

Diaquabis(4-formyl-2-methoxyphenolato)iron(II)

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Key indicators

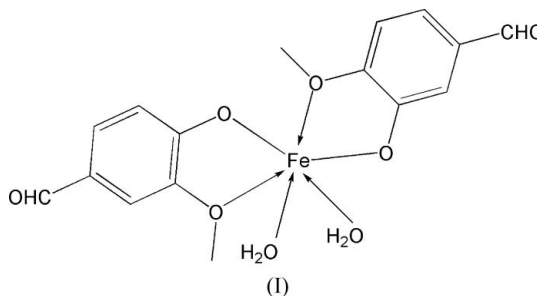
Single-crystal X-ray study
 $T = 291$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.033
 wR factor = 0.103
Data-to-parameter ratio = 16.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

In the title mononuclear iron(II) complex, $[\text{Fe}(\text{C}_8\text{H}_7\text{O}_3)_2(\text{H}_2\text{O})_2]$, the Fe atom, which lies on a twofold rotation axis, is coordinated by four O atoms from two 4-hydroxy-3-methoxybenzaldehyde ligands, and by two O atoms from two water molecules in a distorted octahedral geometry. The molecules are linked by intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds, forming a network.

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Comment

Complexes derived from Schiff bases have played an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures (Costamagna *et al.*, 1992; Bhatia *et al.*, 1981). As an extension of the work on the structural characterization of such complexes, the crystal structure of a mononuclear iron(II) compound, (I), is reported here.



The title complex, (I), is a mononuclear iron(II) compound (Fig. 1), which is isostructural with the manganese(II) complex diaquabis(vanillinato- κ^2O,O')manganese(II) (Gao & Liu, 2005) and the zinc(II) complex *cis*-diaquabis(4-formyl-2-methoxyphenolato)zinc(II) (Lin & Lu, 2005). The Fe^{II} atom, which lies on a twofold rotation axis, is coordinated by two phenolate O atoms and two methoxy O atoms from two 4-hydroxy-3-methoxybenzaldehyde ligands, and by two O atoms from two water molecules in a distorted octahedral geometry (Table 1). The bond lengths are comparable to the values in other iron(II) complexes (Liang *et al.*, 2005; Zhang *et al.*, 2005).

In the crystal structure, the molecules are linked together by intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds, forming a three-dimensional network (Table 2 and Fig. 2).

Experimental

4-Hydroxy-3-methoxybenzaldehyde (0.1 mmol, 15.2 mg) and FeCl_2 (0.1 mmol, 12.7 mg) were dissolved in an aqueous solution (10 ml). The mixture was stirred at room temperature for 30 min and filtered.

After leaving the filtrate to stand in air for 13 d, brown block-shaped crystals were formed.

Crystal data

[Fe(C₈H₇O₃)₂(H₂O)₂]
M_r = 394.15
 Monoclinic, *C*2/*c*
a = 22.431 (2) Å
b = 10.551 (2) Å
c = 7.8463 (7) Å
 β = 106.545 (1)°
V = 1780.1 (4) Å³

Z = 4
D_x = 1.471 Mg m⁻³
 Mo *K*α radiation
 μ = 0.89 mm⁻¹
T = 291 (2) K
 Block, brown
 0.38 × 0.30 × 0.30 mm

Data collection

Bruker APEX area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.733, *T_{max}* = 0.767

6990 measured reflections
 1848 independent reflections
 1738 reflections with *I* > 2σ(*I*)
R_{int} = 0.018
 θ_{\max} = 26.5°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.033
wR (*F*²) = 0.103
S = 1.12
 1848 reflections
 115 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0588P)^2 + 1.5762P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.30 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.30 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Fe1—O1	2.0882 (13)	Fe1—O2	2.3452 (14)
Fe1—O4	2.1100 (14)		
O1—Fe1—O1 ⁱ	156.76 (8)	O1—Fe1—O4 ⁱ	99.28 (6)
O4—Fe1—O2	168.49 (6)	O2—Fe1—O2 ⁱ	91.92 (8)
O1—Fe1—O2	71.94 (5)	O4—Fe1—O2 ⁱ	88.30 (6)
O1—Fe1—O2 ⁱ	91.72 (5)	O4—Fe1—O4 ⁱ	93.78 (9)
O1—Fe1—O4	96.55 (6)		

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

Table 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>
O4—H4 <i>A</i> ...O3 ⁱⁱⁱ	0.84	1.89	2.718 (2)	174
O4—H4 <i>B</i> ...O1 ⁱⁱⁱ	0.84	1.87	2.689 (2)	163

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

Water H atoms were located in a difference Fourier map and their positional parameters and displacement parameters were fixed [*U*_{iso}(H) = 1.2*U*_{eq}(O)]. Other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 or 0.96 Å and *U*_{iso}(H) = 1.2 or 1.5*U*_{eq}(C).

Data collection: SMART (Bruker, 2002); cell refinement: SAINT-Plus (Bruker, 2002); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2002); software used to prepare material for publication: SHELXTL.

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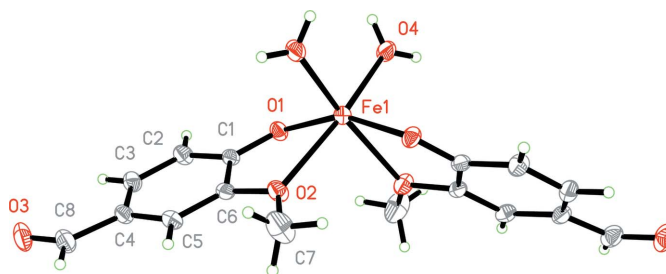


Figure 1

A view of the molecular structure of (I), with the atom-numbering scheme, showing 30% probability displacement ellipsoids and with H atoms are drawn as small spheres of arbitrary radii. Unlabeled atoms are related to labeled atoms by the symmetry operation $(-x + 2, y, -z + \frac{1}{2})$.

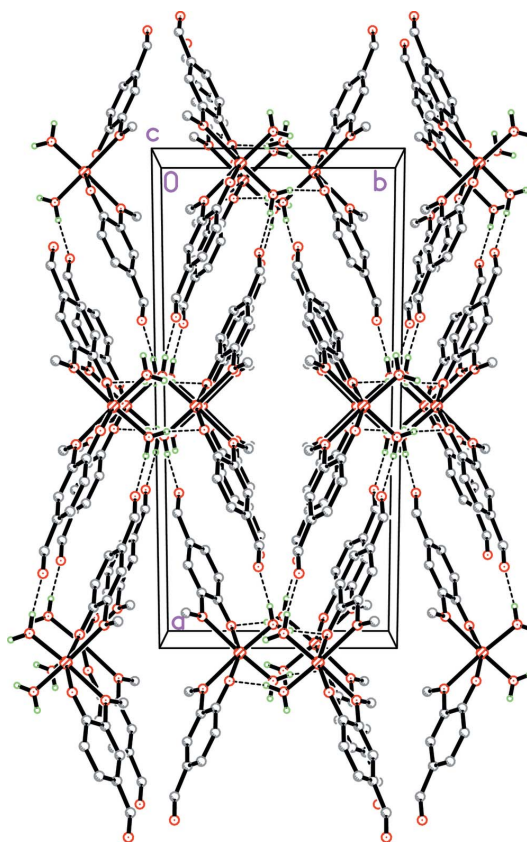


Figure 2

The packing of (I), viewed along the *c* axis. Intermolecular hydrogen bonds are shown as dashed lines.

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