

# Poly[*diaquabis*[ $\mu_2$ -2,4-(dichlorophenoxy)acetato- $\kappa^2$ O:O']iron(II)]

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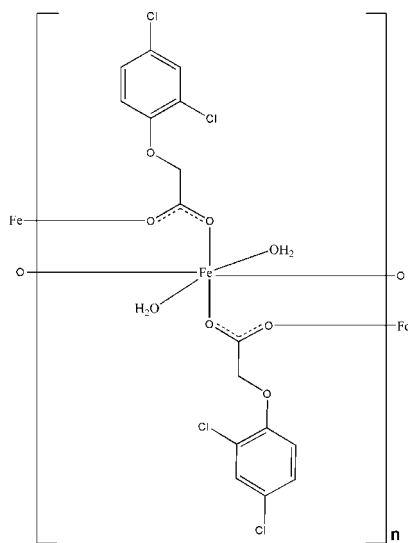
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.035;  $wR$  factor = 0.097; data-to-parameter ratio = 13.5.

In the title compound,  $[\text{Fe}(\text{C}_8\text{H}_5\text{Cl}_2\text{O}_3)_2(\text{H}_2\text{O})_2]_n$ , the  $\text{Fe}^{\text{II}}$  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

$[\text{Fe}(\text{C}_8\text{H}_5\text{Cl}_2\text{O}_3)_2(\text{H}_2\text{O})_2]$   
 $M_r = 531.92$   
 Monoclinic,  $P2_1/c$   
 $a = 17.604$  (2) Å  
 $b = 7.3122$  (8) Å  
 $c = 8.0312$  (9) Å  
 $\beta = 94.258$  (2)°

$V = 1031.0$  (2) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.29$  mm<sup>-1</sup>  
 $T = 296$  (2) K  
 $0.23 \times 0.21 \times 0.20$  mm

### Data collection

Bruker SMART APEXII CCD  
 area-detector diffractometer  
 Absorption correction: multi-scan  
 (SADABS; Bruker, 2001)  
 $T_{\text{min}} = 0.756$ ,  $T_{\text{max}} = 0.782$

5059 measured reflections  
 1849 independent reflections  
 1675 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.021$

### 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  
 $\Delta\rho_{\text{max}} = 0.48$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.48$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Fe1—O3 <sup>i</sup>	2.1654 (17)	Fe1—O1W	2.2297 (18)
Fe1—O2	2.1697 (16)		
O3 <sup>i</sup> —Fe1—O2	80.18 (6)	O3 <sup>iii</sup> —Fe1—O1W	90.64 (7)
O3 <sup>ii</sup> —Fe1—O2	99.82 (6)	O2 <sup>iii</sup> —Fe1—O1W	91.25 (7)
O3 <sup>i</sup> —Fe1—O1W	89.36 (7)	O2—Fe1—O1W	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, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1W...O1 <sup>iv</sup>	0.82	2.41	3.051 (3)	135
O1W—H2W...O3 <sup>iii</sup>	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.

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

## References

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 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

**supplementary materials**

*Acta Cryst.* (2008). E64, m1287 [ doi:10.1107/S1600536808029279 ]

## Poly[diaquabis[ $\mu_2$ -2,4-(dichlorophenoxy)acetato- $\kappa^2O:O'$ ]iron(II)]

W.-B. Pan, X.-H. Xu, X.-H. Huang and R.-H. Zeng

### 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<sup>II</sup> 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<sup>II</sup> 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 $\cdots$ O hydrogen bonds involving the coordinated water molecules and the O atoms from the ligands (Table 2). The adjacent Fe $\cdots$ Fe separation is 5.431 (4) Å.

### Experimental

A mixture of FeCl<sub>2</sub> (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<sup>-1</sup> to afford red block crystals.

### Refinement

H atoms of water molecule were located in difference Fourier maps and fixed with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ . C-bound H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.97 (CH<sub>2</sub>) and 0.93 (CH) Å and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

### Figures

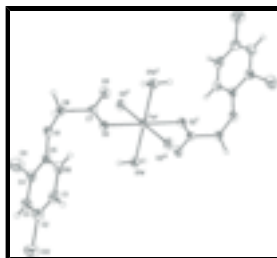


Fig. 1. The asymmetric unit of the title compound, together with symmetry-related atoms to complete the coordination units. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) -x, 1-y, 1-z; (ii) x, 1/2-y, 1/2+z; (iii) -x, 1/2+y, 1/2-z.]

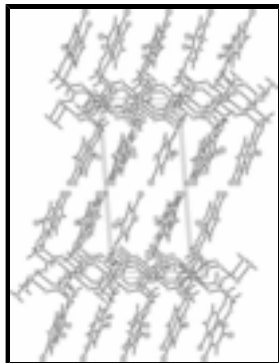


Fig. 2. View of the two-dimensional network in the title compound.

**Poly[*diaquabis*[ $\mu_2$ -(2,4-dichlorophenoxy)acetato- $\kappa^2$ O:O']iron(II)]**

*Crystal data*

[Fe(C<sub>8</sub>H<sub>5</sub>Cl<sub>2</sub>O<sub>3</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]

$M_r = 531.92$

Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$a = 17.604$  (2) Å

$b = 7.3122$  (8) Å

$c = 8.0312$  (9) Å

$\beta = 94.258$  (2)°

$V = 1031.0$  (2) Å<sup>3</sup>

$Z = 2$

$F_{000} = 536$

$D_x = 1.714$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 6377 reflections

$\theta = 1.7$ – $28.0^\circ$

$\mu = 1.29$  mm<sup>-1</sup>

$T = 296$  (2) K

Block, colourless

$0.23 \times 0.21 \times 0.20$  mm

*Data collection*

Bruker SMART APEXII CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 296$ (2) K

$\varphi$  and  $\omega$  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  $I > 2\sigma(I)$

$R_{\text{int}} = 0.021$

$\theta_{\max} = 25.2^\circ$

$\theta_{\min} = 2.3^\circ$

$h = -21 \rightarrow 17$

$k = -8 \rightarrow 8$

$l = -9 \rightarrow 9$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.034$

$wR(F^2) = 0.097$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0473P)^2 + 1.0193P]$

$S = 1.05$

1849 reflections

137 parameters

Primary atom site location: structure-invariant direct methods

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.49 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.48 \text{ e } \text{\AA}^{-3}$

Extinction correction: none

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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 ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
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)

## supplementary materials

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 ( $\text{\AA}$ , $^\circ$ )

Fe1—O3 <sup>i</sup>	2.1654 (17)	C1—H1	0.9300
Fe1—O3 <sup>ii</sup>	2.1654 (17)	C6—H6	0.9300
Fe1—O2 <sup>iii</sup>	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 <sup>iii</sup>	2.2297 (18)	O2—C7	1.250 (3)
C11—C4	1.728 (3)	C7—O3	1.253 (3)
C12—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 <sup>iv</sup>	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 <sup>i</sup> —Fe1—O3 <sup>ii</sup>	180.0	C6—C1—H1	120.1
O3 <sup>i</sup> —Fe1—O2 <sup>iii</sup>	99.82 (6)	C5—C6—C1	120.5 (3)
O3 <sup>ii</sup> —Fe1—O2 <sup>iii</sup>	80.18 (6)	C5—C6—H6	119.8
O3 <sup>i</sup> —Fe1—O2	80.18 (6)	C1—C6—H6	119.8
O3 <sup>ii</sup> —Fe1—O2	99.82 (6)	C1—C2—C3	121.0 (3)
O2 <sup>iii</sup> —Fe1—O2	180.0	C1—C2—C12	119.5 (3)
O3 <sup>i</sup> —Fe1—O1W	89.36 (7)	C3—C2—C12	119.4 (3)
O3 <sup>ii</sup> —Fe1—O1W	90.64 (7)	C2—C3—C4	118.8 (3)
O2 <sup>iii</sup> —Fe1—O1W	91.25 (7)	C2—C3—H3	120.6
O2—Fe1—O1W	88.75 (7)	C4—C3—H3	120.6
O3 <sup>i</sup> —Fe1—O1W <sup>iii</sup>	90.64 (7)	C5—O1—C8	117.4 (2)
O3 <sup>ii</sup> —Fe1—O1W <sup>iii</sup>	89.36 (7)	C7—O2—Fe1	130.51 (15)
O2 <sup>iii</sup> —Fe1—O1W <sup>iii</sup>	88.75 (7)	O2—C7—O3	124.9 (2)
O2—Fe1—O1W <sup>iii</sup>	91.25 (7)	O2—C7—C8	119.4 (2)
O1W—Fe1—O1W <sup>iii</sup>	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—C11	119.6 (2)	C7—C8—H8B	108.6
C5—C4—C11	119.0 (2)	H8A—C8—H8B	107.6
C2—C1—C6	119.7 (3)	C7—O3—Fe1 <sup>iv</sup>	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, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O1W—H1W···O1 <sup>v</sup>	0.82	2.41	3.051 (3)	135
O1W—H2W···O3 <sup>iii</sup>	0.82	2.08	2.797 (3)	145

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

Fig. 1

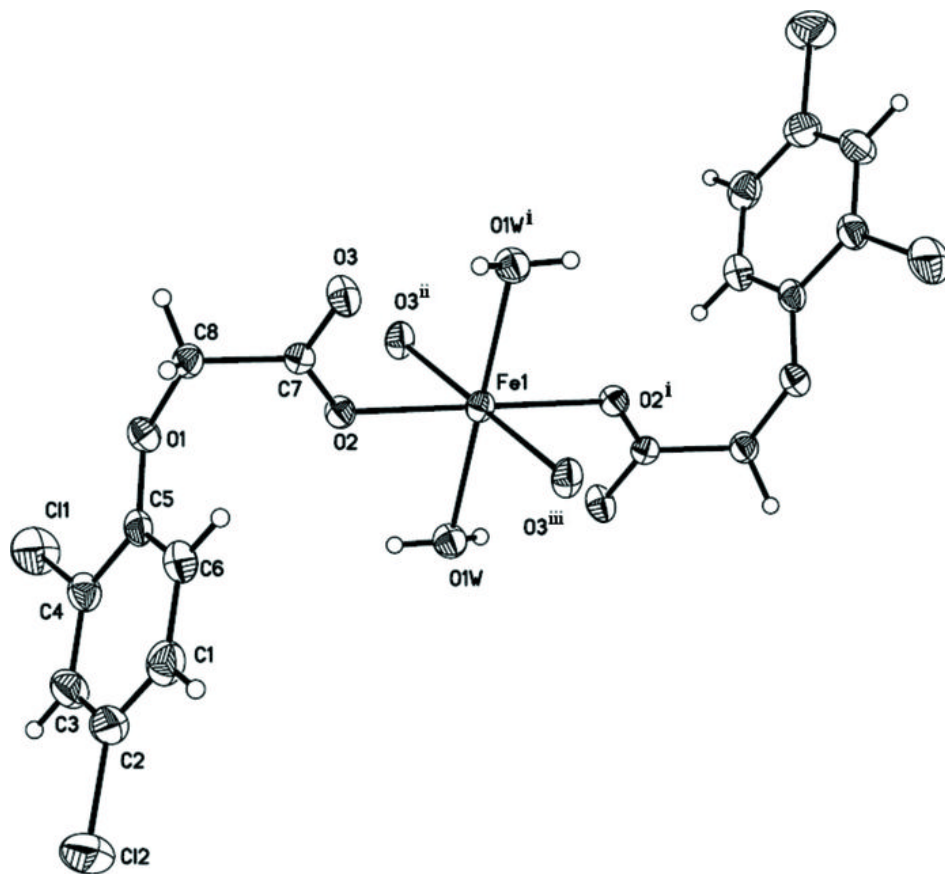


Fig. 2

