$
Cd1	0.3333	0.6667	0.32398 (2)	0.01664 (12)
Fe1	0.3333	0.6667	0.6667	0.0139 (2)
O1	0.47367 (14)	0.75401 (14)	0.59890 (10)	0.0200 (4)
N1	0.59569 (16)	0.90250 (17)	0.52091 (12)	0.0187 (4)
C1	0.4941 (2)	0.8248 (2)	0.54225 (15)	0.0191 (5)
H1	0.431 (2)	0.819 (2)	0.5111 (17)	0.023*
C11	0.6967 (2)	0.9151 (2)	0.56042 (17)	0.0257 (6)
H113	0.7392	0.9902	0.5852	0.039*
H111	0.7435	0.9055	0.5189	0.039*
H112	0.6754	0.8579	0.6038	0.039*
C12	0.6127 (2)	0.9772 (2)	0.45107 (16)	0.0244 (5)
H123	0.6547	0.9645	0.4073	0.037*
H121	0.6553	1.0557	0.4696	0.037*
H122	0.5394	0.9614	0.4295	0.037*
Cl1	0.3333	0.6667	0.1667	0.0233 (3)
Cl2	0.51428 (4)	0.69293 (5)	0.36951 (3)	0.02102 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.01759 (14)	0.01759 (14)	0.01476 (17)	0.00879 (7)	0.000	0.000
Fe1	0.0141 (3)	0.0141 (3)	0.0136 (4)	0.00706 (14)	0.000	0.000
O1	0.0207 (8)	0.0213 (8)	0.0183 (8)	0.0107 (7)	0.0051 (6)	0.0042 (7)
N1	0.0201 (10)	0.0195 (10)	0.0164 (10)	0.0097 (8)	0.0014 (8)	−0.0016 (8)
C1	0.0214 (12)	0.0210 (12)	0.0159 (11)	0.0114 (10)	−0.0012 (9)	−0.0029 (10)
C11	0.0225 (13)	0.0261 (13)	0.0290 (14)	0.0126 (11)	−0.0022 (10)	−0.0020 (11)
C12	0.0248 (13)	0.0267 (13)	0.0217 (13)	0.0129 (11)	0.0041 (10)	0.0036 (10)
Cl1	0.0300 (5)	0.0300 (5)	0.0100 (6)	0.0150 (2)	0.000	0.000
Cl2	0.0191 (3)	0.0249 (3)	0.0201 (3)	0.0119 (2)	−0.0019 (2)	−0.0020 (2)

Geometric parameters (Å, º)

Cd1—Cl2^{i}	2.4358 (5)	N1—C11	1.455 (3)
Cd1—Cl2^{ii}	2.4358 (5)	N1—C12	1.461 (3)
Cd1—Cl2	2.4358 (5)	C1—H1	0.97 (3)
Cd1—Cl1	2.5377 (3)	C11—H113	0.9800
Fe1—O1^{iii}	2.0071 (16)	C11—H111	0.9800
Fe1—O1^{ii}	2.0072 (16)	C11—H112	0.9800
Fe1—O1^{i}	2.0072 (16)	C12—H123	0.9800

Fe1—O1	2.0072 (16)	C12—H121	0.9800
Fe1—O1^{iv}	2.0072 (16)	C12—H122	0.9800
Fe1—O1^{v}	2.0072 (16)	Cl1—Cd1^{vi}	2.5376 (3)
O1—C1	1.258 (3)	Cd1—Cd1^{vi}	5.0752 (3)
N1—C1	1.307 (3)		

Cl2^{i}—Cd1—Cl2^{ii}	111.323 (13)	C1—O1—Fe1	129.31 (16)
Cl2^{i}—Cd1—Cl2	111.325 (13)	C1—N1—C11	123.0 (2)
Cl2^{ii}—Cd1—Cl2	111.324 (13)	C1—N1—C12	120.4 (2)
Cl2^{i}—Cd1—Cl1	107.547 (14)	C11—N1—C12	116.51 (19)
Cl2^{ii}—Cd1—Cl1	107.549 (14)	O1—C1—N1	123.8 (2)
Cl2—Cd1—Cl1	107.547 (14)	O1—C1—H1	117.8 (17)
O1^{iii}—Fe1—O1^{ii}	86.85 (7)	N1—C1—H1	118.4 (17)
O1^{iii}—Fe1—O1^{i}	180.0	N1—C11—H113	109.5
O1^{ii}—Fe1—O1^{i}	93.16 (7)	N1—C11—H111	109.5
O1^{ii}—Fe1—O1	93.15 (7)	H113—C11—H111	109.5
O1^{iii}—Fe1—O1	86.84 (7)	N1—C11—H112	109.5
O1^{i}—Fe1—O1	93.15 (7)	H113—C11—H112	109.5
O1^{iii}—Fe1—O1^{iv}	93.16 (7)	H111—C11—H112	109.5
O1^{ii}—Fe1—O1^{iv}	86.85 (7)	N1—C12—H123	109.5
O1^{i}—Fe1—O1^{iv}	86.84 (7)	N1—C12—H121	109.5
O1—Fe1—O1^{iv}	180.0	H123—C12—H121	109.5
O1^{iii}—Fe1—O1^{v}	93.16 (7)	N1—C12—H122	109.5
O1^{ii}—Fe1—O1^{v}	180.00 (8)	H123—C12—H122	109.5
O1^{i}—Fe1—O1^{v}	86.84 (7)	H121—C12—H122	109.5
O1—Fe1—O1^{v}	86.85 (7)	Cd1^{vi}—Cl1—Cd1	180.0
O1^{iv}—Fe1—O1^{v}	93.15 (7)		

Fe1—O1—C1—N1	156.61 (17)	C12—N1—C1—O1	176.2 (2)
C11—N1—C1—O1	0.4 (4)		

Symmetry codes: (i) −*y*+1, *x*−*y*+1, *z*; (ii) −*x*+*y*, −*x*+1, *z*; (iii) *y*−1/3, −*x*+*y*+1/3, −*z*+4/3; (iv) −*x*+2/3, −*y*+4/3, −*z*+4/3; (v) *x*−*y*+2/3, *x*+1/3, −*z*+4/3; (vi) −*x*+2/3, −*y*+4/3, −*z*+1/3.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H123···Cl2^{vii}	0.98	2.82	3.783 (3)	167
C1—H1···Cl2^{i}	0.97 (3)	2.86 (3)	3.772 (3)	158 (2)
C1—H1···O1^{i}	0.97 (3)	2.62 (3)	3.097 (3)	111 (2)
C12—H122···Cl2^{i}	0.98	2.94	3.861 (3)	157

Symmetry codes: (i) −*y*+1, *x*−*y*+1, *z*; (vii) −*x*+4/3, −*y*+5/3, −*z*+2/3.