Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[diaquabis[μ_2-2,4-(dichlorophenoxy)acetato-κ^2O:O']iron(II)]

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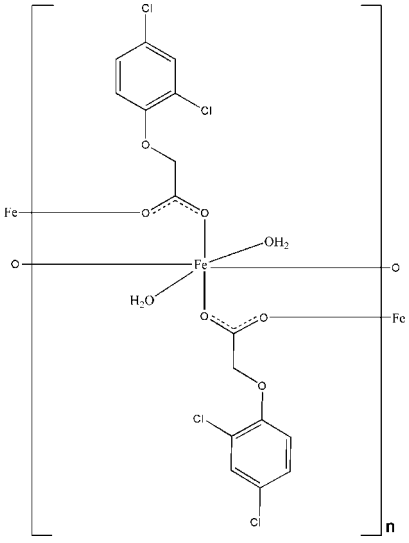
Received 15 August 2008; accepted 12 September 2008

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.035; wR factor = 0.097; data-to-parameter ratio = 13.5.

In the title compound, $[Fe(C_8H_5Cl_2O_3)_2(H_2O)_2]_n$, the Fe^{II} atom is located on an inversion center. It is coordinated by four O atoms from four 2,4-dichlorophenoxyacetate ligands and two water molecules, displaying a distorted octahedral geometry. The carboxylate groups of the 2,4-dichlorophenoxyacetate ligands link the Fe atoms, forming a polymeric layered network in the *bc* plane. Intralayer O—H···O hydrogen bonds enhance the stability of the two-dimensional network.

Related literature

For background on supramolecular networks, see: Eddaoudi *et al.* (2001); Rizk *et al.* (2005).



Experimental

Crystal data

$[Fe(C_8H_5Cl_2O_3)_2(H_2O)_2]$
M_r = 531.92
Monoclinic, $P2_1/c$
a = 17.604 (2) Å
b = 7.3122 (8) Å
c = 8.0312 (9) Å
β = 94.258 (2)°
V = 1031.0 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.29 mm^{-1}
T = 296 (2) K
0.23 × 0.21 × 0.20 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.756, T_{max} = 0.782
5059 measured reflections
1849 independent reflections
1675 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.097
S = 1.05
1849 reflections
137 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Fe1—O3^{i}	2.1654 (17)	Fe1—O1*W*	2.2297 (18)
Fe1—O2	2.1697 (16)		
O3^{i}—Fe1—O2	80.18 (6)	O3^{ii}—Fe1—O1*W*	90.64 (7)
O3^{ii}—Fe1—O2	99.82 (6)	O2^{iii}—Fe1—O1*W*	91.25 (7)
O3^{i}—Fe1—O1*W*	89.36 (7)	O2—Fe1—O1*W*	88.75 (7)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1*W*—H1*W*···O1^{iv}	0.82	2.41	3.051 (3)	135
O1*W*—H2*W*···O3^{iii}	0.82	2.08	2.797 (3)	145

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

The authors acknowledge South China Normal University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2149).

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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2008). E**64**, m1287 [doi:10.1107/S1600536808029279]

Poly[diaquabis[μ_2-2,4-(dichlorophenoxy)acetato-κ^2O:O']iron(II)]

Wei-Bo Pan, Xiao-Hong Xu, Xiao-Hui Huang and Rong-Hua Zeng

S1. Comment

The design, synthesis, characterization and properties of supramolecular networks formed by using functionalized organic molecules as bridges between metal centers are of great interest (Eddaoudi *et al.*, 2001; Rizk *et al.*, 2005). As a building block, 2,4-dichlorophenoxyacetate is an excellent candidate for the construction of supramolecular complexes. Recently, we obtained the title compound, a new coordination polymer.

In the title compound, the Fe^{II} atom is located on an inversion center and coordinated by four O atoms from four 2,4-dichlorophenoxyacetate ligands and two water molecules in an octahedral geometry (Fig. 1; Table 1). The Fe^{II} atoms are linked by 2,4-dichlorophenoxyacetate ligands to form a polymeric layered network in the *bc*-plane (Fig. 2). The two-dimensional network is further stabilized by intralayer O—H···O hydrogen bonds involving the coordinated water molecules and the O atoms from the ligands (Table 2). The adjacent Fe···Fe separation is 5.431 (4) Å.

S2. Experimental

A mixture of $FeCl_2$ (0.127 g, 1 mmol), 2,4-dichlorophenoxyacetic acid (0.221 g, 1 mmol), NaOH (0.04 g, 1 mmol) and water (10 ml) was stirred vigorously for 20 min, and then sealed in a 20 ml Teflon-lined stainless steel autoclave. The autoclave was heated to and maintained at 433 K for 2 d, and then cooled to room temperature at 5 K h^{-1} to afford red block crystals.

S3. Refinement

H atoms of water molecule were located in difference Fourier maps and fixed with $U_{iso}(H) = 1.5U_{eq}(O)$. C-bound H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.97 (CH_2) and 0.93 (CH) Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

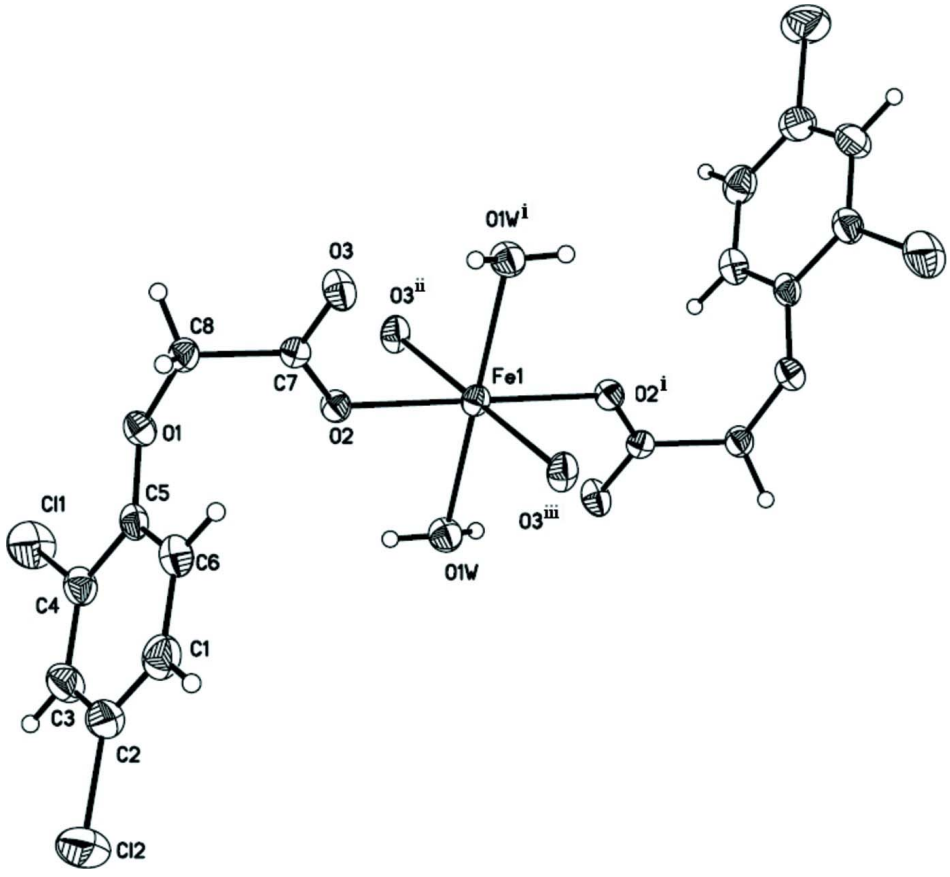

Figure 1

The asymmetric unit of the title compound, together with symmetry-related atoms to complete the coordination units. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i)-x, 1-y, 1-z; (ii) x, 1/2-y, 1/2+z; (iii) -x, 1/2+y, 1/2-z.]

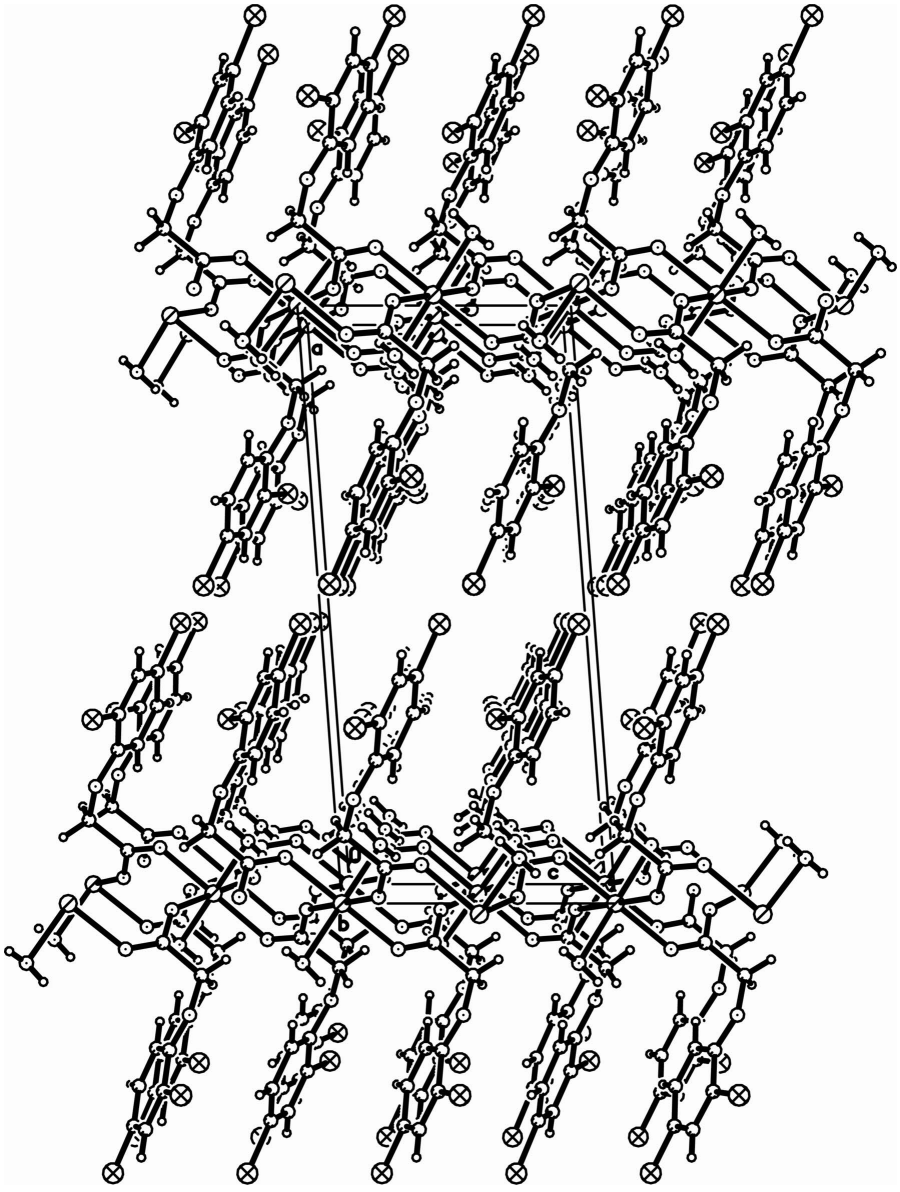

Figure 2

View of the two-dimensional network in the title compound.

Poly[diaquabis[μ_2-(2,4-dichlorophenoxy)acetato-κ^2O:O′]iron(II)]

Crystal data

$[Fe(C_8H_5Cl_2O_3)_2(H_2O)_2]$
M_r = 531.92
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 17.604 (2) Å
b = 7.3122 (8) Å
c = 8.0312 (9) Å
β = 94.258 (2)°
V = 1031.0 (2) Å^3
Z = 2
$F(000)$ = 536
D_x = 1.714 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6377 reflections
θ = 1.7–28.0°
μ = 1.29 mm^{-1}
T = 296 K
Block, colourless
0.23 × 0.21 × 0.20 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.756, T_{max} = 0.782
5059 measured reflections
1849 independent reflections
1675 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 25.2°, θ_{min} = 2.3°
$h = -21 \rightarrow 17$
$k = -8 \rightarrow 8$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.097
S = 1.05
1849 reflections
137 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0473P)^2 + 1.0193P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.0000	0.5000	0.5000	0.03073 (17)
Cl1	0.30460 (6)	0.78166 (12)	0.11801 (14)	0.0735 (3)
Cl2	0.46770 (6)	0.2467 (2)	0.43433 (14)	0.0928 (4)
C5	0.24797 (14)	0.4477 (4)	0.1746 (3)	0.0356 (6)
C4	0.31062 (16)	0.5621 (4)	0.1975 (4)	0.0431 (6)
C1	0.32151 (18)	0.2103 (5)	0.3170 (4)	0.0530 (8)
H1	0.3253	0.0913	0.3575	0.064*
C6	0.25386 (16)	0.2715 (4)	0.2358 (4)	0.0435 (6)
H6	0.2122	0.1932	0.2226	0.052*
C2	0.38251 (18)	0.3256 (5)	0.3371 (4)	0.0565 (8)
C3	0.37794 (18)	0.5028 (5)	0.2792 (4)	0.0553 (8)
H3	0.4195	0.5812	0.2948	0.066*
O1	0.18551 (10)	0.5189 (2)	0.0859 (2)	0.0385 (4)
O2	0.07809 (9)	0.4569 (2)	0.3070 (2)	0.0323 (4)
C7	0.07058 (13)	0.3655 (3)	0.1753 (3)	0.0277 (5)
C8	0.12459 (15)	0.3979 (4)	0.0403 (3)	0.0367 (6)
H8A	0.1456	0.2812	0.0092	0.044*
H8B	0.0958	0.4467	−0.0575	0.044*
O3	0.01927 (10)	0.2497 (2)	0.1419 (2)	0.0407 (4)
O1W	0.09385 (11)	0.6384 (3)	0.6535 (2)	0.0416 (4)
H1W	0.1227	0.6879	0.5917	0.062*
H2W	0.0708	0.7130	0.7070	0.062*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0341 (3)	0.0280 (3)	0.0304 (3)	0.00233 (19)	0.0045 (2)	0.00195 (19)
Cl1	0.0771 (6)	0.0489 (5)	0.0935 (7)	−0.0269 (4)	−0.0007 (5)	0.0116 (4)
Cl2	0.0567 (6)	0.1397 (11)	0.0803 (7)	0.0293 (6)	−0.0068 (5)	0.0080 (7)
C5	0.0338 (13)	0.0400 (13)	0.0344 (13)	−0.0029 (11)	0.0113 (10)	−0.0048 (11)
C4	0.0430 (15)	0.0433 (15)	0.0439 (15)	−0.0095 (12)	0.0089 (12)	−0.0045 (12)
C1	0.0574 (19)	0.0538 (18)	0.0493 (17)	0.0108 (15)	0.0136 (14)	0.0055 (14)
C6	0.0434 (15)	0.0410 (15)	0.0474 (16)	−0.0046 (12)	0.0119 (12)	0.0001 (12)
C2	0.0435 (17)	0.081 (2)	0.0451 (17)	0.0115 (16)	0.0060 (13)	−0.0031 (16)
C3	0.0384 (16)	0.073 (2)	0.0546 (18)	−0.0126 (15)	0.0041 (13)	−0.0088 (16)
O1	0.0344 (10)	0.0370 (10)	0.0444 (10)	−0.0064 (7)	0.0052 (8)	0.0011 (8)
O2	0.0327 (9)	0.0342 (9)	0.0305 (9)	−0.0017 (7)	0.0056 (7)	−0.0074 (7)
C7	0.0291 (12)	0.0234 (11)	0.0305 (12)	0.0049 (9)	0.0025 (9)	0.0012 (9)
C8	0.0369 (13)	0.0429 (15)	0.0306 (12)	−0.0072 (11)	0.0052 (10)	−0.0047 (11)
O3	0.0423 (10)	0.0358 (10)	0.0456 (11)	−0.0128 (8)	0.0140 (8)	−0.0149 (8)
O1W	0.0415 (11)	0.0412 (10)	0.0419 (10)	−0.0042 (9)	0.0030 (8)	−0.0053 (9)

Geometric parameters (Å, º)

Fe1—O3^{i}	2.1654 (17)	C1—H1	0.9300
Fe1—O3^{ii}	2.1654 (17)	C6—H6	0.9300
Fe1—O2^{iii}	2.1697 (16)	C2—C3	1.377 (5)
Fe1—O2	2.1697 (16)	C3—H3	0.9300
Fe1—O1W	2.2297 (18)	O1—C8	1.417 (3)
Fe1—O1W^{iii}	2.2297 (18)	O2—C7	1.250 (3)
Cl1—C4	1.728 (3)	C7—O3	1.253 (3)
Cl2—C2	1.737 (3)	C7—C8	1.513 (3)
C5—O1	1.368 (3)	C8—H8A	0.9700
C5—C6	1.380 (4)	C8—H8B	0.9700
C5—C4	1.386 (4)	O3—Fe1^{iv}	2.1654 (17)
C4—C3	1.381 (4)	O1W—H1W	0.8200
C1—C2	1.365 (5)	O1W—H2W	0.8200
C1—C6	1.389 (4)		
O3^{i}—Fe1—O3^{ii}	180.0	C6—C1—H1	120.1
O3^{i}—Fe1—O2^{iii}	99.82 (6)	C5—C6—C1	120.5 (3)
O3^{ii}—Fe1—O2^{iii}	80.18 (6)	C5—C6—H6	119.8
O3^{i}—Fe1—O2	80.18 (6)	C1—C6—H6	119.8
O3^{ii}—Fe1—O2	99.82 (6)	C1—C2—C3	121.0 (3)
O2^{iii}—Fe1—O2	180.0	C1—C2—Cl2	119.5 (3)
O3^{i}—Fe1—O1W	89.36 (7)	C3—C2—Cl2	119.4 (3)
O3^{ii}—Fe1—O1W	90.64 (7)	C2—C3—C4	118.8 (3)
O2^{iii}—Fe1—O1W	91.25 (7)	C2—C3—H3	120.6
O2—Fe1—O1W	88.75 (7)	C4—C3—H3	120.6
O3^{i}—Fe1—O1W^{iii}	90.64 (7)	C5—O1—C8	117.4 (2)
O3^{ii}—Fe1—O1W^{iii}	89.36 (7)	C7—O2—Fe1	130.51 (15)

O2^{iii}—Fe1—O1W^{iii}	88.75 (7)	O2—C7—O3	124.9 (2)
O2—Fe1—O1W^{iii}	91.25 (7)	O2—C7—C8	119.4 (2)
O1W—Fe1—O1W^{iii}	180.00 (7)	O3—C7—C8	115.7 (2)
O1—C5—C6	125.3 (2)	O1—C8—C7	114.6 (2)
O1—C5—C4	116.1 (2)	O1—C8—H8A	108.6
C6—C5—C4	118.6 (3)	C7—C8—H8A	108.6
C3—C4—C5	121.3 (3)	O1—C8—H8B	108.6
C3—C4—Cl1	119.6 (2)	C7—C8—H8B	108.6
C5—C4—Cl1	119.0 (2)	H8A—C8—H8B	107.6
C2—C1—C6	119.7 (3)	C7—O3—Fe1^{iv}	139.91 (16)
C2—C1—H1	120.1	H1W—O1W—H2W	112

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O1^{v}	0.82	2.41	3.051 (3)	135
O1*W*—H2*W*···O3^{iii}	0.82	2.08	2.797 (3)	145

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