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## Structure Reports

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Diaquabis(4-methylbenzoato- $\kappa$ O)zinc(II)De-Yun Ma,<sup>a</sup> Guo-Hua Deng<sup>a\*</sup> and Wen-Dong Song<sup>b</sup>

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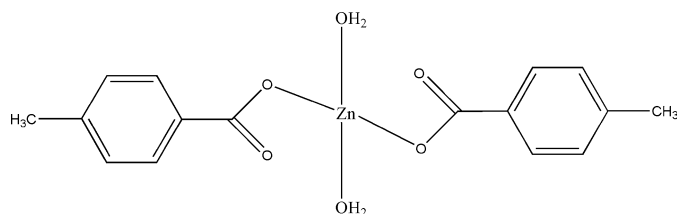
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Key indicators: single-crystal X-ray study;  $T = 273$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.031;  $wR$  factor = 0.076; data-to-parameter ratio = 15.9.

The Zn atom in the title mononuclear complex,  $[\text{Zn}(\text{C}_8\text{H}_7\text{O}_2)_2(\text{H}_2\text{O})_2]$ , lies on a special position of site symmetry 2. The carboxylate group binds in a monodentate manner so that the geometry is best described as tetrahedral. Adjacent molecules are linked by  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds into a three-dimensional network.

## Related literature

For related literature, see: Song *et al.* (2007).

## Experimental

## Crystal data

 $[\text{Zn}(\text{C}_8\text{H}_7\text{O}_2)_2(\text{H}_2\text{O})_2]$  $M_r = 371.70$ Monoclinic,  $C2/c$  $a = 26.8432$  (5) Å $b = 5.0600$  (1) Å $c = 12.0609$  (2) Å $\beta = 106.806$  (1)° $V = 1568.22$  (5) Å<sup>3</sup> $Z = 4$ Mo  $K\alpha$  radiation $\mu = 1.59$  mm<sup>-1</sup> $T = 273$  (2) K $0.32 \times 0.29 \times 0.26$  mm

## Data collection

Bruker APEXII area-detector diffractometer

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

 $T_{\min} = 0.605$ ,  $T_{\max} = 0.660$ 

9051 measured reflections

1784 independent reflections

1566 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.036$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.031$  $wR(F^2) = 0.076$  $S = 1.05$ 

1784 reflections

112 parameters

3 restraints

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.25$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.43$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1W}-\text{H1W}\cdots\text{O1}^{\text{i}}$	0.813 (9)	1.973 (10)	2.774 (2)	168 (3)
$\text{O1W}-\text{H2W}\cdots\text{O2}^{\text{ii}}$	0.803 (9)	1.931 (11)	2.726 (2)	171 (3)

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

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.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2397).

## References

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## supporting information

*Acta Cryst.* (2008). E64, m32 [https://doi.org/10.1107/S1600536807062460]

**Diaquabis(4-methylbenzoato- $\kappa$ O)zinc(II)****De-Yun Ma, Guo-Hua Deng and Wen-Dong Song****S1. Comment**

In the structural investigation of 4-methylbenzoate complexes, it has been found that the 4-methylbenzoic acid functions as a multidentate ligand [(Song *et al.* (2007)], 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 4-methylbenzoic acid with zinc chloride in alkaline aqueous solution.

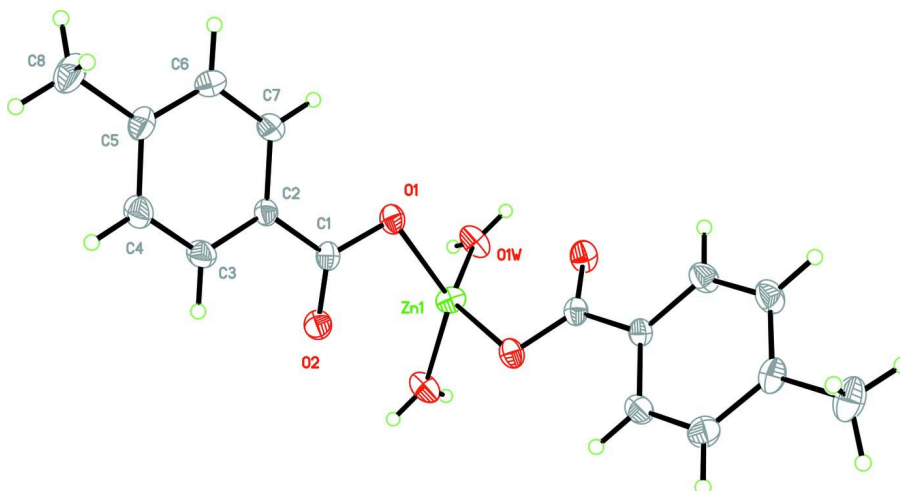
As illustrated in Figure 1, the Zn<sup>II</sup> atom, possesses crystallographically imposed C<sub>2</sub> symmetry, which is coordinated by two O atoms from two 4-methylbenzoate ligands and two water molecules, and displays a tetrahedral geometry. Intermolecular O—H $\cdots$ O hydrogen bonding interactions (Table 1) between the coordinated water molecules and the carboxyl O atoms of 4-methylbenzoate ligands stabilize the structural packing (Fig. 2).

**S2. Experimental**

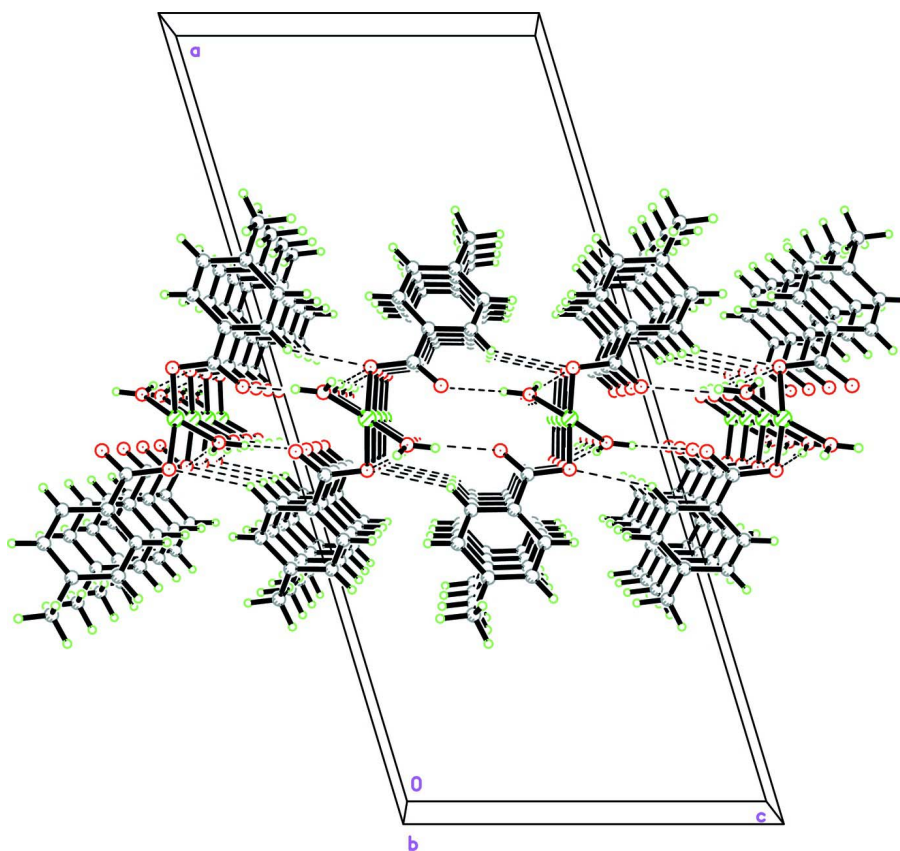
A mixture of zinc nitrate(1 mmol), 4-methylbenzoic acid (1 mmol) NaOH (1.5 mmol) and H<sub>2</sub>O (12 ml) was placed in a 23 ml Teflon reactor, which was heated to 433 K for three days and then cooled to room temperature at a rate of 10 K h<sup>-1</sup>. The crystals obtained were washed with water and dried in air.

**S3. Refinement**

Carbon-bound H atoms were placed at calculated positions and were treated as riding on the parent C atoms with C—H = 0.93 - 0.97 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ . Water H atoms were tentatively located in difference Fourier maps and were refined with distance restraints of O—H = 0.82 Å and H $\cdots$ H = 1.29 Å, each within a standard deviation of 0.01 Å, and with  $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{O})$ .

**Figure 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  $(-x, y, 0.5 - z)$ .

**Figure 2**

A packing view of the title compound. The intermolecular hydrogen bonds are shown as dashed lines.

Diaquabis(4-methylbenzoato- $\kappa$ O)zinc(II)

## Crystal data

[Zn(C<sub>8</sub>H<sub>7</sub>O<sub>2</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>] $M_r = 371.70$ Monoclinic,  $C2/c$ Hall symbol:  $-C\ 2yc$  $a = 26.8432$  (5) Å $b = 5.0600$  (1) Å $c = 12.0609$  (2) Å $\beta = 106.806$  (1)° $V = 1568.22$  (5) Å<sup>3</sup> $Z = 4$  $F(000) = 768$  $D_x = 1.574$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 3600 reflections

 $\theta = 3.0$ – $27.5$ ° $\mu = 1.59$  mm<sup>-1</sup> $T = 273$  K

Block, colorless

 $0.32 \times 0.29 \times 0.26$  mm

## Data collection

Bruker APEXII area-detector

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 $\varphi$  and  $\omega$  scan

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

 $T_{\min} = 0.605$ ,  $T_{\max} = 0.660$ 

9051 measured reflections

1784 independent reflections

1566 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.036$  $\theta_{\max} = 27.5$ °,  $\theta_{\min} = 3.2$ ° $h = -34 \rightarrow 34$  $k = -6 \rightarrow 6$  $l = -15 \rightarrow 15$ 

## Refinement

Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.031$  $wR(F^2) = 0.076$  $S = 1.05$ 

1784 reflections

112 parameters

3 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

 $w = 1/[\sigma^2(F_o^2) + (0.0378P)^2 + 0.8633P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} < 0.001$  $\Delta\rho_{\max} = 0.25$  e Å<sup>-3</sup> $\Delta\rho_{\min} = -0.43$  e Å<sup>-3</sup>

## 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<sup>2</sup>)

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.06512 (8)	0.6273 (4)	0.40073 (18)	0.0311 (4)
C2	0.10484 (7)	0.4299 (4)	0.46142 (17)	0.0300 (4)
C3	0.10475 (9)	0.3264 (4)	0.56687 (19)	0.0409 (5)

H3	0.0795	0.3813	0.6009	0.049*
C4	0.14146 (9)	0.1422 (5)	0.6231 (2)	0.0437 (5)
H4	0.1408	0.0771	0.6948	0.052*
C5	0.17921 (8)	0.0533 (4)	0.5741 (2)	0.0384 (5)
C6	0.17872 (9)	0.1556 (5)	0.4675 (2)	0.0463 (6)
H6	0.2036	0.0985	0.4329	0.056*
C7	0.14237 (8)	0.3399 (5)	0.4110 (2)	0.0416 (5)
H7	0.1429	0.4044	0.3391	0.050*
C8	0.21820 (10)	-0.1520 (5)	0.6349 (2)	0.0550 (6)
H8A	0.2226	-0.1445	0.7166	0.082*
H8B	0.2510	-0.1183	0.6204	0.082*
H8C	0.2059	-0.3243	0.6062	0.082*
O1	0.05926 (5)	0.6655 (3)	0.29258 (12)	0.0356 (3)
O2	0.03766 (6)	0.7481 (3)	0.45086 (13)	0.0415 (4)
O1W	0.02917 (7)	1.2004 (3)	0.16969 (14)	0.0450 (4)
H1W	0.0402 (11)	1.342 (3)	0.199 (2)	0.067*
H2W	0.0326 (10)	1.199 (5)	0.1058 (12)	0.067*
Zn1	0.0000	0.92389 (6)	0.2500	0.03485 (13)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0344 (10)	0.0256 (9)	0.0297 (11)	-0.0033 (8)	0.0038 (9)	-0.0014 (7)
C2	0.0319 (9)	0.0304 (9)	0.0257 (10)	0.0002 (8)	0.0053 (8)	-0.0020 (8)
C3	0.0470 (12)	0.0430 (11)	0.0362 (12)	0.0136 (10)	0.0177 (10)	0.0066 (9)
C4	0.0527 (13)	0.0423 (12)	0.0365 (13)	0.0112 (10)	0.0135 (11)	0.0113 (9)
C5	0.0369 (11)	0.0322 (10)	0.0392 (12)	0.0039 (9)	0.0000 (9)	-0.0018 (9)
C6	0.0383 (11)	0.0568 (13)	0.0453 (14)	0.0146 (11)	0.0142 (11)	-0.0009 (11)
C7	0.0425 (12)	0.0514 (12)	0.0328 (12)	0.0069 (10)	0.0139 (10)	0.0041 (10)
C8	0.0494 (14)	0.0459 (13)	0.0588 (17)	0.0159 (11)	-0.0015 (12)	-0.0005 (12)
O1	0.0428 (8)	0.0325 (7)	0.0296 (8)	0.0029 (6)	0.0074 (6)	0.0073 (6)
O2	0.0459 (8)	0.0389 (8)	0.0379 (9)	0.0135 (7)	0.0094 (7)	-0.0002 (7)
O1W	0.0727 (11)	0.0285 (7)	0.0383 (9)	-0.0127 (7)	0.0232 (9)	-0.0040 (6)
Zn1	0.0361 (2)	0.02136 (17)	0.0484 (2)	0.000	0.01423 (16)	0.000

*Geometric parameters (Å, °)*

C1—O2	1.241 (2)	C6—H6	0.9300
C1—O1	1.283 (2)	C7—H7	0.9300
C1—C2	1.490 (3)	C8—H8A	0.9600
C2—C3	1.376 (3)	C8—H8B	0.9600
C2—C7	1.395 (3)	C8—H8C	0.9600
C3—C4	1.383 (3)	O1—Zn1	2.0078 (14)
C3—H3	0.9300	O1W—Zn1	1.9867 (14)
C4—C5	1.387 (3)	O1W—H1W	0.813 (9)
C4—H4	0.9300	O1W—H2W	0.803 (9)
C5—C6	1.383 (3)	Zn1—O1W <sup>i</sup>	1.9867 (14)
C5—C8	1.506 (3)	Zn1—O1 <sup>i</sup>	2.0078 (14)

C6—C7	1.379 (3)		
O2—C1—O1	120.38 (18)	C6—C7—H7	119.9
O2—C1—C2	122.17 (19)	C2—C7—H7	119.9
O1—C1—C2	117.43 (17)	C5—C8—H8A	109.5
C3—C2—C7	118.26 (19)	C5—C8—H8B	109.5
C3—C2—C1	121.13 (17)	H8A—C8—H8B	109.5
C7—C2—C1	120.59 (18)	C5—C8—H8C	109.5
C2—C3—C4	121.21 (19)	H8A—C8—H8C	109.5
C2—C3—H3	119.4	H8B—C8—H8C	109.5
C4—C3—H3	119.4	C1—O1—Zn1	102.32 (12)
C3—C4—C5	121.0 (2)	Zn1—O1W—H1W	123.8 (18)
C3—C4—H4	119.5	Zn1—O1W—H2W	129.3 (18)
C5—C4—H4	119.5	H1W—O1W—H2W	106.9 (15)
C6—C5—C4	117.58 (19)	O1W <sup>i</sup> —Zn1—O1W	90.48 (9)
C6—C5—C8	121.9 (2)	O1W <sup>i</sup> —Zn1—O1 <sup>i</sup>	100.86 (7)
C4—C5—C8	120.5 (2)	O1W—Zn1—O1 <sup>i</sup>	136.77 (7)
C7—C6—C5	121.8 (2)	O1W <sup>i</sup> —Zn1—O1	136.77 (7)
C7—C6—H6	119.1	O1W—Zn1—O1	100.86 (6)
C5—C6—H6	119.1	O1 <sup>i</sup> —Zn1—O1	98.74 (8)
C6—C7—C2	120.1 (2)		

Symmetry code: (i)  $-x, y, -z+1/2$ .

#### Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1W $\cdots$ O1 <sup>ii</sup>	0.81 (1)	1.97 (1)	2.774 (2)	168 (3)
O1W—H2W $\cdots$ O2 <sup>iii</sup>	0.80 (1)	1.93 (1)	2.726 (2)	171 (3)

Symmetry codes: (ii)  $x, y+1, z$ ; (iii)  $x, -y+2, z-1/2$ .