Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tetraaquabis(1-hydroxy-2-naphthoato-κO)zinc(II)

Wen-Dong Song,* Jian-Bin Yan, Hao Wang and Li-Li Ji

College of Science, Guang Dong Ocean University, Zhanjiang 524088, People's Republic of China
Correspondence e-mail: songwd60@126.com

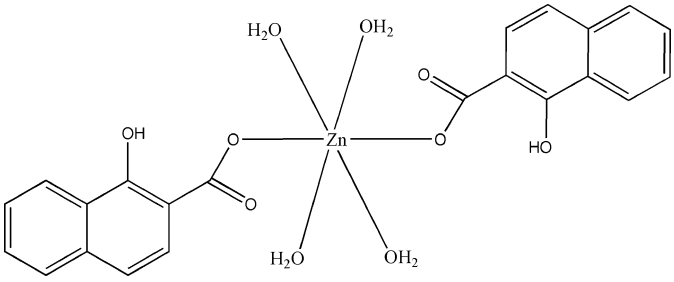
Received 21 November 2007; accepted 21 November 2007

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.033; wR factor = 0.078; data-to-parameter ratio = 11.6.

In the title mononuclear complex, $[Zn(C_{11}H_7O_3)_2(H_2O)_4]$, the Zn^{II} atom is located on a centre of inversion and is coordinated by two O atoms from two 1-hydroxy-2-naphthoate ligands and four water molecules in an octahedral geometry. The structure is consolidated by intermolecular O—H···O hydrogen bonding, as well as by a π–π stacking interaction [centroid–centroid distance 3.762 (2)Å] between adjacent naphthyl ring systems.

Related literature

For metal derivatives of 2-hydroxynaphthoic acid, see: Ohki *et al.* (1986, 1987); Schmidt *et al.* (2005); Xue *et al.* (2005)).



Experimental

Crystal data

$[Zn(C_{11}H_7O_3)_2(H_2O)_4]$
M_r = 511.77
Monoclinic, $P2_1/n$
a = 6.7499 (2) Å
b = 5.2239 (1) Å
c = 29.9876 (8) Å
β = 94.733 (2)°
V = 1053.78 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.22 mm^{-1}
T = 296 (2) K
0.26 × 0.25 × 0.23 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.736, T_{max} = 0.756
7878 measured reflections
1903 independent reflections
1583 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.078
S = 1.07
1903 reflections
164 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O1	0.82	1.75	2.482 (2)	147
O1W—H1W···O2^{i}	0.814 (10)	1.912 (10)	2.714 (2)	168 (3)
O1W—H2W···O3^{ii}	0.810 (9)	2.091 (15)	2.814 (2)	149 (3)
O2W—H3W···O1W^{iii}	0.808 (10)	2.104 (11)	2.889 (3)	164 (3)
O2W—H4W···O2^{iv}	0.809 (10)	1.994 (15)	2.712 (3)	148 (3)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); software used to prepare material for publication: *SHELXTL*.

The authors acknowledge Guang Dong Ocean University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2392).

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 doi:10.1107/S1600536807061442

supplementary materials

Acta Cryst. (2008). E**64**, m5 [**doi:10.1107/S1600536807061442**]

Tetraaquabis(1-hydroxy-2-naphthoato-*κO*)zinc(II)

W.-D. Song, J.-B. Yan, H. Wang and L.-L. Ji

Comment

In the structural investigation of 1-hydroxy-2-naphthoate complexes, it has been found that the 1-hydroxy-2-naphthoate functions as a multidentate ligand (Ohki *et al.* 1986, 1987; Schmidt *et al.* (2005); Xue *et al.* (2005)), with versatile binding and coordination modes. In this paper, we report the crystal structure of the title compound, (I), a new Zn complex obtained by the reaction of 1-naphthol-2-carboxylic acid with zinc chloride in alkaline aqueous solution.

As illustrated in Figure 1, the Zn^{II} atom, lies on a centre of inversion, has a disordered octahedral geometry, which is defined by two O atoms from two 1-hydroxy-2-naphthoate ligands and four water molecules (Fig. 1). The structural components are governed by intermolecular O—H···O hydrogen bond (Table 1) involving the coordinated water molecules, the hydroxy and carboxyl O atoms of 1-hydroxy-2-naphthoate ligands, and *via* π-π stacking interaciton. The centroid to centroid distance between parallel naphthoate rings of neighboring complexes (at *X*, 1+Y, *Z*) is 3.762 (2)A%, thus indicating a weak π-π stacking interaction.

Experimental

A mixture of zinc chloride(1 mmol), 1-hydroxy-2-naphthoate (1 mmol) NaOH (1.5 mmol) and H_2O (12 ml) was placed in a 23 ml Teflon reactor, which was heated to 433 K for three days and then cooled to room temperature at a rate of 10 K h^{-1}. The crystals obtained were washed with water and dryed in air.

Refinement

Carbon-bound and hydroxyl H atoms were placed at calculated positions and were treated as riding on the parent C atoms with C—H = 0.93 Å, O—H = 0.82 Å and with U_{iso}(H) = 1.2 U_{eq}(C, O). Water H atoms were tentatively located in difference Fourier maps and were refined with distance restraints of O–H = 0.82 Å and H···H = 1.29 Å, each within a standard deviation of 0.01 Å, and with U_{iso}(H) = 1.5 U_{eq}(O).

Figures

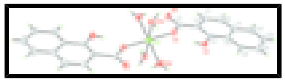

Fig. 1. The structure of (I), showing the atomic numbering scheme. Non-H atoms are shown with 30% probability displacement ellipsoids. Unlabeled atoms are related to the labelled atoms by the symmetry operator (1 - *x*, 1 - *y*, -*z*).

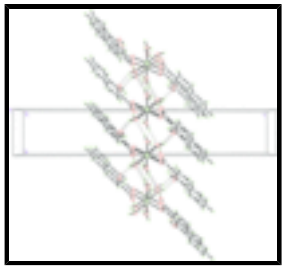

Fig. 2. A packing view of the title compound. The intermolecluar hydrogen bonds are shown with dashed lines.

Tetraaquabis(1-hydroxy-2-naphthoato-κ*O*)zinc(II)

Crystal data

$[Zn(C_{11}H_7O_3)_2(H_2O)_4]$	F_{000} = 528
M_r = 511.77	D_x = 1.613 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3500 reflections
a = 6.7499 (2) Å	θ = 1.3–26º
b = 5.22390 (10) Å	μ = 1.22 mm^{-1}
c = 29.9876 (8) Å	T = 296 (2) K
β = 94.733 (2)º	Block, colorless
V = 1053.78 (5) Å^3	0.26 × 0.25 × 0.23 mm
Z = 2	

Data collection

Bruker APEXII area-detector diffractometer	1903 independent reflections
Radiation source: fine-focus sealed tube	1583 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.025
T = 296(2) K	θ_{max} = 25.5º
φ and ω scan	θ_{min} = 2.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −8→8
T_{min} = 0.736, T_{max} = 0.756	k = −6→5
7878 measured reflections	l = −36→28

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.033	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.078	$w = 1/[\sigma^2(F_o^2) + (0.0333P)^2 + 0.6372P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max}$ = 0.001

1903 reflections	$\Delta\rho_{max}$ = 0.25 e Å^{-3}
164 parameters	$\Delta\rho_{min}$ = −0.28 e Å^{-3}
6 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8379 (3)	0.3495 (5)	0.06924 (7)	0.0306 (6)
C2	0.8996 (3)	0.1561 (5)	0.10400 (7)	0.0291 (5)
C3	0.7639 (3)	−0.0133 (5)	0.11983 (8)	0.0316 (5)
C4	0.8218 (4)	−0.1956 (5)	0.15378 (8)	0.0347 (6)
C5	1.0231 (4)	−0.1986 (5)	0.17178 (8)	0.0406 (6)
C6	1.1595 (4)	−0.0253 (6)	0.15493 (9)	0.0457 (7)
H6	1.2918	−0.0279	0.1664	0.055*
C7	1.1001 (3)	0.1446 (5)	0.12234 (8)	0.0379 (6)
H7	1.1929	0.2561	0.1118	0.045*
C8	0.6851 (4)	−0.3712 (5)	0.16959 (9)	0.0432 (7)
H8	0.5535	−0.3702	0.1576	0.052*
C9	0.7452 (5)	−0.5427 (6)	0.20239 (9)	0.0546 (8)
H9	0.6547	−0.6587	0.2126	0.066*
C10	0.9424 (5)	−0.5439 (6)	0.22056 (10)	0.0602 (9)
H10	0.9816	−0.6596	0.2432	0.072*
C11	1.0768 (5)	−0.3799 (6)	0.20586 (9)	0.0543 (8)
H11	1.2076	−0.3858	0.2183	0.065*
O1	0.6516 (2)	0.3475 (3)	0.05507 (5)	0.0383 (4)
O2	0.9567 (2)	0.5030 (3)	0.05494 (6)	0.0429 (5)
O3	0.5689 (2)	−0.0105 (3)	0.10473 (6)	0.0406 (4)
H3	0.5493	0.1032	0.0860	0.061*
O1W	0.3164 (2)	0.7122 (4)	0.04289 (6)	0.0374 (4)
H1W	0.217 (3)	0.637 (5)	0.0494 (8)	0.056*
H2W	0.379 (3)	0.743 (6)	0.0665 (5)	0.056*
O2W	0.2956 (2)	0.2023 (4)	−0.00189 (7)	0.0448 (5)
H3W	0.280 (4)	0.060 (3)	0.0077 (10)	0.067*
H4W	0.194 (3)	0.239 (5)	−0.0166 (9)	0.067*

Zn1	0.5000	0.5000	0.0000	0.03273 (15)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0296 (12)	0.0319 (16)	0.0306 (13)	−0.0008 (11)	0.0051 (10)	−0.0011 (11)
C2	0.0314 (12)	0.0263 (15)	0.0297 (12)	0.0026 (11)	0.0038 (9)	−0.0018 (11)
C3	0.0343 (12)	0.0306 (15)	0.0303 (12)	0.0014 (12)	0.0051 (9)	−0.0035 (12)
C4	0.0474 (14)	0.0279 (15)	0.0299 (13)	0.0058 (12)	0.0100 (11)	−0.0012 (11)
C5	0.0496 (15)	0.0394 (17)	0.0331 (14)	0.0130 (13)	0.0053 (11)	−0.0005 (12)
C6	0.0352 (13)	0.054 (2)	0.0467 (16)	0.0106 (14)	−0.0027 (11)	0.0050 (15)
C7	0.0305 (12)	0.0418 (17)	0.0416 (15)	−0.0003 (12)	0.0043 (11)	0.0037 (13)
C8	0.0561 (17)	0.0342 (17)	0.0410 (15)	0.0035 (14)	0.0138 (13)	0.0014 (14)
C9	0.086 (2)	0.0347 (19)	0.0465 (17)	0.0019 (16)	0.0252 (16)	0.0072 (14)
C10	0.090 (3)	0.050 (2)	0.0425 (17)	0.0199 (18)	0.0126 (17)	0.0145 (15)
C11	0.0639 (19)	0.055 (2)	0.0432 (17)	0.0194 (17)	−0.0004 (14)	0.0084 (16)
O1	0.0283 (8)	0.0410 (12)	0.0443 (10)	−0.0048 (8)	−0.0038 (7)	0.0136 (9)
O2	0.0299 (9)	0.0482 (12)	0.0508 (11)	−0.0076 (9)	0.0038 (8)	0.0166 (10)
O3	0.0329 (9)	0.0413 (12)	0.0470 (11)	−0.0077 (8)	0.0000 (7)	0.0131 (9)
O1W	0.0295 (9)	0.0389 (11)	0.0440 (10)	−0.0070 (8)	0.0053 (7)	−0.0008 (9)
O2W	0.0343 (9)	0.0292 (11)	0.0694 (14)	−0.0077 (8)	−0.0054 (9)	0.0116 (10)
Zn1	0.0286 (2)	0.0282 (3)	0.0411 (3)	−0.00204 (18)	0.00111 (16)	0.0060 (2)

Geometric parameters (Å, °)

C1—O2	1.236 (3)	C9—C10	1.396 (5)
C1—O1	1.294 (3)	C9—H9	0.9300
C1—C2	1.486 (3)	C10—C11	1.348 (4)
C2—C3	1.385 (3)	C10—H10	0.9300
C2—C7	1.420 (3)	C11—H11	0.9300
C3—O3	1.356 (3)	O1—Zn1	2.0323 (16)
C3—C4	1.425 (3)	O3—H3	0.8200
C4—C8	1.411 (4)	O1W—Zn1	2.1635 (17)
C4—C5	1.420 (3)	O1W—H1W	0.814 (10)
C5—C6	1.414 (4)	O1W—H2W	0.810 (9)
C5—C11	1.418 (4)	O2W—Zn1	2.0767 (16)
C6—C7	1.356 (4)	O2W—H3W	0.808 (10)
C6—H6	0.9300	O2W—H4W	0.809 (10)
C7—H7	0.9300	Zn1—O1^{i}	2.0323 (16)
C8—C9	1.367 (4)	Zn1—O2W^{i}	2.0767 (16)
C8—H8	0.9300	Zn1—O1W^{i}	2.1635 (17)
O2—C1—O1	122.2 (2)	C11—C10—H10	119.5
O2—C1—C2	122.2 (2)	C9—C10—H10	119.5
O1—C1—C2	115.6 (2)	C10—C11—C5	121.4 (3)
C3—C2—C7	118.5 (2)	C10—C11—H11	119.3
C3—C2—C1	121.3 (2)	C5—C11—H11	119.3
C7—C2—C1	120.2 (2)	C1—O1—Zn1	132.37 (15)
O3—C3—C2	122.0 (2)	C3—O3—H3	109.5

O3—C3—C4	116.6 (2)	Zn1—O1W—H1W	115 (2)
C2—C3—C4	121.4 (2)	Zn1—O1W—H2W	110 (2)
C8—C4—C5	119.8 (2)	H1W—O1W—H2W	105.2 (15)
C8—C4—C3	121.7 (2)	Zn1—O2W—H3W	142 (2)
C5—C4—C3	118.5 (2)	Zn1—O2W—H4W	111.7 (19)
C6—C5—C11	123.4 (3)	H3W—O2W—H4W	106.4 (16)
C6—C5—C4	119.2 (2)	$O1^{i}$—Zn1—O1	180.00 (13)
C11—C5—C4	117.5 (3)	$O1^{i}$—Zn1—$O2W^{i}$	90.99 (7)
C7—C6—C5	121.0 (2)	O1—Zn1—$O2W^{i}$	89.01 (7)
C7—C6—H6	119.5	$O1^{i}$—Zn1—O2W	89.01 (7)
C5—C6—H6	119.5	O1—Zn1—O2W	90.99 (7)
C6—C7—C2	121.5 (2)	$O2W^{i}$—Zn1—O2W	180.0
C6—C7—H7	119.3	$O1^{i}$—Zn1—$O1W^{i}$	89.56 (7)
C2—C7—H7	119.3	O1—Zn1—$O1W^{i}$	90.44 (7)
C9—C8—C4	120.3 (3)	$O2W^{i}$—Zn1—$O1W^{i}$	89.33 (7)
C9—C8—H8	119.8	O2W—Zn1—$O1W^{i}$	90.67 (7)
C4—C8—H8	119.8	$O1^{i}$—Zn1—O1W	90.44 (7)
C8—C9—C10	120.0 (3)	O1—Zn1—O1W	89.56 (7)
C8—C9—H9	120.0	$O2W^{i}$—Zn1—O1W	90.67 (7)
C10—C9—H9	120.0	O2W—Zn1—O1W	89.33 (7)
C11—C10—C9	121.0 (3)	$O1W^{i}$—Zn1—O1W	180.00 (11)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O1	0.82	1.75	2.482 (2)	147
O1W—H1W···$O2^{ii}$	0.814 (10)	1.912 (10)	2.714 (2)	168 (3)
O1W—H2W···$O3^{iii}$	0.810 (9)	2.091 (15)	2.814 (2)	149 (3)
O2W—H3W···$O1W^{iv}$	0.808 (10)	2.104 (11)	2.889 (3)	164 (3)
O2W—H4W···$O2^{i}$	0.809 (10)	1.994 (15)	2.712 (3)	148 (3)

Symmetry codes: (ii) *x*−1, *y*, *z*; (iii) *x*, *y*+1, *z*; (iv) *x*, *y*−1, *z*; (i) −*x*+1, −*y*+1, −*z*.

Fig. 1

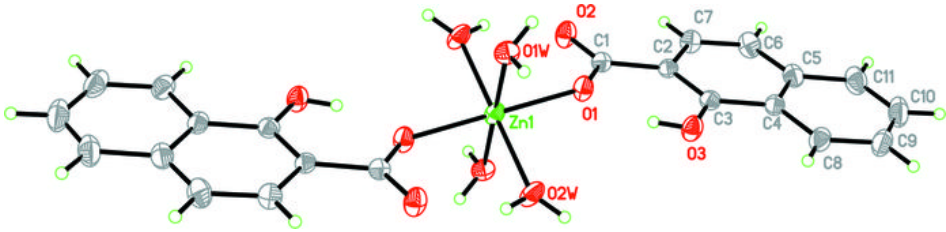

Fig. 2