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## Diaquabis(2-oxo-2H-chromene-3-carboxylato)zinc(II)

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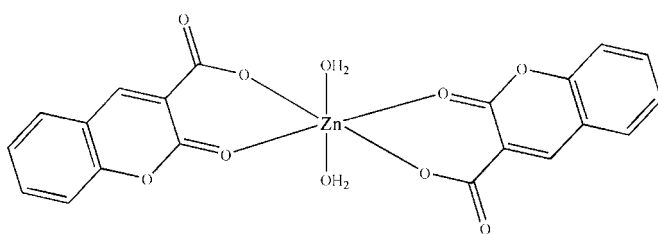
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.022;  $wR$  factor = 0.061; data-to-parameter ratio = 12.7.

In the title compound,  $[\text{Zn}(\text{C}_{10}\text{H}_5\text{O}_4)_2(\text{H}_2\text{O})_2]$ , the  $\text{Zn}^{\text{II}}$  atom lies on a crystallographic inversion center and is six-coordinated by two O atoms from water molecules in the axial positions and four O atoms from two deprotonated coumarin-3-carboxylate ligands in the equatorial plane, forming a slightly distorted octahedral coordination geometry. O—H...O hydrogen-bonding interactions involving the water molecules form infinite chains parallel to [010].

## Related literature

For related structures, see: Chu *et al.* (2010). For hydrogen-bond motifs, see: Bernstein *et al.* (1995); Etter (1990).



## Experimental

## Crystal data

 $[\text{Zn}(\text{C}_{10}\text{H}_5\text{O}_4)_2(\text{H}_2\text{O})_2]$  $M_r = 479.70$ Triclinic,  $P\bar{1}$  $a = 6.6113$  (13) Å $b = 6.8404$  (14) Å $c = 10.392$  (2) Å $\alpha = 85.64$  (3)° $\beta = 89.47$  (3)° $\gamma = 66.09$  (3)° $V = 428.27$  (18) Å<sup>3</sup> $Z = 1$   
Mo  $K\alpha$  radiation  
 $\mu = 1.50$  mm<sup>-1</sup> $T = 293$  K  
 $0.2 \times 0.2 \times 0.2$  mm

## Data collection

Bruker APEXII CCD diffractometer  
Absorption correction: multi-scan (SADABS; Bruker, 2005)  
 $T_{\text{min}} = 0.741$ ,  $T_{\text{max}} = 0.748$ 2642 measured reflections  
1808 independent reflections  
1793 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.013$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.022$   
 $wR(F^2) = 0.061$   
 $S = 1.12$   
1808 reflections142 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.42$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.28$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1W}-\text{H1}\cdots\text{O3}^{\text{i}}$	0.82	1.88	2.6950 (17)	179
$\text{O1W}-\text{H2}\cdots\text{O3}^{\text{ii}}$	0.93	1.83	2.7473 (19)	168

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

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT (Bruker, 2005); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP3 (Burnett & Johnson, 1996), ORTEP-3 for Windows (Farrugia, 1997) and PLATON (Spek, 2009); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

This work was supported by the National Natural Science Foundation of China (No. 21075114), the Science and Technology Development Project of Beijing Education Committee and the Special Environmental Protection Fund for Public Welfare project (201009015).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2633).

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**supplementary materials**

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## Diaquabis(2-oxo-2H-chromene-3-carboxylato)zinc(II)

Y. Cui, Q. Gao, H.-H. Wang, L. Wang and Y.-B. Xie

### Comment

In the past decades, numerous papers dealing with mononuclear zinc complexes have been published (Chu *et al.* 2010). Herein, we report the synthesis and crystal structure of a new mononuclear zinc complex.

In the title compound,  $[\text{Zn}(\text{C}_{10}\text{H}_5\text{O}_4)_2(\text{H}_2\text{O})_2]$ , each  $\text{Zn}^{\text{II}}$  atom lies on a crystallographic inversion center and is six-coordinated by two O atoms from water molecules in the axial positions and four O atoms from two deprotonated coumarin-3-carboxylic acid ligands in the equatorial plane, forming an octahedral coordination geometry (Fig. 1). O—H $\cdots$ O hydrogen bonds involving the water molecules build up chain parallel to the [0 1 0] axis (Table 1, Fig. 2). The O—H $\cdots$ O interactions results in the formation of  $\text{R}^4_2(8)$  rings (Etter, 1990; Bernstein *et al.*, 1995).

### Experimental

The title complex was synthesized by carefully layering a solution of  $\text{ZnSO}_4 \cdot 7\text{H}_2\text{O}$  (28.8 mg, 0.1 mmol) in ethanol solution (10 ml) on top of a solution of coumarin-3-carboxylic acid (19.0 mg, 0.1 mmol) and LiOH (8.4 mg, 0.2 mmol) in  $\text{H}_2\text{O}$  (10 ml) in a test-tube. After about one month at room temperature, colorless block-shaped single crystals suitable for X-ray investigation appeared at the boundary between ethanol solution and water with a yield of 27%.

### Refinement

The H atoms were placed geometrically (C—H = 0.93 Å) and treated as riding with  $U_{\text{iso}(\text{H})} = 1.2_{\text{eq}}(\text{C})$ . H atoms of water molecule were located in difference Fourier maps and included in the subsequent refinement using restraints (O—H = 0.85 (1) Å and H $\cdots$ H = 1.40 (2) Å) with  $U_{\text{iso}(\text{H})} = 1.5U_{\text{eq}}(\text{O})$ . In the last cycle of refinement they were treated as riding on their parent O atom.

### Figures

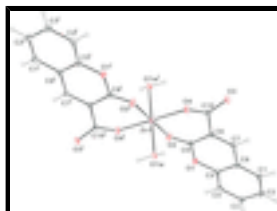


Fig. 1. Molecular view of (I) with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii. [Symmetry code: (i)  $-x+1, -y+1, -z+1$ ]

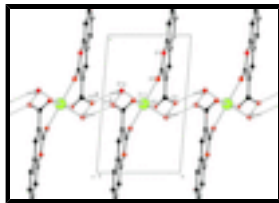


Fig. 2. Partial packing view of compound ( I ), showing the formation of chains along [010] built from hydrogen bonds, and the formation of R<sup>2</sup><sub>4</sub>(8) rings. For the sake of clarity, H atoms not involved in hydrogen bonding have been omitted. [Symmetry codes: (ii) -x, -y+1, -z+1; (iii) x+1, y-1, z]

## Diaquabis(2-oxo-2H-chromene-3-carboxylato)zinc(II)

### Crystal data

[Zn(C<sub>10</sub>H<sub>5</sub>O<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]

*M<sub>r</sub>* = 479.70

Triclinic, *P* $\bar{1}$

Hall symbol: -P 1

*a* = 6.6113 (13) Å

*b* = 6.8404 (14) Å

*c* = 10.392 (2) Å

$\alpha$  = 85.64 (3)°

$\beta$  = 89.47 (3)°

$\gamma$  = 66.09 (3)°

*V* = 428.27 (18) Å<sup>3</sup>

*Z* = 1

*F*(000) = 244

*D<sub>x</sub>* = 1.860 Mg m<sup>-3</sup>

Mo *K*α radiation,  $\lambda$  = 0.71073 Å

Cell parameters from 2271 reflections

$\theta$  = 3.4–28.4°

$\mu$  = 1.50 mm<sup>-1</sup>

*T* = 293 K

Block, colourless

0.2 × 0.2 × 0.2 mm

### Data collection

Bruker APEXII CCD  
diffractometer

Radiation source: fine-focus sealed tube  
graphite

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(*SADABS*; Sheldrick, 2008)

*T<sub>min</sub>* = 0.741, *T<sub>max</sub>* = 0.748

2642 measured reflections

1808 independent reflections

1793 reflections with *I* > 2σ(*I*)

*R<sub>int</sub>* = 0.013

$\theta_{\max}$  = 27.1°,  $\theta_{\min}$  = 3.4°

*h* = -8→8

*k* = -8→8

*l* = 0→13

### Refinement

Refinement on *F*<sup>2</sup>

Least-squares matrix: full

*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.022

*wR*(*F*<sup>2</sup>) = 0.061

*S* = 1.12

1808 reflections

142 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0216P)^2 + 0.2757P]$

where  $P = (F_o^2 + 2F_c^2)/3$

( $\Delta/\sigma$ )<sub>max</sub> < 0.001

$\Delta\rho_{\max} = 0.42 \text{ e \AA}^{-3}$

0 restraints

$$\Delta\rho_{\min} = -0.28 \text{ e } \text{\AA}^{-3}$$

*Special details*

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.5000	0.5000	0.5000	0.01047 (10)
O1	0.30343 (17)	0.68964 (17)	0.87151 (10)	0.0127 (2)
O1W	0.49536 (17)	0.22209 (17)	0.59641 (10)	0.0133 (2)
H1	0.3972	0.1951	0.5649	0.020*
H2	0.6183	0.1022	0.5763	0.020*
O2	0.45061 (18)	0.64366 (18)	0.68157 (10)	0.0141 (2)
O3	-0.17320 (17)	0.86870 (17)	0.50573 (10)	0.0134 (2)
O4	0.16868 (17)	0.63230 (18)	0.47583 (10)	0.0132 (2)
C1	-0.2479 (3)	0.7880 (2)	0.99672 (15)	0.0146 (3)
H1A	-0.3880	0.8073	0.9679	0.018*
C2	-0.2071 (3)	0.7889 (3)	1.12660 (15)	0.0168 (3)
H3A	-0.3203	0.8111	1.1850	0.020*
C3	0.0042 (3)	0.7564 (2)	1.17064 (15)	0.0161 (3)
H2A	0.0305	0.7567	1.2584	0.019*
C4	0.1753 (3)	0.7237 (2)	1.08507 (15)	0.0148 (3)
H11A	0.3160	0.7015	1.1143	0.018*
C5	0.1306 (2)	0.7250 (2)	0.95493 (14)	0.0119 (3)
C6	-0.0780 (2)	0.7579 (2)	0.90792 (14)	0.0122 (3)
C7	-0.1088 (2)	0.7641 (2)	0.77180 (14)	0.0120 (3)
H7A	-0.2480	0.7893	0.7385	0.014*
C8	0.0600 (2)	0.7342 (2)	0.68973 (14)	0.0109 (3)
C9	0.2798 (2)	0.6861 (2)	0.74172 (14)	0.0113 (3)
C10	0.0171 (2)	0.7468 (2)	0.54635 (14)	0.0105 (3)

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Zn1	0.00736 (13)	0.01189 (14)	0.01013 (13)	-0.00175 (9)	0.00122 (8)	-0.00152 (9)
O1	0.0106 (5)	0.0164 (5)	0.0101 (5)	-0.0041 (4)	0.0009 (4)	-0.0028 (4)
O1W	0.0105 (5)	0.0139 (5)	0.0143 (5)	-0.0036 (4)	0.0005 (4)	-0.0016 (4)
O2	0.0099 (5)	0.0185 (5)	0.0133 (5)	-0.0048 (4)	0.0021 (4)	-0.0041 (4)

## supplementary materials

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O3	0.0093 (5)	0.0143 (5)	0.0138 (5)	-0.0018 (4)	-0.0009 (4)	-0.0012 (4)
O4	0.0091 (5)	0.0168 (5)	0.0116 (5)	-0.0026 (4)	0.0013 (4)	-0.0032 (4)
C1	0.0139 (7)	0.0135 (7)	0.0155 (7)	-0.0046 (6)	0.0028 (6)	-0.0014 (6)
C2	0.0204 (8)	0.0135 (7)	0.0147 (7)	-0.0051 (6)	0.0069 (6)	-0.0015 (6)
C3	0.0247 (8)	0.0122 (7)	0.0098 (7)	-0.0059 (6)	0.0016 (6)	-0.0012 (5)
C4	0.0166 (7)	0.0133 (7)	0.0129 (7)	-0.0043 (6)	-0.0009 (6)	-0.0014 (6)
C5	0.0129 (7)	0.0092 (6)	0.0117 (7)	-0.0024 (5)	0.0034 (5)	-0.0017 (5)
C6	0.0133 (7)	0.0095 (6)	0.0129 (7)	-0.0036 (5)	0.0020 (5)	-0.0008 (5)
C7	0.0110 (7)	0.0108 (7)	0.0135 (7)	-0.0037 (5)	-0.0002 (5)	-0.0008 (5)
C8	0.0105 (7)	0.0100 (6)	0.0113 (6)	-0.0032 (5)	0.0004 (5)	-0.0016 (5)
C9	0.0123 (7)	0.0096 (6)	0.0105 (6)	-0.0026 (5)	0.0004 (5)	-0.0015 (5)
C10	0.0097 (6)	0.0108 (6)	0.0120 (7)	-0.0051 (5)	0.0006 (5)	-0.0009 (5)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

Zn1—O4	2.0122 (12)	C1—C6	1.406 (2)
Zn1—O4 <sup>i</sup>	2.0122 (12)	C1—H1A	0.9300
Zn1—O1W <sup>i</sup>	2.0918 (12)	C2—C3	1.398 (2)
Zn1—O1W	2.0918 (12)	C2—H3A	0.9300
Zn1—O2	2.1548 (12)	C3—C4	1.388 (2)
Zn1—O2 <sup>i</sup>	2.1548 (12)	C3—H2A	0.9300
O1—C9	1.3623 (18)	C4—C5	1.386 (2)
O1—C5	1.3801 (18)	C4—H11A	0.9300
O1W—H1	0.8200	C5—C6	1.391 (2)
O1W—H2	0.9269	C6—C7	1.426 (2)
O2—C9	1.2241 (18)	C7—C8	1.356 (2)
O3—C10	1.2501 (19)	C7—H7A	0.9300
O4—C10	1.2617 (19)	C8—C9	1.454 (2)
C1—C2	1.380 (2)	C8—C10	1.509 (2)
O4—Zn1—O4 <sup>i</sup>	180.0	C3—C2—H3A	119.9
O4—Zn1—O1W <sup>i</sup>	88.05 (5)	C4—C3—C2	120.84 (15)
O4 <sup>i</sup> —Zn1—O1W <sup>i</sup>	91.95 (5)	C4—C3—H2A	119.6
O4—Zn1—O1W	91.95 (5)	C2—C3—H2A	119.6
O4 <sup>i</sup> —Zn1—O1W	88.05 (5)	C5—C4—C3	118.17 (15)
O1W <sup>i</sup> —Zn1—O1W	180.00 (3)	C5—C4—H11A	120.9
O4—Zn1—O2	87.20 (5)	C3—C4—H11A	120.9
O4 <sup>i</sup> —Zn1—O2	92.80 (5)	O1—C5—C4	117.34 (14)
O1W <sup>i</sup> —Zn1—O2	90.89 (5)	O1—C5—C6	120.25 (13)
O1W—Zn1—O2	89.11 (5)	C4—C5—C6	122.41 (14)
O4—Zn1—O2 <sup>i</sup>	92.80 (5)	C5—C6—C1	118.34 (14)
O4 <sup>i</sup> —Zn1—O2 <sup>i</sup>	87.20 (5)	C5—C6—C7	118.03 (14)
O1W <sup>i</sup> —Zn1—O2 <sup>i</sup>	89.11 (5)	C1—C6—C7	123.62 (14)
O1W—Zn1—O2 <sup>i</sup>	90.89 (5)	C8—C7—C6	121.59 (14)
O2—Zn1—O2 <sup>i</sup>	180.000 (1)	C8—C7—H7A	119.2
C9—O1—C5	122.65 (12)	C6—C7—H7A	119.2
Zn1—O1W—H1	109.5	C7—C8—C9	119.36 (14)

Zn1—O1W—H2	110.7	C7—C8—C10	119.39 (13)
H1—O1W—H3	99.9	C9—C8—C10	121.24 (13)
C9—O2—Zn1	122.37 (10)	O2—C9—O1	114.78 (13)
C10—O4—Zn1	131.42 (10)	O2—C9—C8	127.30 (14)
C2—C1—C6	120.10 (15)	O1—C9—C8	117.92 (13)
C2—C1—H1A	119.9	O3—C10—O4	124.05 (14)
C6—C1—H1A	119.9	O3—C10—C8	116.41 (13)
C1—C2—C3	120.13 (15)	O4—C10—C8	119.51 (13)
C1—C2—H3A	119.9		

Symmetry codes: (i)  $-x+1, -y+1, -z+1$ .

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1 $\cdots$ O3 <sup>ii</sup>	0.82	1.88	2.6950 (17)	179
O1W—H2 $\cdots$ O3 <sup>iii</sup>	0.93	1.83	2.7473 (19)	168

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

Fig. 1

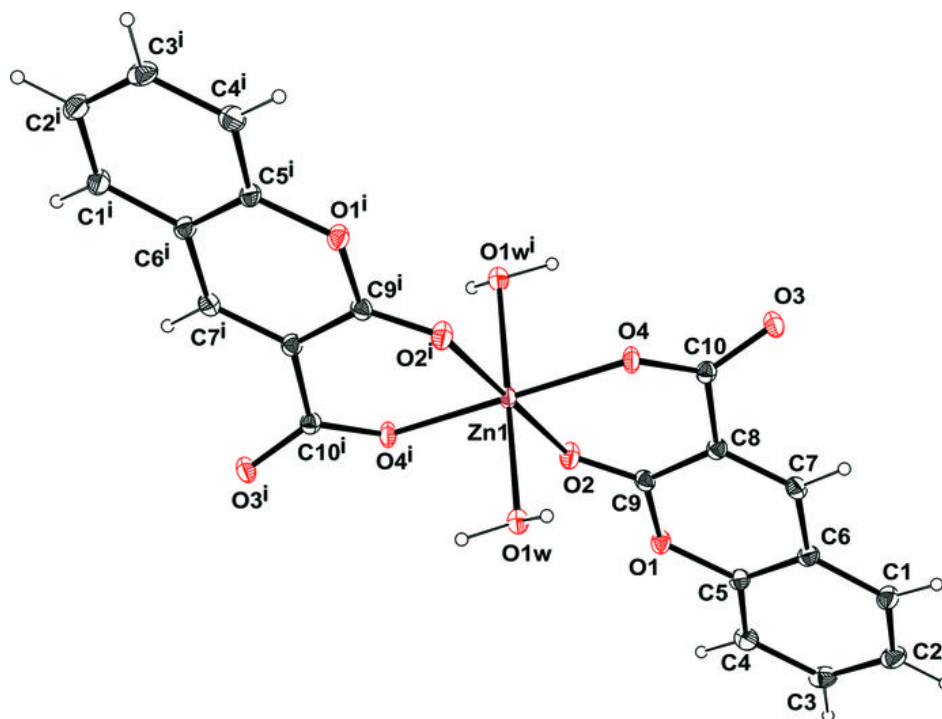




Fig. 2

