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

# Diaquabis(8-quinolinolato-$\kappa^2N,O$)zinc(II)

**Zhen-Feng Chen,[a] Ming Zhang,[a] Shao-Ming Shi,[a] Ling Huang,[a] Hong Liang[a]* and Zhong-Yuan Zhou[b]**

[a]College of Chemistry and Chemical Engineering, Guangxi Normal University, Guilin 541004, People's Republic of China, and [b]Department of Applied Biology and Chemical Technology Chemistry, Hong Kong Polytechnic University, Hong Kong, People's Republic of China

Correspondence e-mail:
chenzfgxnu@yahoo.com

Received 18 July 2003
Accepted 18 August 2003
Online 30 August 2003

The crystal structure of the title compound, $[Zn(C_9H_6NO)_2(H_2O)_2]$, has been redetermined with better $R$ factors ($R_1$ = 0.0471) and higher accuracy than in previous publications. The molecule is centrosymmetric.

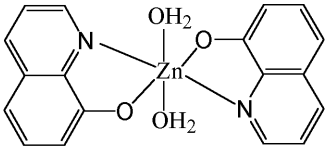
**Key indicators**

Single-crystal X-ray study
$T$ = 294 K
Mean $\sigma$(C–C) = 0.004 Å
$R$ factor = 0.042
$wR$ factor = 0.117
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.

## Comment

8-Quinolinol has been widely used in the quantitative analysis of W and Mo (Marcel & Rene, 1950). The complexes of 8-quinolinol with Nb, Mo, W and Hf emit interesting fluorescence (Schneider & Roselli, 1970). The crystal structure of the title compound, (I), was originally determined by Merrit *et al.* (1954) with $R_1$ = 0.226, and was then refined by Palenik (1964) to $R_1$ = 0.13. Here, we present the results of a redetermination of the structure of (I) with better $R$ factors ($R_1$ = 0.0471) and higher accuracy. The molecule is centrosymmetric.



(I)

In (I), the Zn$^{II}$ atom is six-coordinate, to one N and one O atom from each of the two 8-quinolinolate ligands and to one O atom from each of the two aqua ligands. This $ZnO_4N_2$ coordination forms an octahedral geometry (Fig. 1). The chelate ligands are connected to the central atom through a Zn—O [1.9655 (18) Å] single bond and a Zn—N [2.011 (2) Å] coordinative bond, with a bite angle of 83.88 (8)°, and they occupy the equatorial plane. The two aqua ligands occupy the apical positions of the octahedron.

The bond angles in the aromatic ring system of (I) are between 118.2 (5) and 121.7 (5)°. In the 8-quinolinolate ligands, the absence of any unusually long bonds and the

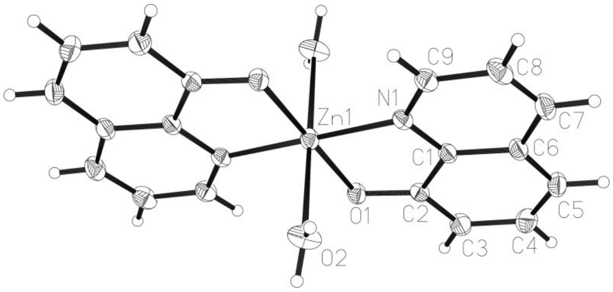


**Figure 1**
A view of the molecule of (I) showing the atom-numbering scheme and with 30% probability displacement ellipsoids.

marginally longer carbonyl bond [1.355 (6) Å *versus* 1.28 Å], shorter than the normal single bond in ether and alcohols (>1.4 Å), suggest that the delocalization extends over the entire molecule and will therefore withdraw more negative charge from the cation (Barton *et al.*, 1983).

The coordinated water molecules of (I) interact with the O atom of the 8-quinolinolato ligands *via* intermolecular hydrogen bonds (Table 1). These hydrogen bonds interconnect the molecules into chains along the **c** direction (Fig. 2).

## Experimental

An ethanolic solution of 8-quinolinol (2 mmol in 20 ml of ethanol) was mixed with $Zn(OAc)_2$ (1 mmol in 20 ml of $H_2O$). The resulting solution was left to stand for 5 h and a pale-yellowish solid was obtained. The product was recrystallized from ethanol–water. After several days, pale-yellowish crystals of (I) were harvested. Analysis, found: C 55.41, H 4.23, N 7.42%; calculated: C 55.48, H 4.14, N 7.19%.

*Crystal data*

$[Zn(C_9H_6NO)_2(H_2O)_2]$
$M_r = 389.70$
Monoclinic, $P2_1/c$
$a = 12.955$ (2) Å
$b = 5.5463$ (10) Å
$c = 11.423$ (2) Å
$\beta = 106.288$ (4)°
$V = 787.8$ (2) Å$^3$
$Z = 2$
$D_x = 1.643$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 2881 reflections
$\theta = 1$–27.5°
$\mu = 1.59$ mm$^{-1}$
$T = 294$ (2) K
Plate, yellow
0.30 × 0.24 × 0.12 mm

*Data collection*

Siemens SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.648$, $T_{max} = 0.833$
5060 measured reflections
1820 independent reflections
1382 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 27.6°$
$h = -15 \rightarrow 16$
$k = -5 \rightarrow 7$
$l = -14 \rightarrow 14$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.117$
$S = 1.02$
1820 reflections
115 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0725P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.60$ e Å$^{-3}$
$\Delta\rho_{min} = -0.37$ e Å$^{-3}$

**Table 1**
Hydrogen-bonding geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2—H2$A$···O1$^{i}$ | 0.85 | 1.99 | 2.841 (3) | 174 |
| O2—H2$B$···O1$^{ii}$ | 0.85 | 1.99 | 2.829 (3) | 169 |

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

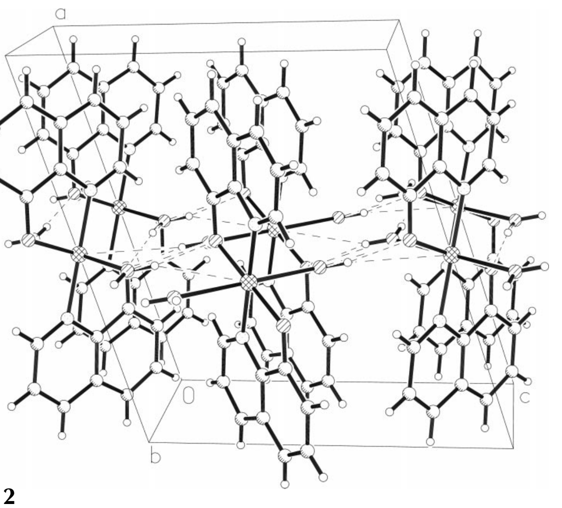


**Figure 2**
Packing view of (I). Hydrogen bonds are indicated by dashed lines.

The H atoms of the water ligands were located in a difference Fourier map and refined with a common isotropic displacement parameter. O—H and H···H distances were restrained to ensure a reasonable geometry for the water molecules. H atoms bound to C atoms were fixed geometrically and were treated as riding on the parent C atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2$–$1.5U_{eq}(C)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SHELXTL* (Siemens, 1996); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors thank the Youth Science Foundation of Guangxi of the People's Republic of China and the Natural Science Foundation of the Guangxi Chuang Autonomous Region of the People's Republic of China, as well as the project of the One Hundred Plan of Guangxi Universities, People's Republic of China.

## References

Barton, R. J., Dabeka, R. W., Shengzhi, H., Mihichuk, L. M., Pizzey, M., Robertson, B. E. & Wallace, W. J. (1983). *Acta Cryst.* C**39**, 714–717.
Marcel, B. & Rene, P. (1950). *Anal. Chim. Acta*, **4**, 476–479.
Merrit, L. L., Cady, R. T. & Mundy, B. W. (1954). *Acta Cryst.* **7**, 473–476.
Palenik, G. J. (1964). *Acta Cryst.* **17**, 696–700.
Schneider, H. O. & Roselli, M. E. (1970). *An. Asoc. Quim. Argent.* **58**, 191–205.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Siemens (1996). *SMART* (Version 4.0) and *SHELXTL* (Version 5.06). Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

*Acta Cryst.* (2003). E**59**, m814–m815 Zhen-Feng Chen *et al.* • $[Zn(C_9H_6NO)_2(H_2O)_2]$ **m815**