trans-Diaquabis(isoquinoline-1-carboxylato-κ^2N,O)iron(II) dihydrate

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The title complex, [Fe(C$_{10}$H$_6$NO$_2$)$_2$(H$_2$O)$_2$]·2(H$_2$O), has a six-coordinate Fe atom at a center of symmetry, with two bidentate isoquinoline ligands and two water molecules in a *trans* configuration. The coordination bond length of the aqua O atom [2.180 (2) Å] in the axial direction is longer than those of the carboxylato O atom and the ring N atom of the bidentate isoquinoline-1-carboxylate ligand in the equatorial plane [2.091 (2) and 2.153 (2) Å, respectively].

## Comment

Isoquinoline-1-carboxylic acid (IQCA) inhibits the copper enzyme, dopamine β-hydroxylase, which catalyses the biosynthesis of norepinephrine, and lowers endogeneous levels of norepinephrine and epinephrine in the brain, heart, spleen and adrenal glands (Townes *et al.*, 1990). These authors reported the strong binding affinity of IQCA to dopamine β-hydroxylase as compared with the analogous compound, quinoline-2-carboxylic acid (quinaldinic acid) (QCA), which is also a inhibitor of the same enzyme. Based on these findings, it is important to clarify the coordination modes of complexes of IQCA with transition metal ions. Previously, the crystal structures of Cu^{II} (Tomas *et al.*, 1999), Sn^{IV} (Smith *et al.*, 1995), Co^{II} and Ni^{II} (Okabe & Muranishi, 2002) and Zn^{II} (Okabe & Muranishi, 2003) complexes of IQCA have been reported. In this study, we aimed to determine the structure of the Fe^{II} complex of IQCA, (I), in order to clarify the coordination mode of the complex and compare it with other transition metal ion complexes.

(I)
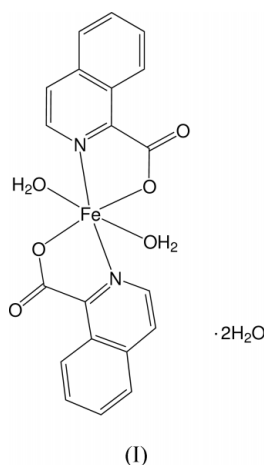
The molecular structure of (I) is shown in Fig. 1. The Fe atom has a distorted octahedral coordination geometry in the *trans* form, defined by two N atoms and two O atoms of two

metal-organic papers
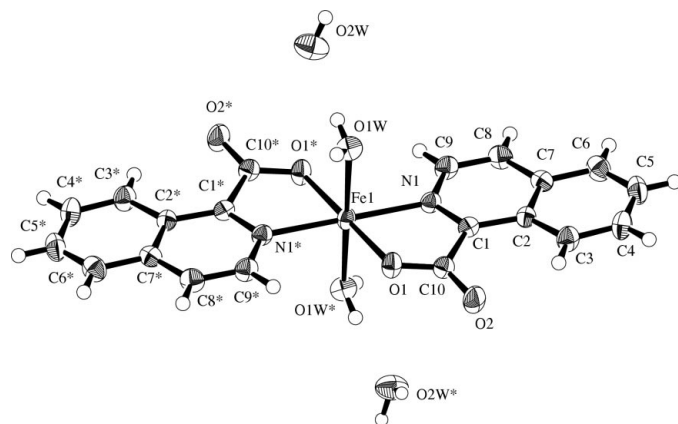
Figure 1
*ORTEP*II (Johnson, 1976) drawing of (I), with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level. Atoms marked with an asterisk (*) are at the symmetry position $(1 - x, 1 - y, 1 - z)$. One of the H atoms of O2W is not visible.

bidentate ligand molecules in the equatorial plane, and two axial aqua O atoms. The Fe atom lies on a center of symmetry. The coordination bond length in the axial direction is longer than those in the equatorial plane (Table 1). A similar coordination geometry is observed in the Co^{II} and Ni^{II} (Okabe & Muranishi, 2002) and Zn^{II} (Okabe & Muranishi, 2003) complexes.

The equatorial M—N(IQCA) coordination bond lengths decrease in the order Fe^{II} [Fe—N = 2.153 (2) Å; this work] > Co^{II} [Co—N = 2.096 (2) Å; Okabe & Muranishi, 2002] > Ni^{II} [Ni—N = 2.039 (3) Å; Okabe & Muranishi, 2002] > Cu^{II} [Cu—N = 1.969 (3) and 1.957 (3) Å; Tomas *et al.*, 1999] < Zn^{II} [Zn—N = 2.084 (3) Å; Okabe & Muranishi, 2003]. The M—O(IQCA) bond lengths also decrease in the same order: Fe^{II} [Fe—O = 2.091 (2) Å; this work] > Co^{II} [Co—O = 2.055 (2) Å; Okabe & Muranishi, 2002] > Ni^{II} [Ni—O = 2.036 (2) Å; Okabe & Muranishi, 2002] > Cu^{II} [Cu—O = 1.927 (3) & 1.928 (3) Å; Tomas *et al.*, 1999] < Zn^{II} [Zn—O = 2.068 (2) Å; Okabe & Muranishi, 2003]. These results indicate that the order of stability of these complexes corresponds to the well known Irving–Williams series, Fe < Co < Ni < Cu > Zn. As observed in the tin(IV) complex of isoquinoline-1-carboxylate (Smith *et al.*, 1995), the C1—C10 distance of 1.535 (4) Å is longer than the normal Csp^2—Csp^2 bond length.

In the crystal structure, neighbouring isoquinoline rings are stacked in the **c** direction, the distance between the centroids of benzene rings at the symmetry position $(-x, 1 - y, 1 - z)$ being 3.988 (3) Å. Hydrogen bonds are formed between the carboxylate group, the coordinated water and the uncoordinated water molecules (Table 2).

Experimental

Red plate-shaped crystals of (I) were obtained by slow evaporation of a methanol–water solution (50:50%, *v/v*) of a mixture of IQCA and FeCl$_2$·6H$_2$O (molar ratio 4:1).

Table 1
Selected geometric parameters (Å, °).

Fe1—O1	2.091 (2)	Fe1—N1	2.153 (2)
Fe1—O1W	2.180 (2)		
O1—Fe1—O1W	89.74 (7)	O1W—Fe1—N1	89.00 (8)
O1—Fe1—N1	76.47 (8)		

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1W—H1A$\cdots$O1^i	0.80	2.02	2.810 (3)	170
O1W—H1B$\cdots$O2W	0.81	2.01	2.822 (3)	177
O2W—H2A$\cdots$O2W^{ii}	0.80	2.20	2.949 (3)	156
O2W—H2B$\cdots$O2^{iii}	0.80	1.93	2.717 (3)	171

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

All H atoms were located in a difference Fourier maps, and treated using a riding model [O—H = 0.80–0.82 Å, C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(parent atom)].

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1994); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation & Rigaku Corporation, 2000); program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *TEXSAN*.

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