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

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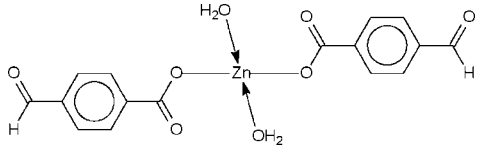
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.030; wR factor = 0.082; data-to-parameter ratio = 13.5.

The Zn^{II} atom in the title compound, $[Zn(C_8H_5O_3)_2(H_2O)_2]$, which lies on a twofold rotation axis, is coordinated by two monodentate carboxylate groups and two water molecules in a tetrahedral geometry; the geometry is distorted towards octahedral owing to two long $Zn\cdots O_{carbonyl}$ contacts [2.512 (2) Å]. Hydrogen-bonding interactions give rise to a three-dimensional network. The formyl group is disordered approximately equally over two positions.

Related literature

A pseudo-polymorph of the title compound containing a solvent water molecule exists in a $P2/c$ modification, which features zinc in an unambiguous tetrahedral coordination geometry; see Deng *et al.* (2006).



Experimental

Crystal data

$[Zn(C_8H_5O_3)_2(H_2O)_2]$
M_r = 399.64
Monoclinic, $C2/c$
a = 27.537 (1) Å
b = 5.0039 (2) Å
c = 12.0930 (6) Å
β = 110.039 (2)°
V = 1565.4 (1) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.61 mm^{-1}
T = 295 (2) K
0.34 × 0.26 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.532, T_{max} = 0.760
7203 measured reflections
1785 independent reflections
1448 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.082
S = 1.09
1785 reflections
132 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—O1W	1.983 (2)	Zn1—O2	2.512 (2)
Zn1—O1	2.005 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W1···O1^{i}	0.84 (1)	1.93 (1)	2.761 (2)	174 (3)
O1W—H1W2···O2^{ii}	0.84 (1)	1.88 (1)	2.720 (2)	174 (3)

Symmetry codes: (i) $-x+1, y-1, -z+\frac{3}{2}$; (ii) $-x+1, -y, -z+1$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2669).

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supporting information

Acta Cryst. (2008). E**64**, m447 [doi:10.1107/S1600536808003152]

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

Zhao-Peng Deng, Shan Gao, Li-Hua Huo and Seik Weng Ng

S1. Comment

A pseuodpolymorph of the title compound containing a solvent water molecule was isolated from the reaction of zinc acetate and 4-formylbenzoic acid in the presence of sodium hydroxide (Deng *et al.*, 2006). The reaction with pyridine in place of sodium hydroxide yielded the title polymorph.

S2. Experimental

Zinc diacetate dihydrate (2.2 g, 10 mmol) was added to anaqueous solution of 4-formylbenzoic acid (3.0 g, 20 mmol) that has earlier been treated with 1 ml pyridine to give a pH of 6. The solution was allowed to evaporate at room temperature; colorless prismatic crystals separated from the filtered solution after several days. C&N elemental analysis. Calc. $C_{16}H_{14}O_8Zn$: C 48.08, H3.53%. Found: C 48.06, H 3.56%.

S3. Refinement

The formyl group is disordered over two sites; the ratio of the site occupation factors refined to a 0.508 (5):0.492 (5) ratio.

The carbon-bound H atoms were placed in calculated positions [C–H 0.93 Å and U_{iso}(H) 1.2U_{eq}(C)], and were included in the refinement in the riding-model approximation. The water H-atoms were located in a difference Fourier map, and were refined with distance restraints of O–H 0.85±0.01 Å and H···H 1.39±0.01 Å; their displacement parameters were freely refined.

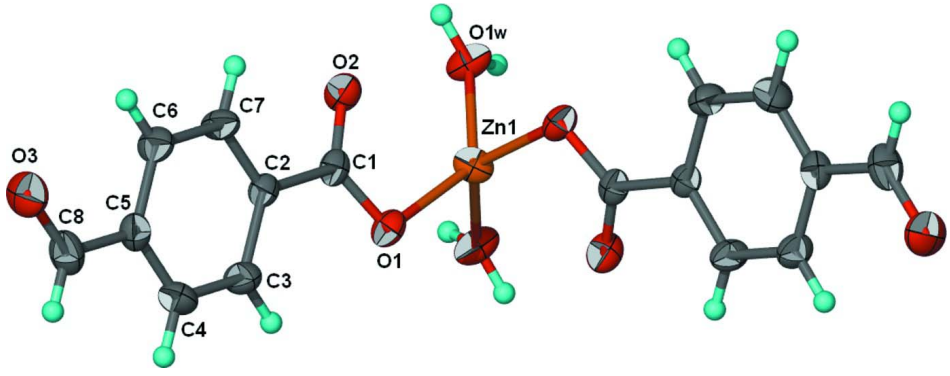

Figure 1

Anisotropic displacement parameter plot of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms as spheres of arbitrary radius.

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Crystal data

$[Zn(C_8H_5O_3)_2(H_2O)_2]$
$M_r = 399.64$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 27.537$ (1) Å
$b = 5.0039$ (2) Å
$c = 12.0930$ (6) Å
$\beta = 110.039$ (2)°
$V = 1565.4$ (1) Å^3
$Z = 4$
$F(000) = 816$
$D_x = 1.696$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5776 reflections
$\theta = 3.2$–$27.5°$
$\mu = 1.61$ mm^{-1}
$T = 295$ K
Block, colorless
0.34 × 0.26 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.532$, $T_{max} = 0.760$
7203 measured reflections
1785 independent reflections
1448 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$
$h = -35 \rightarrow 35$
$k = -6 \rightarrow 6$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.082$
$S = 1.09$
1785 reflections
132 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
$w = 1/[\sigma^2(F_o^2) + (0.0444P)^2 + 0.5739P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.59$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Zn1	0.5000	0.07300 (7)	0.7500	0.03500 (15)	
O1W	0.52887 (7)	−0.2045 (3)	0.67306 (15)	0.0420 (4)	
O1	0.44080 (6)	0.3312 (3)	0.69827 (13)	0.0347 (4)	
O2	0.46297 (6)	0.2522 (3)	0.54394 (14)	0.0396 (4)	
O3	0.28940 (13)	1.2782 (7)	0.2481 (3)	0.0537 (13)	0.508 (5)
O3′	0.25060 (16)	1.2320 (10)	0.3707 (4)	0.0757 (18)	0.492 (5)
H1W1	0.5398 (10)	−0.346 (3)	0.7104 (19)	0.051 (8)*	
H1W2	0.5313 (11)	−0.208 (5)	0.6055 (12)	0.062 (9)*	
C1	0.43534 (8)	0.3714 (4)	0.59025 (19)	0.0299 (5)	
C2	0.39595 (8)	0.5736 (4)	0.52428 (18)	0.0283 (4)	
C3	0.35743 (9)	0.6552 (5)	0.5675 (2)	0.0396 (5)	
H3	0.3554	0.5809	0.6363	0.048*	

C4	0.32199 (9)	0.8489 (6)	0.5070 (2)	0.0444 (6)	
H4	0.2963	0.9046	0.5357	0.053*	
C5	0.32469 (8)	0.9588 (4)	0.4047 (2)	0.0348 (5)	
C6	0.36283 (9)	0.8759 (5)	0.3612 (2)	0.0373 (5)	
H6	0.3645	0.9485	0.2919	0.045*	
C7	0.39830 (9)	0.6846 (5)	0.4219 (2)	0.0358 (5)	
H7	0.4240	0.6303	0.3932	0.043*	
C8	0.28767 (9)	1.1697 (5)	0.3399 (2)	0.0460 (6)	
H8	0.2621	1.2233	0.3691	0.055*	0.508 (5)
H8′	0.2924	1.2551	0.2760	0.055*	0.492 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0384 (2)	0.02089 (19)	0.0487 (3)	0.000	0.01878 (17)	0.000
O1W	0.0676 (11)	0.0278 (8)	0.0359 (10)	0.0119 (8)	0.0247 (8)	0.0052 (7)
O1	0.0445 (9)	0.0313 (8)	0.0266 (8)	−0.0005 (7)	0.0101 (6)	0.0054 (6)
O2	0.0460 (9)	0.0351 (8)	0.0355 (9)	0.0121 (7)	0.0111 (7)	−0.0003 (7)
O3	0.051 (2)	0.055 (2)	0.052 (2)	0.0156 (17)	0.0141 (17)	0.0215 (19)
O3′	0.058 (3)	0.086 (4)	0.079 (3)	0.036 (2)	0.019 (2)	0.008 (3)
C1	0.0335 (11)	0.0244 (10)	0.0276 (11)	−0.0051 (8)	0.0051 (8)	−0.0011 (8)
C2	0.0318 (10)	0.0251 (10)	0.0264 (10)	−0.0022 (8)	0.0078 (8)	−0.0022 (9)
C3	0.0413 (12)	0.0478 (13)	0.0338 (13)	0.0033 (11)	0.0180 (10)	0.0055 (10)
C4	0.0356 (12)	0.0557 (15)	0.0458 (15)	0.0093 (11)	0.0190 (10)	−0.0025 (12)
C5	0.0314 (11)	0.0341 (12)	0.0337 (12)	0.0016 (9)	0.0044 (9)	−0.0032 (10)
C6	0.0418 (12)	0.0386 (12)	0.0322 (12)	0.0061 (10)	0.0135 (9)	0.0093 (10)
C7	0.0417 (12)	0.0366 (11)	0.0342 (12)	0.0106 (10)	0.0196 (10)	0.0037 (10)
C8	0.0368 (13)	0.0432 (13)	0.0497 (16)	0.0091 (11)	0.0043 (11)	−0.0036 (12)

Geometric parameters (Å, º)

Zn1—O1w	1.983 (2)	C2—C3	1.395 (3)
Zn1—O1w^{i}	1.983 (2)	C3—C4	1.392 (4)
Zn1—O1^{i}	2.005 (2)	C3—H3	0.9300
Zn1—O1	2.005 (2)	C4—C5	1.379 (4)
Zn1—O2	2.512 (2)	C4—H4	0.9300
O1W—H1W1	0.84 (1)	C5—C6	1.389 (3)
O1W—H1W2	0.84 (1)	C5—C8	1.490 (3)
O1—C1	1.279 (3)	C6—C7	1.385 (3)
O2—C1	1.241 (3)	C6—H6	0.9300
O3—C8	1.251 (4)	C7—H7	0.9300
O3′—C8	1.240 (5)	C8—H8	0.9300
C1—C2	1.498 (3)	C8—H8′	0.9300
C2—C7	1.379 (3)		
O1W—Zn1—O1W^{i}	91.11 (10)	C5—C4—H4	119.8
O1W—Zn1—O1^{i}	100.59 (7)	C3—C4—H4	119.8
O1W^{i}—Zn1—O1^{i}	135.95 (7)	C4—C5—C6	120.0 (2)

O1W—Zn1—O1	135.95 (7)	C4—C5—C8	121.1 (2)
O1W^{i}—Zn1—O1	100.59 (7)	C6—C5—C8	118.9 (2)
O1^{i}—Zn1—O1	99.75 (9)	C7—C6—C5	119.6 (2)
Zn1—O1W—H1W1	117.8 (17)	C7—C6—H6	120.2
Zn1—O1W—H1W2	130.4 (17)	C5—C6—H6	120.2
H1W1—O1W—H1W2	111.8 (16)	C2—C7—C6	120.8 (2)
C1—O1—Zn1	102.62 (13)	C2—C7—H7	119.6
O2—C1—O1	120.65 (19)	C6—C7—H7	119.6
O2—C1—C2	121.9 (2)	O3—C8—O3′	116.3 (3)
O1—C1—C2	117.42 (19)	O3—C8—C5	123.1 (3)
C7—C2—C3	119.6 (2)	O3′—C8—C5	120.4 (3)
C7—C2—C1	120.14 (19)	O3—C8—H8	118.4
C3—C2—C1	120.2 (2)	C5—C8—H8	118.4
C4—C3—C2	119.5 (2)	O3′—C8—H8′	119.8
C4—C3—H3	120.2	C5—C8—H8′	119.8
C2—C3—H3	120.2	H8—C8—H8′	121.5
C5—C4—C3	120.4 (2)		

O1W—Zn1—O1—C1	−27.75 (17)	C3—C4—C5—C6	0.1 (4)
O1W^{i}—Zn1—O1—C1	−130.56 (13)	C3—C4—C5—C8	−178.9 (2)
O1^{i}—Zn1—O1—C1	88.73 (13)	C4—C5—C6—C7	−0.6 (4)
Zn1—O1—C1—O2	2.0 (2)	C8—C5—C6—C7	178.5 (2)
Zn1—O1—C1—C2	−175.83 (14)	C3—C2—C7—C6	−0.1 (3)
O2—C1—C2—C7	−17.2 (3)	C1—C2—C7—C6	−178.6 (2)
O1—C1—C2—C7	160.7 (2)	C5—C6—C7—C2	0.6 (4)
O2—C1—C2—C3	164.4 (2)	C4—C5—C8—O3	178.6 (3)
O1—C1—C2—C3	−17.8 (3)	C6—C5—C8—O3	−0.5 (4)
C7—C2—C3—C4	−0.3 (4)	C4—C5—C8—O3′	−7.0 (5)
C1—C2—C3—C4	178.2 (2)	C6—C5—C8—O3′	173.9 (3)
C2—C3—C4—C5	0.3 (4)		

Symmetry code: (i) −*x*+1, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O1^{ii}	0.84 (1)	1.93 (1)	2.761 (2)	174 (3)
O1*W*—H1*W*2···O2^{iii}	0.84 (1)	1.88 (1)	2.720 (2)	174 (3)

Symmetry codes: (ii) −*x*+1, *y*−1, −*z*+3/2; (iii) −*x*+1, −*y*, −*z*+1.