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Diaquabis(3-hydroxynaphthalene-2-carboxylato-κO)zinc(II)

Bing Deng,[a] Zhao-Di Liu,[b] Xiu-Ying Liu,[a] Min-Yu Tan[b] and Hai-Liang Zhu[a]*

[a]Department of Chemistry, Wuhan University of Science and Engineering, Wuhan 430073, People's Republic of China, and [b]Department of Chemistry, Lanzhou University, Lanzhou 730000, People's Republic of China

Correspondence e-mail: hailiang_zhu@163.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.015 Å
R factor = 0.057
wR factor = 0.158
Data-to-parameter ratio = 8.4

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

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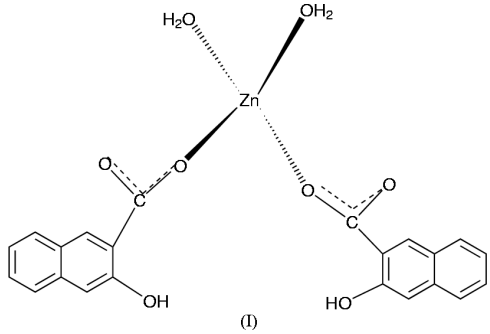
The title compound, $[Zn(C_{11}H_7O_3)_2(H_2O)_2]$, is a mononuclear zinc(II) complex, with the Zn atom on a twofold rotation axis, coordinated by two O atoms from two water molecules and two O atoms from two 3-hydroxynaphthalene-2-carboxylate ligands, in a distorted tetrahedral geometry. The crystal structure is stabilized by O—H···O hydrogen bonds, forming a two-dimensional network.

Comment

Recently, there has been growing interest in the photochemistry of luminescent Zn(II) coordination complexes. As colourless d^{10} metal ions, zinc(II) can assume coordination geometries from tetrahedral through trigonal–bipyramidal and square-pyramidal to octahedral, and hence is suitable for the construction of luminescent coordination complexes (Zheng & Chen, 2004). Our interest in the luminescent properties of zinc(II) complexes has led us to the title complex, (I), a new mononuclear zinc(II) complex of the 3-hydroxynaphthalene-2-carboxylate (H-na) ligand. We report here the crystal structure of (I).



(I)

The asymmetric unit of (I) consists of a half-molecule, with the Zn atom lying on a crystallographic twofold axis; the other half of the molecule is generated by the twofold axis. In this four-coordinate complex (Fig. 1), the Zn atom is in a severely distorted tetrahedral geometry, with the bond angles around it ranging from 93.3 (2) to 128.6 (4)° (Table 1). The Zn—O bond lengths show normal values. In the crystal structure, O—H···O hydrogen bonding involving the water, carboxylate and hydroxyl O atoms forms a two-dimensional network parallel to the (001) plane (Fig. 2 and Table 2).

Experimental

A $C_2H_5OH{\cdot}H_2O$ (1/1 v/v, 10 ml) solution containing $Zn(NO_3)_2{\cdot}4H_2O$ (0.131 g, 0.5 mmol) and 3-hydroxynaphthalene-2-carboxylic acid (0.188 g, 1 mmol) was stirred for 1 h in air, and then placed in a Parr Teflon-lined stainless steel vessel (18 ml). The vessel was sealed and

heated at 423 K for 24 h, cooled to 373 K at a rate of 8 K h^{-1} and held at that temperature for 12 h, followed by further cooling to room temperature. Pale-yellow crystals of (I) were collected, washed with water, and dried in a vacuum using $CaCl_2$ (yield 50%). Elemental analysis found: C 55.32, H 3.68, O 27.03%; calculated for $C_{22}H_{18}O_8Zn$: C 55.54, H 3.81, O 26.90%.

Crystal data

$[Zn(C_{11}H_7O_3)_2(H_2O)_2]$	D_x = 1.459 Mg m^{-3}
M_r = 475.73	Mo $K\alpha$ radiation
Monoclinic, $C2$	Cell parameters from 25 reflections
a = 15.597 (9) Å	θ = 7.5–15.0°
b = 5.509 (4) Å	μ = 1.18 mm^{-1}
c = 12.648 (7) Å	T = 293 (2) K
β = 95.06 (2)°	Block, pale yellow
V = 1082.5 (12) $Å^3$	0.52 × 0.20 × 0.18 mm
Z = 2	

Data collection

Siemens $R3m$ diffractometer	R_{int} = 0.089
ω scans	θ_{max} = 26.0°
Absorption correction: ψ scan (North *et al.*, 1968)	$h = 0 \rightarrow 19$
T_{min} = 0.579, T_{max} = 0.816	$k = 0 \rightarrow 6$
1227 measured reflections	$l = -15 \rightarrow 15$
1180 independent reflections	2 standard reflections
879 reflections with $I > 2\sigma(I)$	every 200 reflections
	intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0945P)^2 + 0.6786P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.057	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.158	$\Delta\rho_{max}$ = 0.41 e $Å^{-3}$
S = 1.02	$\Delta\rho_{min}$ = −0.54 e $Å^{-3}$
1180 reflections	Absolute structure: Flack (1983); 0 Friedel pairs
141 parameters	Flack parameter = 0.00 (4)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Zn1—O1*W*	1.996 (6)	Zn1—O2	2.010 (6)
O1*W*—Zn1—O1*W*^{i}	101.3 (4)	O1*W*—Zn1—O2	93.3 (2)
O1*W*—Zn1—O2^{i}	119.5 (2)	O2^{i}—Zn1—O2	128.6 (4)

Symmetry code: (i) $2-x, y, -z$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1*W*···O1^{ii}	0.82	1.89	2.688 (9)	165
O1*W*—H2*W*···O3^{iii}	0.87	1.89	2.747 (8)	173
O3—H3···O2	0.82	1.86	2.591 (8)	148

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

Water H atoms were located in a difference Fourier map and were allowed to ride on the O atom, with $U_{iso}(H) = 1.5U_{eq}(O)$. All other H atoms were placed in geometrically idealized positions (O—H = 0.85 Å and C—H = 0.93 Å) and allowed to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(O)$.

Data collection: *SHELXTL-Plus* (Siemens, 1990); cell refinement: *SHELXTL-Plus*; data reduction: *SHELXTL-Plus*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL*97.

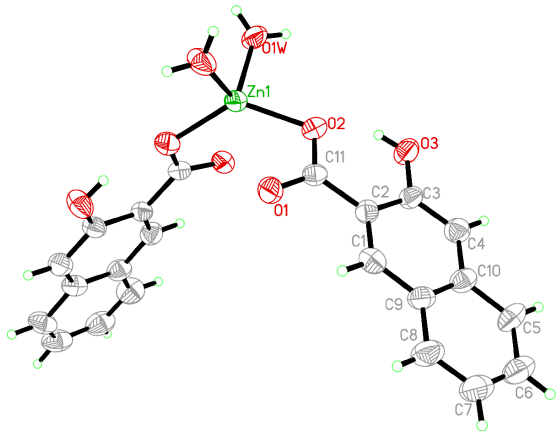


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atomic numbering for the contents of the asymmetric unit. Atom Zn1 lies on a crystallographic twofold axis. Unlabelled atoms are related to labelled atoms by $2-x, y, -z$.

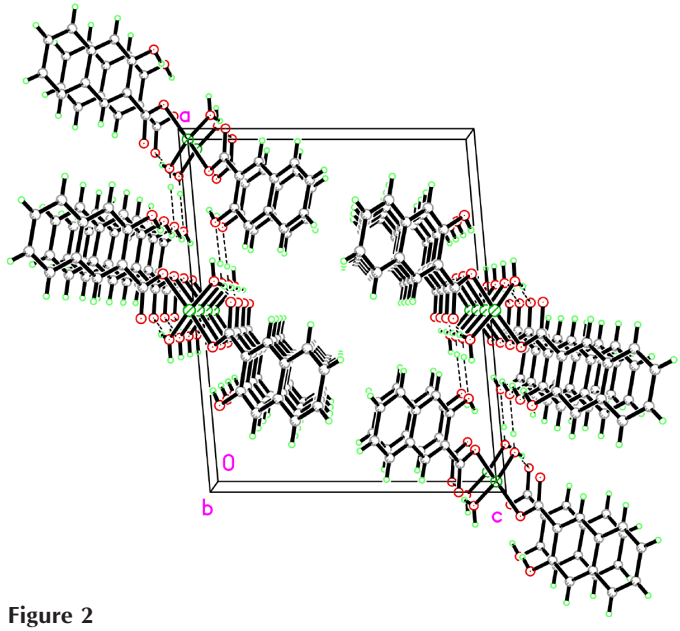


Figure 2
The crystal packing of (I), showing O—H···O hydrogen-bonding interactions as dashed lines.

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