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

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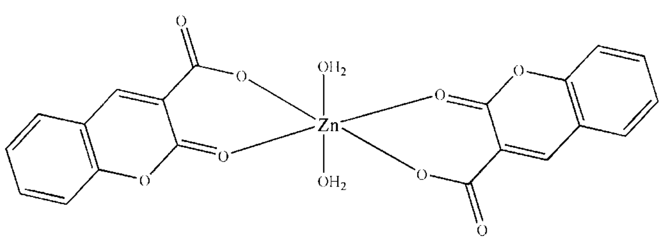
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.022; wR factor = 0.061; data-to-parameter ratio = 12.7.

In the title compound, $[Zn(C_{10}H_5O_4)_2(H_2O)_2]$, the Zn^{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

$[Zn(C_{10}H_5O_4)_2(H_2O)_2]$
M_r = 479.70
Triclinic, $P\bar{1}$
a = 6.6113 (13) Å
b = 6.8404 (14) Å
c = 10.392 (2) Å
α = 85.64 (3)°
β = 89.47 (3)°
γ = 66.09 (3)°
V = 428.27 (18) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.50 mm^{-1}
T = 293 K
0.2 × 0.2 × 0.2 mm

Data collection

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

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.061
S = 1.12
1808 reflections
142 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.42 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
O1W—H1···O3^{i}	0.82	1.88	2.6950 (17)	179
O1W—H2···O3^{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: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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

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supporting information

Acta Cryst. (2011). E**67**, m69   [https://doi.org/10.1107/S1600536810050865]

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

Yue Cui, Qian Gao, Huan-Huan Wang, Lin Wang and Ya-Bo Xie

S1. 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, $[Zn(C_{10}H_5O_4)_2(H_2O)_2]$, each Zn^{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···O hydrogen bonds involving the water molecules build up chain parllel to the [0 1 0] axis (Table 1, Fig. 2). The O-H···O interactions results in the formation of $R^4_2(8)$ rings (Etter, 1990; Bernstein *et al.*, 1995).

S2. Experimental

The title complex was synthesized by carefully layering a solution of $ZnSO_4.7H_2O$ (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 H_2O (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%.

S3. Refinement

The H atoms were placed geometrically (C—H = 0.93 Å) and treated as riding with $U_{iso(H)} = 1.2_{eq}(C)$. 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···H= 1.40 (2)Å) with $U_{iso}(H) = 1.5U_{eq}(O)$. In the last cycle of refinement they were treated as riding on their parent O atom.

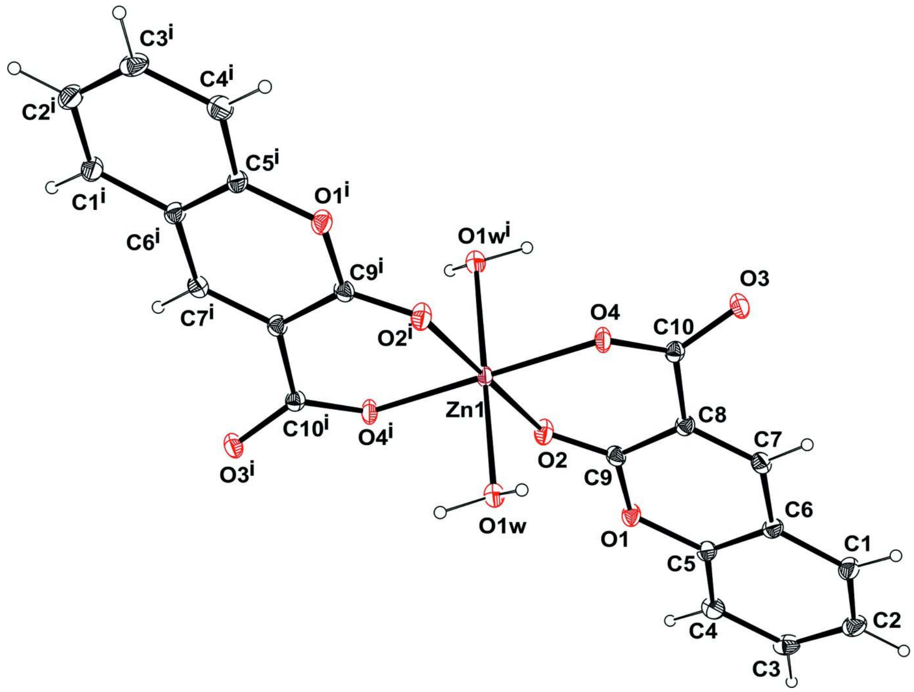

Figure 1

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]

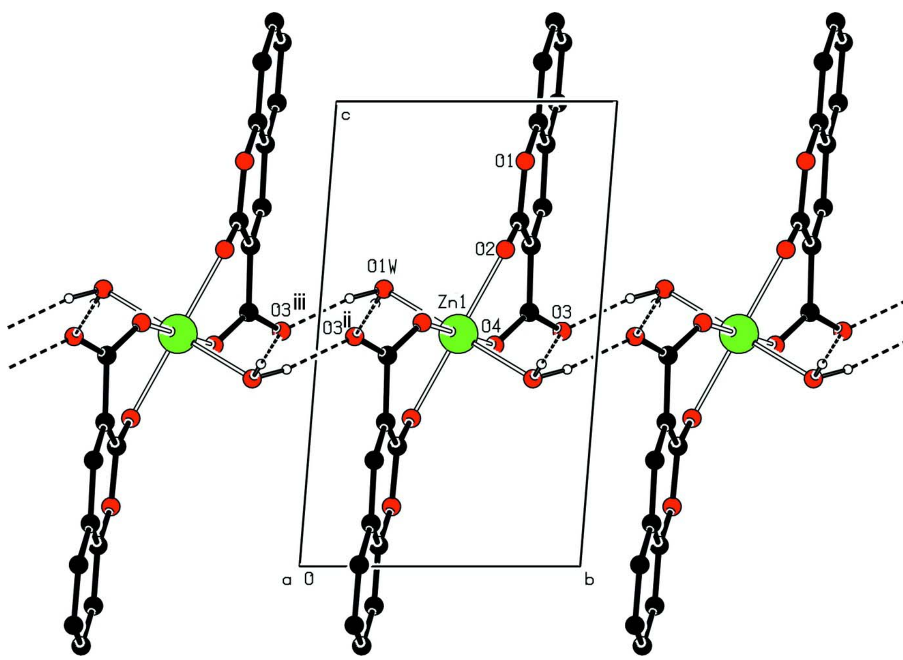

Figure 2

Partial packing view of compound (I), showing the formation of chains along [010] built from hydrogen bonds, and the formation of $R_2^4(8)$ 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-2*H*-chromene-3-carboxylato)zinc(II)

Crystal data

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c = 10.392 (2) Å
α = 85.64 (3)°
β = 89.47 (3)°
γ = 66.09 (3)°
V = 428.27 (18) Å^3
Z = 1
F(000) = 244
D_x = 1.860 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2271 reflections
θ = 3.4–28.4°
μ = 1.50 mm^{-1}
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 monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008)
T_{min} = 0.741, T_{max} = 0.748
2642 measured reflections
1808 independent reflections
1793 reflections with $I > 2\sigma(I)$
R_{int} = 0.013
θ_{max} = 27.1°, θ_{min} = 3.4°
h = −8→8
k = −8→8
l = 0→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.061
S = 1.12
1808 reflections
142 parameters
0 restraints
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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-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 (Å^2)

	x	y	z	$U_{iso}*/U_{eq}$
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 (Å²)

	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)
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 (Å, º)

Zn1—O4	2.0122 (12)	C1—C6	1.406 (2)
Zn1—O4^{i}	2.0122 (12)	C1—H1A	0.9300
Zn1—O1W^{i}	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^{i}	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^{i}	180.0	C3—C2—H3A	119.9
O4—Zn1—O1W^{i}	88.05 (5)	C4—C3—C2	120.84 (15)
O4^{i}—Zn1—O1W^{i}	91.95 (5)	C4—C3—H2A	119.6
O4—Zn1—O1W	91.95 (5)	C2—C3—H2A	119.6
O4^{i}—Zn1—O1W	88.05 (5)	C5—C4—C3	118.17 (15)
O1W^{i}—Zn1—O1W	180.00 (3)	C5—C4—H11A	120.9
O4—Zn1—O2	87.20 (5)	C3—C4—H11A	120.9
O4^{i}—Zn1—O2	92.80 (5)	O1—C5—C4	117.34 (14)
O1W^{i}—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^{i}	92.80 (5)	C5—C6—C1	118.34 (14)
O4^{i}—Zn1—O2^{i}	87.20 (5)	C5—C6—C7	118.03 (14)
O1W^{i}—Zn1—O2^{i}	89.11 (5)	C1—C6—C7	123.62 (14)
O1W—Zn1—O2^{i}	90.89 (5)	C8—C7—C6	121.59 (14)
O2—Zn1—O2^{i}	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 code: (i) $-x+1, -y+1, -z+1$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1···O3^{ii}	0.82	1.88	2.6950 (17)	179
O1*W*—H2···O3^{iii}	0.93	1.83	2.7473 (19)	168

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