Acta Crystallographica Section E
**Structure Reports**
**Online**
ISSN 1600-5368

# Aquabis(quinoline-2-carboxylato-$\kappa^2N,O$)zinc(II)

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Received 31 March 2003
Accepted 7 April 2003
Online 16 April 2003

**Key indicators**

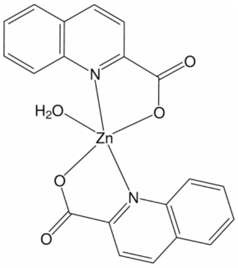
Single-crystal X-ray study
$T$ = 296 K
Mean $\sigma$(C–C) = 0.008 Å
$R$ factor = 0.049
$wR$ factor = 0.170
Data-to-parameter ratio = 15.8

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

In the title compound, $[Zn(C_{10}H_7NO_3)_2(H_2O)]$, the Zn atom is pentacoordinated and has a square pyramidal geometry. The Zn atom is coordinated by two N and two O atoms of the two organic ligands, forming the square plane. One aqua O atom occupies the vertex of the square pyramid. The N and O atoms of the ligands lie in *trans* positions with respect to each other.

## Comment

Quinoline-2-carboxylic acid is a tryptophan metabolite (Martell & Smith, 1974). The crystal structures of its metal complexes have been determined for copper(II) (Haendler, 1986), manganese(II) (Haendler, 1996; Okabe & Koizumi, 1997), iron(II), cobalt(II) (Okabe & Makino, 1998, 1999), zinc(II) (Zevaco *et al.*, 1998), nickel(II) (Odoko *et al.*, 2001) and vanadium(IV) (Okabe & Muranishi, 2002) complexes. Of these complexes, the Zn complex is considered to be an efficient catalyst for potential carbon dioxide activation (Zevaco *et al.*, 1998). The Zn complex has been characterized as the anhydrous complex (Zevaco *et al.*, 1998), $[Zn(2\text{-quinolinecarboxylato})_2(1\text{-methylimidazole})_2]$, in which the Zn atom is hexacoordinated, and exhibits a slightly distorted octahedral geometry. The structure of the title Zn complex, (I), with a square-pyramidal geometry is shown in Fig. 1, and selected geometric parameters are listed in Table 1.



(I)

The Zn atom is pentacoordinated. The structure of (I) resembles the Cu complex (Haendler, 1986). The Zn atom is coordinated by two N and two O atoms of the two quinaldinate ligands, which form the square plane, and one aqua O atom occupies the vertex of the square pyramid. The N and O atoms of the ligands lie in *trans* positions with respect to each other. The organic ligands and the central Zn atom form five-membered rings, which are usually observed in metal compounds of quinoline-2-carboxylic acid (Okabe & Makino, 1999). The Zn—O(carboxylate) and Zn—N distances in (I) (Table 1) are shorter than those in the hexacoordinated Zn complex with octahedral geometry (Zevaco *et al.*, 1998), which

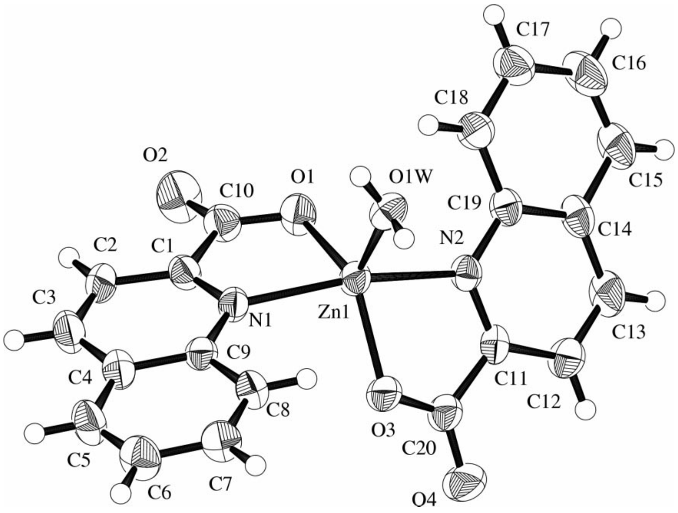


**Figure 1**
*ORTEP*II (Johnson, 1976) drawing of the title compound, with the atomic numbering scheme and 50% probability ellipsoids.

may indicate a greater stability of the Zn complex in a square pyramidal coordination than in a distorted octahedral geometry. In the crystal packing, shown in Fig. 2, quinoline rings of the complex form stacks along the *b* axis. The water molecules form a hydrogen-bonding network (Table 2).

## Experimental

The purple plate crystal was obtained by slow evaporation from a mixture of quinoline-2-carboxylic acid and $Fe(NH_4)_2(SO_4)_2 \cdot 6H_2O$ (4:1) dissolved in water.

*Crystal data*

$[Zn(C_{10}H_7NO_3)_2(H_2O)]$
$M_r = 427.72$
Monoclinic, $P2_1/c$
$a = 7.716$ (4) Å
$b = 7.564$ (6) Å
$c = 30.037$ (3) Å
$\beta = 95.97$ (2)°
$V = 1743.6$ (17) Å$^3$
$Z = 4$

$D_x = 1.629$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 22 reflections
$\theta = 12.2$–14.4°
$\mu = 1.45$ mm$^{-1}$
$T = 296.2$ K
Plate, purple
0.20 × 0.15 × 0.10 mm

*Data collection*

Rigaku AFC-5*R* diffractometer
$\omega$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{\min} = 0.771$, $T_{\max} = 0.865$
4602 measured reflections
3985 independent reflections
2001 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.048$
$\theta_{\max} = 27.5°$
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 9$
$l = -39 \rightarrow 38$
3 standard reflections
every 150 reflections
intensity decay: none

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.170$
$S = 0.89$
3985 reflections
253 parameters

H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.72$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.45$ e Å$^{-3}$

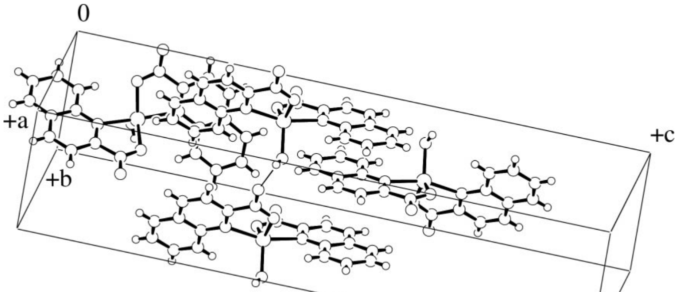


**Figure 2**
Molecular packing of (I).

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Zn1—O1 | 2.017 (4) | Zn1—N1 | 2.144 (4) |
| Zn1—O1*W* | 1.986 (3) | Zn1—N2 | 2.147 (4) |
| Zn1—O3 | 1.994 (4) | | |
| O1—Zn1—O1*W* | 112.2 (1) | O1*W*—Zn1—N1 | 101.4 (1) |
| O1—Zn1—O3 | 127.3 (2) | O1*W*—Zn1—N2 | 97.0 (1) |
| O1—Zn1—N1 | 79.9 (1) | O3—Zn1—N1 | 92.5 (1) |
| O1—Zn1—N2 | 92.0 (1) | O3—Zn1—N2 | 79.2 (1) |
| O1*W*—Zn1—O3 | 120.4 (2) | N1—Zn1—N2 | 161.6 (1) |

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H1*B*···O2$^{\rm i}$ | 0.82 | 1.81 | 2.616 (5) | 168 |
| O1*W*—H1*A*···O4$^{\rm ii}$ | 0.82 | 1.82 | 2.620 (5) | 165 |

Symmetry codes: (i) $x, 1+y, z$; (ii) $1+x, y, z$.

All H atoms were located from a difference Fourier map, and the H atoms of the quinoline rings were replaced at ideal positions by riding models using *SHELXL* defaults. The H atoms of the water molecules were left at the positions located in the Fourier map, and were not idealized.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation and Rigaku, 1999); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation and Rigaku, 1999); program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1999) and *DIRDIF*94 (Beurskens *et al.*, 1992); 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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