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Aquabis(2-methylquinolin-8-olato-κ^2N,O)zinc(II)

Luiz Everson da Silva,[a] Antonio Carlos Joussef,[b] Ricardo Andrade Rebelo,[c] Sabine Foro[d] and Boris Schmidt[d]*

[a]Departamento de Química–UFSC, 88040-900 Florianópolis, SC, Brazil, and Clemens Schöpf-Institut für Organische Chemie und Biochemie, Technische Universität Darmstadt, Petersenstrasse 22, D-64287 Darmstadt, Germany, [b]Departamento de Química–UFSC, 88040-900 Florianópolis, SC, Brazil, [c]Fundação Universidade Regional de Blumenau, Centro de Ciências Exatas e Naturais, Brazil, and [d]Clemens Schöpf-Institut für Organische Chemie und Biochemie, Technische Universität Darmstadt, Petersenstrasse 22, D-64287 Darmstadt, Germany

Correspondence e-mail: foro@tu-darmstadt.de

Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.012 Å
R factor = 0.062
wR factor = 0.154
Data-to-parameter ratio = 12.3

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

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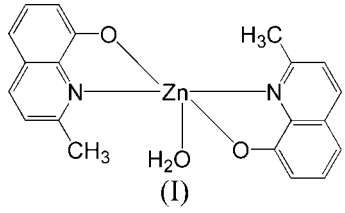
The title molecule, $[Zn(C_{10}H_8NO)_2(H_2O)]$, lies on a crystallographic twofold axis. The Zn^{II} atom is in a trigonal–bipyramidal coordination geometry formed by two N atoms of two quinoline groups, two O atoms and a water molecule. In the crystal structure, intermolecular hydrogen bonds link molecules into a two-dimensional network.

Comment

Hydroxyquinolines and their derivatives are well known complexing agents in analytical chemistry (Czugler *et al.*, 2001). In addition, metal chelators based on the quinoline core have been developed as potential agents for neuroprotection in neurogenerative diseases (Zheng *et al.*, 2005). In this context, clioquinol is a leading compound being investigated as a biomarker for β-amyloid Zn^{II} complexes in Alzheimer's disease (Opazo *et al.*, 2006). We have an interest in investigating new metal-chelator probes for neuroprotection in neurogenerative diseases (da Silva *et al.*, 2006*a*,*b*,*c*,*d*,*e*). The crystal structure of the title compound, (I), is reported here.



(I)

The molecular structure of (I) is shown in Fig. 1. The Zn atom is in a trigonal–bipyramidal coordination geometry formed by two N atoms of two quinoline groups, two O atoms and a water molecule. The Zn atom and the water O atom both lie on a crystallographic twofold axis. Selected bond distances and angles are given in Table 1. The hydroxyquinoline ligands are bis-chelating through the quinoline N atom and the O atom, forming a five-membered ring including the Zn atom.

In the crystal structure, two intermolecular hydrogen bonds link the molecules into a two-dimensional network (Fig. 2 and Table 2).

Experimental

The title compound was prepared according to a literature procedure (Macías *et al.*, 2003). 2-Methyl-8-quinolinol (1.5 mmol) was dissolved in methanol (75 ml) and aqueous ammonia (2 ml M NH_4OH) aqueous ammonia was added. During stirring of this solution, $ZnCl_2$ (0.75 mmol) dissolved in methanol (50 ml) was added dropwise. When the addition was complete, a green precipitate was formed

which was separated by filtration (yield 80%). Single crystals of (I) suitable for X-ray data collection appeared after 2 d from a methanol solution.

Crystal data

$[Zn(C_{10}H_8NO)_2(H_2O)]$
M_r = 399.73
Orthorhombic, *Pbcn*
a = 7.284 (1) Å
b = 9.131 (2) Å
c = 25.199 (5) Å
V = 1676.0 (5) Å^3
Z = 4
D_x = 1.584 Mg m^{-3}
Cu $K\alpha$ radiation
μ = 2.23 mm^{-1}
T = 299 (2) K
Block, light red
0.20 × 0.10 × 0.08 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.615, T_{max} = 0.841
2878 measured reflections
1499 independent reflections
655 reflections with $I > 2\sigma(I)$
R_{int} = 0.198
θ_{max} = 67.0°
3 standard reflections
frequency: 120 min
intensity decay: 1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.154
S = 0.93
1499 reflections
122 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.010
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—Zn1	2.114 (5)	O2—Zn1	2.103 (6)
O1—Zn1	2.022 (5)		
O1^i—Zn1—O1	125.0 (3)	O1—Zn1—N1	80.4 (2)
O1—Zn1—O2	117.48 (14)	O2—Zn1—N1	89.97 (18)
O1^i—Zn1—N1	99.6 (2)	N1—Zn1—N1^i	179.9 (4)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2O···O1^{ii}	0.92 (7)	1.82 (7)	2.736 (6)	176 (7)
C10—H10A···N1^{iii}	0.96	2.61	3.555 (10)	169

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

The symmetry-independent O-bound H atom was located in a difference map and its positional parameters were refined. The other H atoms were positioned with idealized geometry using a riding model, with C—H = 0.93 Å (aromatic) or 0.96 Å (methyl). For all H atoms, U_{iso}(H) = 1.2U_{eq}(parent atom). The ratio of observed to unique reflections is lower than normal and this has resulted in a higher than normal value for R_{int} (0.198). This in turn can lower the precision of the results.

Data collection: *CAD-4-PC* Software (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC* Software; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

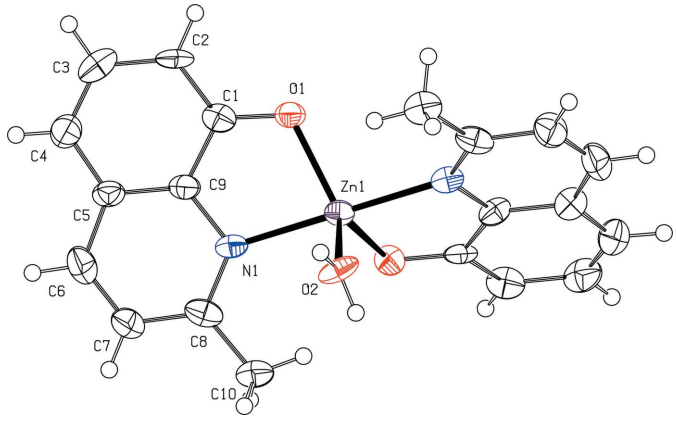


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. Unlabelled atoms are related to the corresponding labelled atoms by the symmetry operation $(-x, y, -z+\frac{1}{2})$.

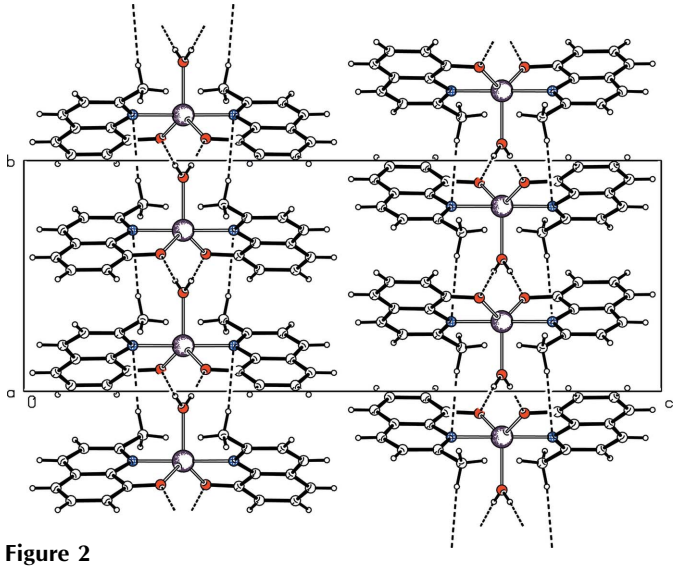


Figure 2
Part of the crystal structure of (I), with hydrogen bonds shown as dashed lines.

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References

Czugler, M., Neumann, R. & Weber, E. (2001). *Inorg. Chim. Acta*, **313**, 100–108.
Enraf–Nonius (1996). *CAD-4-PC* Software. Version 1.2. Enraf–Nonius, Delft, The Netherlands.
Macías, B., García, I., Villa, M. V., Borrás, J., Castiñeiras, A. & Sanz, F. (2003). *Z. Anorg. Allg. Chem.* **629**, 255–260.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Opazo, C., Luza, S., Villemagne, V. L., Volitakis, I., Rowe, C., Barnham, K. J., Strozyk, D., Masters, C. L., Cherny, R. A. & Bush, A. I. (2006). *Aging Cell*, **5**, 69–79.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Silva, L. E. da, Joussef, A. C., Foro, S. & Schmidt, B. (2006*a*). *Acta Cryst.* E**62**, m516–m517.
Silva, L. E. da, Joussef, A. C., Foro, S. & Schmidt, B. (2006*b*). *Acta Cryst.* E**62**, m912–m913.

Silva, L. E. da, Joussef, A. C., Foro, S. & Schmidt, B. (2006*c*). *Acta Cryst.* E**62**, m999–m1001.
Silva, L. E. da, Joussef, A. C., Foro, S. & Schmidt, B. (2006*d*). *Acta Cryst.* E**62**, m1719–m1721.
Silva, L. E. da, Joussef, A. C., Foro, S. & Schmidt, B. (2006*e*). *Acta Cryst.* E**62**, m1773–m1775.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stoe & Cie (1987). *REDU4*. Version 6.2c. Stoe & Cie GmbH, Darmstadt, Germany.
Zheng, H., Weiner, L. M., Bar-Am, O., Epsztejn, S., Cabantchik, Z. I., Warshawsky, A., Youdim, M. B. H. & Fridkin, M. (2005). *Bioorg. Med. Chem.* **13**, 773–783.