

***trans*-Diaquabis(isoquinoline-1-carboxylato- $\kappa^2$ N,O)zinc(II) dihydrate****Nobuo Okabe\* and Yasunori Muranishi**

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**Key indicators**

Single-crystal X-ray study

 $T = 296$  KMean  $\sigma(\text{C}-\text{C}) = 0.005$  Å $R$  factor = 0.036 $wR$  factor = 0.129

Data-to-parameter ratio = 15.8

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title complex,  $[\text{Zn}(\text{C}_{10}\text{H}_6\text{NO}_2)_2(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$ , has a distorted octahedral coordination, in which the  $\text{Zn}^{\text{II}}$  atom lies on a centre of symmetry. The coordination bond length of the aqua O atom, 2.208 (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 [2.068 (2) and 2.084 (3) Å, respectively].

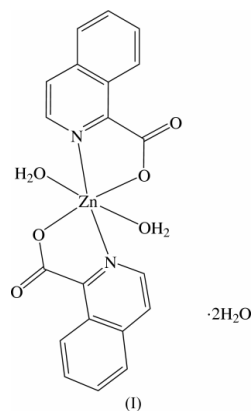
Received 2 April 2003

Accepted 8 April 2003

Online 23 April 2003

**Comment**

Isoquinoline-1-carboxylic acid (IQCA) inhibits the copper enzyme, dopamine  $\beta$ -hydroxylase (Townes *et al.*, 1990). Previously, the crystal structures of the  $\text{Cu}^{\text{II}}$  (Tomas *et al.*, 1999),  $\text{Sn}^{\text{IV}}$  (Smith *et al.*, 1995),  $\text{Co}^{\text{II}}$  and  $\text{Ni}^{\text{II}}$  complexes (Okabe & Muranishi, 2002) of IQCA have been reported, establishing the coordination modes of the complexes. In this study, we sought to determine the structure of the  $\text{Zn}^{\text{II}}$  complex (I), because  $\text{Zn}^{\text{II}}$  has many important biological functions, for example as a catalytic ion in many enzymes such as alcohol dehydrogenase (Esposito *et al.*, 2002), or a zinc finger motif in a ribosomal protein (Dresios *et al.*, 2002) or an insulin-mimetic complex in metallopharmaceutical compounds (Sakurai *et al.*, 2002).



The molecular structure of (I) is shown in Fig. 1. The  $\text{Zn}^{\text{II}}$  atom has a distorted octahedral coordination, in the *trans* form, defined by two N atoms and two O atoms of the two bidentate ligands in the equatorial plane, and two axial aqua O atoms. The Zn atom lies on a centre of symmetry. The coordination mode of (I) strongly resembles that of the  $\text{Co}^{\text{II}}$  and  $\text{Ni}^{\text{II}}$  complexes (Okabe & Muranishi, 2002). The coordination bond length in the axial direction [ $\text{Zn1}-\text{O1W}$  2.208 (2) Å] is longer than those in the equatorial plane (Table 1). The O—Zn—N chelate angle of the five-membered ring, 78.91 (10)°, is larger than in the  $\text{Co}^{\text{II}}$  complex, 78.25 (7)°, but smaller than in both the  $\text{Ni}^{\text{II}}$  complex, 80.00 (9)° (Okabe & Muranishi, 2002), and the  $\text{Cu}^{\text{II}}$  complex, 82.96 (12)° for one of

the two isoquinoline-1-carboxylate ligands and 83.15 (12)° for the second (Tomas *et al.*, 1999). The coordinated *M*–*N* bond lengths are 2.096 (2) (Co<sup>II</sup>), 2.039 (3) (Ni<sup>II</sup>), 2.084 (3) (Zn<sup>II</sup>), and 1.957 (3) and 1.969 (3) Å (Cu<sup>II</sup>). These results indicate that the order of stability of these complexes corresponds to the well known Irving–Williams series, Co<sup>II</sup> < Ni<sup>II</sup> < Cu<sup>II</sup> > Zn<sup>II</sup>. In the crystal structure, the isoquinoline rings are stacked with respect to each other, with a mean separation distance of 3.392 (5) Å, in a manner similar to that in the Co<sup>II</sup> and Ni<sup>II</sup> complexes (Okabe & Muranishi, 2002). Hydrogen bonds are formed between the coordinated water, the carboxylate group and the uncoordinated water molecules (Table 2).

### Experimental

Colorless plate-shaped crystals of (I) were obtained by slow evaporation of a methanol–water solution (90:10%, v/v) of a mixture of isoquinoline-1-carboxylic acid and ZnSO<sub>4</sub>·7H<sub>2</sub>O (molar ratio 4:1).

#### Crystal data

[Zn(C <sub>10</sub> H <sub>6</sub> NO <sub>2</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> ] <sub>2</sub> ·2H <sub>2</sub> O	<i>D</i> <sub>x</sub> = 1.628 Mg m <sup>-3</sup>
<i>M</i> <sub>r</sub> = 481.77	Mo Kα radiation
Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>n</i>	Cell parameters from 25 reflections
<i>a</i> = 12.224 (1) Å	<i>θ</i> = 12.8–14.5°
<i>b</i> = 5.341 (2) Å	<i>μ</i> = 1.30 mm <sup>-1</sup>
<i>c</i> = 15.191 (1) Å	<i>T</i> = 296.2 K
<i>β</i> = 97.625 (7)°	Plate, colorless
<i>V</i> = 983.0 (4) Å <sup>3</sup>	0.30 × 0.10 × 0.05 mm
<i>Z</i> = 2	

#### Data collection

Rigaku AFC-5R diffractometer	<i>R</i> <sub>int</sub> = 0.026
<i>ω</i> –2 <i>θ</i> scans	<i>θ</i> <sub>max</sub> = 27.5°
Absorption correction: <i>ψ</i> scan (North <i>et al.</i> , 1968)	<i>h</i> = 0 → 15
<i>T</i> <sub>min</sub> = 0.855, <i>T</i> <sub>max</sub> = 0.937	<i>k</i> = 0 → 6
2598 measured reflections	<i>l</i> = –19 → 19
2247 independent reflections	3 standard reflections
1477 reflections with <i>I</i> > 2σ( <i>I</i> )	every 150 reflections
	intensity decay: 0.4%

#### Refinement

Refinement on <i>F</i> <sup>2</sup>	H-atom parameters constrained
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )] = 0.036	<i>w</i> = 1/[σ <sup>2</sup> ( <i>F</i> <sub>o</sub> <sup>2</sup> ) + (0.1 <i>P</i> ) <sup>2</sup> ]
<i>wR</i> ( <i>F</i> <sup>2</sup> ) = 0.129	where <i>P</i> = ( <i>F</i> <sub>o</sub> <sup>2</sup> + 2 <i>F</i> <sub>c</sub> <sup>2</sup> )/3
<i>S</i> = 0.82	(Δ/σ) <sub>max</sub> < 0.001
2247 reflections	Δ <i>ρ</i> <sub>max</sub> = 0.32 e Å <sup>-3</sup>
142 parameters	Δ <i>ρ</i> <sub>min</sub> = –0.33 e Å <sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

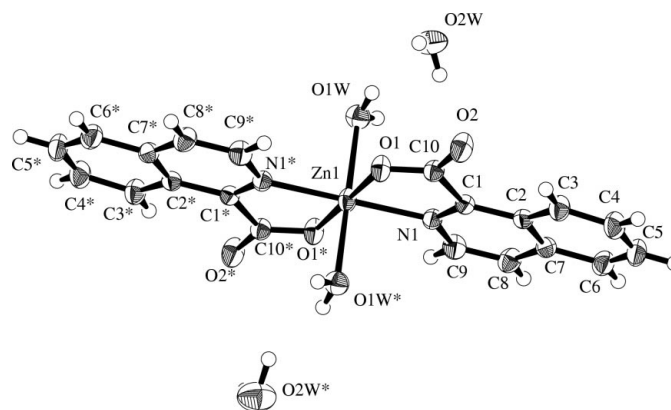
Zn1–O1	2.068 (2)	Zn1–N1	2.084 (3)
Zn1–O1W	2.208 (2)		
O1–Zn1–O1W	90.11 (9)	O1W–Zn1–N1	91.71 (9)
O1–Zn1–N1	78.91 (10)	Zn1–O1–C10	115.4 (2)

**Table 2**

Hydrogen-bonding 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–H1A...O1 <sup>i</sup>	0.81	2.03	2.831 (3)	169
O1W–H1B...O2W <sup>ii</sup>	0.82	2.01	2.830 (4)	172
O2W–H2A...O2	0.82	1.90	2.721 (4)	175
O2W–H2B...O2W <sup>iii</sup>	0.82	2.17	2.944 (3)	157

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



**Figure 1**

ORTEP (Johnson, 1976) drawing of (I), with the atomic numbering scheme. Ellipsoids for non-H atoms are drawn at the 50% probability level. Atoms marked with an asterisk (\*) are at the symmetry-related positions (–*x*, –*y*, –*z*).

H atoms were treated in the riding model approximation.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, Rigaku Corporation, 2000); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999) & *DIRDIF94* (Beurskens *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP* (Johnson, 1976); software used to prepare material for publication: *TEXSAN*.

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