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Diaquabis(4-formylbenzoato-κO)zinc(II) monohydrate

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
R factor = 0.026
wR factor = 0.074
Data-to-parameter ratio = 15.3

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

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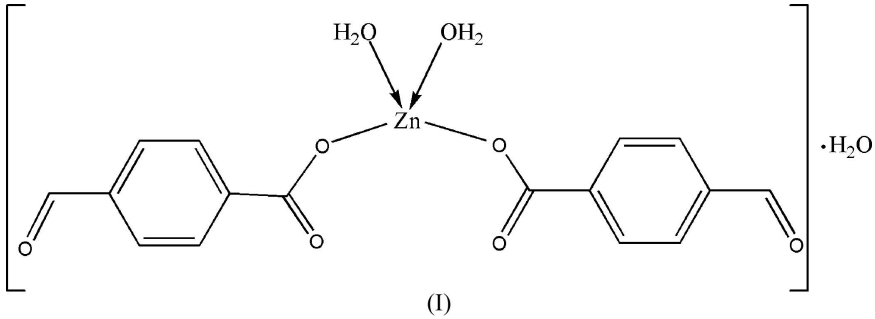
In the title complex, $[Zn(C_8H_5O_3)_2(H_2O)_2]\cdot H_2O$, the Zn atom exhibits a distorted tetrahedral coordination environment defined by two carboxylate O atoms and two water molecules. The coordinated and uncoordinated water molecules participate in a three-dimensional supramolecular network of O—H···O hydrogen bonds.

Comment

This report is part of a continuation of our studies on metal complexes of 4-formylbenzoic acid. In our previous work, we reported two metal complexes of 4-formylbenzoic acid with nickel(II) (Deng *et al.*, 2006*a*) and copper(II) (Deng *et al.*, 2006*b*), in which the 4-formylbenzoate ligand coordinated to the metal centers in a monodentate mode. Using zinc in a similar reaction leads to the formation of the title compound, (I), a monohydrated diaqua complex. As depicted in Fig. 1, the Zn^{II} atom exists in a distorted tetrahedral geometry. There is a long Zn1···O2 contact [2.5976 (13) Å]; if this were considered to be a bond, then an extremely acute O2—Zn1—O3 bond angle of 55.43 (6)° would arise.



(I)

We can see from Fig. 2 that all the adjacent mononuclear units parallel to the *a* axis are linked by hydrogen bonds formed by atoms O1*W* and O2*W*, giving rise to a one-dimensional chain, with a Zn···Zn separation of 7.9390 (16) Å. In addition, O1*W* forms another kind of hydrogen bond with O1, which connects these infinite hydrogen-bonded chains to produce a two-dimensional architecture in the crystallographic *ac* plane; the shortest distance between the Zn atoms of adjacent chains is 11.1762 (17) Å. The layers are further linked into a three-dimensional supramolecular network *via* hydrogen-bonding interactions between O1*W* and O2 (Table 2).

Experimental

Zinc diacetate dihydrate (0.11 g, 0.5 mmol) was added to an aqueous solution (15 ml) of 4-formylbenzoic acid (0.15 g, 1 mmol) that had

earlier been treated with 0.1 *M* sodium hydroxide to attain a pH of 5. The solution was allowed to evaporate at room temperature and colorless prismatic crystals of (I) were separated from the filtered solution after several days. Analysis calculated for $C_{16}H_{16}O_9Zn$: C 46.01, H 3.86%; found: C 46.06, H 3.83%.

Crystal data

$[Zn(C_8H_5O_3)_2(H_2O)_2]\cdot H_2O$	$Z = 2$
$M_r = 417.66$	$D_x = 1.628$ Mg m^{-3}
Monoclinic, $P2/c$	Mo $K\alpha$ radiation
$a = 7.9390$ (16) Å	$\mu = 1.49$ mm^{-1}
$b = 5.7474$ (11) Å	$T = 295$ (2) K
$c = 18.736$ (4) Å	Prism, colorless
$\beta = 94.69$ (3)°	0.36 × 0.24 × 0.18 mm
$V = 852.0$ (3) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	7940 measured reflections
	1959 independent reflections
ω scans	1820 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$R_{int} = 0.026$
	$\theta_{max} = 27.5°$
$T_{min} = 0.646$, $T_{max} = 0.768$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0453P)^2 + 0.1686P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.026$	
$wR(F^2) = 0.074$	
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
1959 reflections	$\Delta\rho_{max} = 0.31$ e Å^{-3}
128 parameters	$\Delta\rho_{min} = -0.26$ e Å^{-3}
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

Zn1—O3	1.9676 (13)		
Zn1—O2*W*	2.0076 (12)		
O3^i—Zn1—O3	141.88 (8)	O3—Zn1—O2*W*	97.93 (6)
O3—Zn1—O2*W*^{i}	106.94 (6)	O2*W*^{i}—Zn1—O2*W*	97.79 (7)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O1^{ii}	0.841 (6)	1.917 (6)	2.7319 (15)	163.0 (16)
O2*W*—H2*W*1···O1*W*	0.839 (9)	1.867 (9)	2.7047 (15)	177 (2)
O2*W*—H2*W*2···O2^{iii}	0.845 (9)	1.806 (10)	2.6460 (18)	172 (2)

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

The carbon-bound H atoms were placed in calculated positions, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$, and were refined in the riding-model approximation. The H atoms of the water molecules were located in a difference map and refined with O—H and H···H distance restraints of 0.85 (1) and 1.39 (1) Å, respectively, and with $U_{iso}(H) = 1.5U_{eq}(O)$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

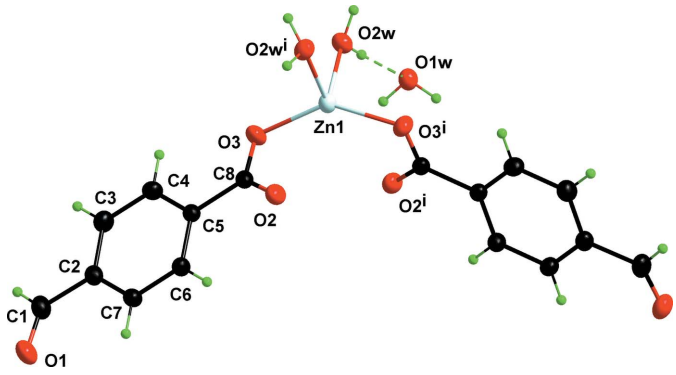


Figure 1
The molecular structure of the title complex showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. The dashed line indicates a hydrogen bond. [Symmetry code: (i) $-x+1, y, -z+\frac{1}{2}$.]

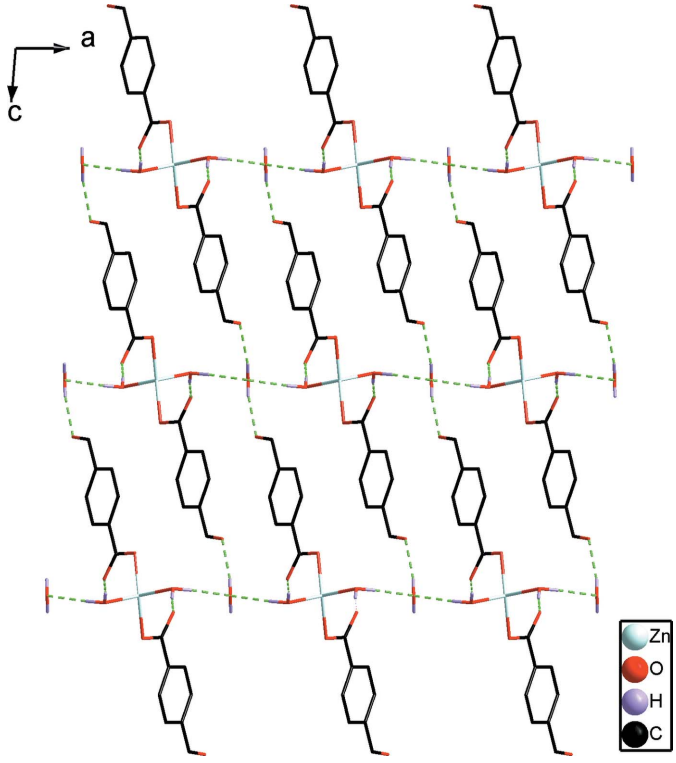


Figure 2
The three-dimensional supramolecular structure of (I), with the O—H···O hydrogen bonds denoted by dashed lines. H atoms not involved in hydrogen bonding have been omitted.

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