

catena-Poly[[diaquazinc(II)]- μ -4,4'-(methylenedioxy)dibenzoato]

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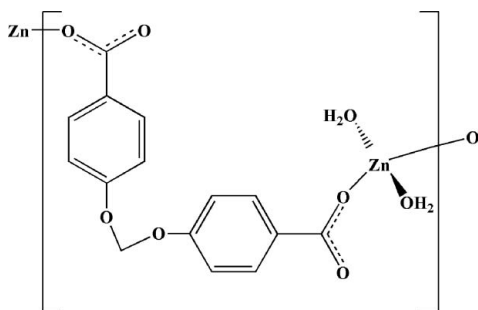
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.032; wR factor = 0.075; data-to-parameter ratio = 14.4.

In the title complex, $[\text{Zn}(\text{C}_{15}\text{H}_{10}\text{O}_6)(\text{H}_2\text{O})_2]_n$, the Zn^{II} atom is located on a twofold rotation axis and exhibits a distorted tetrahedral coordination environment defined by two O atoms from two 4,4'-(methylenedioxy)dibenzoate ligands and two O atoms from two coordinated water molecules. In the crystal structure, molecules are linked into a three-dimensional framework by $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds and $\text{C}-\text{H}\cdots\pi$ interactions.

Related literature

For the potential properties and structural topologies of metal-organic complexes involving polycarboxylate ligands, see: Chen & Liu (2002); Han *et al.* (2009); Li *et al.* (2007).



Experimental

Crystal data

$[\text{Zn}(\text{C}_{15}\text{H}_{10}\text{O}_6)(\text{H}_2\text{O})_2]$
 $M_r = 387.63$
Monoclinic, $P2_1/c$
 $a = 13.496$ (1) Å
 $b = 4.931$ (1) Å
 $c = 12.357$ (1) Å
 $\beta = 113.352$ (1)°

$V = 755.0$ (2) Å³
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 1.67$ mm⁻¹
 $T = 293$ K
0.21 × 0.19 × 0.15 mm

Data collection

Rigaku R-Axis RAPID diffractometer
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{\text{min}} = 0.707$, $T_{\text{max}} = 0.780$

4318 measured reflections
1696 independent reflections
1461 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.075$
 $S = 1.06$
1696 reflections
118 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.25$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.30$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Zn1—O1	1.9582 (18)	Zn1—O4	1.975 (2)
O1—Zn1—O1 ⁱ	102.26 (11)	O1 ⁱ —Zn1—O4	132.40 (8)
O1—Zn1—O4	99.87 (9)	O4—Zn1—O4 ⁱ	95.27 (13)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O4—H1 ⁱ \cdots O1 ⁱⁱ	0.74 (3)	2.13 (3)	2.851 (3)	167 (3)
O4—H2 ⁱ \cdots O2 ⁱⁱⁱ	0.88 (4)	1.78 (4)	2.657 (3)	177 (4)
C8—H8A ⁱ \cdots Cg3 ^{iv}	0.97	2.97	3.741 (3)	137
C8—H8B ⁱ \cdots Cg3 ^v	0.97	2.97	3.741 (3)	137

Symmetry codes: (ii) $x, y - 1, z$; (iii) $x, -y, z - \frac{1}{2}$; (iv) $x, y + 1, z$; (v) $-x + 1, y + 1, -z + \frac{3}{2}$. Cg3 is the centroid of the C2–C7 benzene ring.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL-Plus* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2728).

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supplementary materials

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Comment

Recently, the area of metal-organic framework materials has become one of the intense research activity for their fascinating structural diversities and potential applications in catalysis, nonlinear optics and molecular sensing. As an important family of multidentate O-donor ligands, organic aromatic polycarboxylate ligands have been extensively employed in the preparation of metal-organic complexes because of their potential properties and intriguing structural topologies (Han *et al.*, 2009; Li *et al.*, 2007; Chen *et al.*, 2002). Herein, we report the structure of the title complex with bis(4-benzoateoxyl)methane and zinc, [Zn(C₁₅H₁₀O₆)(H₂O)₂] (I).

Single-crystal X-ray diffraction analyses revealed Zn(II) is tetra-coordinated and exhibits tetrahedral coordination environment supplied by two bis(4-benzoateoxyl)methane O atoms and two water molecules (Fig. 1). The Zn—O bond lengths are in the normal range (Table 1). The bis(4-benzoateoxyl)methane ligand adopts bidentate coordinated modes and bond with two zinc ions to form a chain. Adjacent chains are linked by O—H \cdots O hydrogen bonds and C—H \cdots π interactions into a three-dimensional supramolecular network structure (Fig. 2, Table 2).

Experimental

Zinc(II) acetate dihydrate (0.066 g, 0.3 mol), bis(4-benzoateoxyl)methane (0.058 g, 0.2 mmol), sodium hydroxide (0.016 g, 0.4 mmol) and water (14 ml) were placed in a 23 ml Teflon-lined autoclave, and the autoclave was heated at 423 K for 3 d. After cooling slowly to room temperature at a rate of 10 K h⁻¹, colourless crystals of (I) were obtained.

Refinement

C-bound H atoms were treated as riding, with C—H = 0.93 and 0.97 Å and $U_{\text{iso}}(\text{H}) = 1.2$ times $U_{\text{eq}}(\text{C})$. O-bound H atoms were located in a difference Fourier map and refined as riding in their as-found relative positions; $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$.

Figures

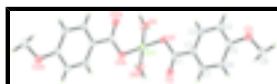


Fig. 1. View of the local coordination of Zn(II) with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

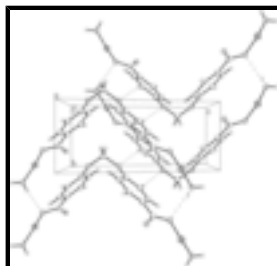


Fig. 2. A packing diagram for the three-dimensional supramolecular framework *via* O—H \cdots O interactions. The view direction is parallel to the *a* axis. Hydrogen bonds are indicated by dashed lines.

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Crystal data

[Zn(C ₁₅ H ₁₀ O ₆)(H ₂ O) ₂]	$F_{000} = 396$
$M_r = 387.63$	$D_x = 1.705 \text{ Mg m}^{-3}$
Monoclinic, $P2/c$	Mo $K\alpha$ radiation
Hall symbol: -P 2yc	$\lambda = 0.71069 \text{ \AA}$
$a = 13.496 (1) \text{ \AA}$	Cell parameters from 3185 reflections
$b = 4.931 (1) \text{ \AA}$	$\theta = 2.1\text{--}27.4^\circ$
$c = 12.357 (1) \text{ \AA}$	$\mu = 1.67 \text{ mm}^{-1}$
$\beta = 113.352 (1)^\circ$	$T = 293 \text{ K}$
$V = 755.0 (2) \text{ \AA}^3$	Block, colourless
$Z = 2$	$0.21 \times 0.19 \times 0.15 \text{ mm}$

Data collection

Rigaku R-Axis RAPID diffractometer	1696 independent reflections
Radiation source: fine-focus sealed tube	1461 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.027$
Detector resolution: 10 pixels mm^{-1}	$\theta_{\text{max}} = 27.5^\circ$
$T = 293 \text{ K}$	$\theta_{\text{min}} = 3.3^\circ$
ω scans	$h = -10 \rightarrow 17$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -6 \rightarrow 5$
$T_{\text{min}} = 0.707$, $T_{\text{max}} = 0.780$	$l = -15 \rightarrow 15$
4318 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.032$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.075$	$w = 1/[\sigma^2(F_o^2) + (0.0304P)^2 + 0.2993P]$
$S = 1.06$	where $P = (F_o^2 + 2F_c^2)/3$
1696 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
118 parameters	$\Delta\rho_{\text{max}} = 0.25 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.30 \text{ e \AA}^{-3}$
	Extinction correction: none

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Zn1	0.0000	0.02532 (7)	0.2500	0.03611 (14)	
O3	0.48509 (13)	1.0388 (3)	0.65056 (14)	0.0430 (4)	
O4	0.06484 (17)	-0.2446 (4)	0.17945 (17)	0.0484 (5)	
O2	0.07014 (13)	0.2515 (3)	0.46679 (14)	0.0420 (4)	
O1	0.12200 (13)	0.2746 (3)	0.31887 (13)	0.0406 (4)	
C5	0.39531 (18)	0.8759 (5)	0.60267 (19)	0.0351 (5)	
C7	0.22564 (18)	0.6856 (4)	0.58165 (19)	0.0356 (5)	
H7	0.1685	0.6754	0.6055	0.043*	
C1	0.13275 (18)	0.3401 (4)	0.42419 (18)	0.0331 (5)	
C8	0.5000	1.1980 (7)	0.7500	0.0451 (8)	
H8A	0.4375	1.3138	0.7330	0.054*	0.50
H8B	0.5625	1.3138	0.7670	0.054*	0.50
C2	0.22362 (18)	0.5269 (4)	0.48823 (19)	0.0328 (5)	
C6	0.31099 (19)	0.8591 (5)	0.6403 (2)	0.0379 (5)	
H6	0.3119	0.9624	0.7037	0.046*	
C3	0.3096 (2)	0.5481 (5)	0.4528 (2)	0.0434 (6)	
H3	0.3092	0.4453	0.3896	0.052*	
C4	0.3942 (2)	0.7180 (5)	0.5100 (2)	0.0447 (6)	
H4	0.4515	0.7273	0.4863	0.054*	
H2	0.069 (3)	-0.244 (7)	0.110 (3)	0.100 (13)*	
H1	0.085 (2)	-0.374 (6)	0.210 (2)	0.046 (8)*	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0455 (2)	0.0276 (2)	0.0380 (2)	0.000	0.01943 (18)	0.000
O3	0.0416 (9)	0.0491 (10)	0.0364 (9)	-0.0115 (8)	0.0132 (7)	0.0005 (7)
O4	0.0832 (14)	0.0311 (10)	0.0397 (10)	0.0128 (9)	0.0338 (10)	0.0040 (8)
O2	0.0471 (9)	0.0448 (9)	0.0359 (9)	-0.0096 (8)	0.0183 (7)	0.0003 (7)
O1	0.0538 (10)	0.0371 (9)	0.0338 (9)	-0.0057 (8)	0.0205 (8)	-0.0074 (7)
C5	0.0361 (12)	0.0332 (11)	0.0337 (12)	-0.0026 (10)	0.0114 (10)	0.0052 (10)
C7	0.0367 (12)	0.0370 (12)	0.0370 (12)	-0.0021 (10)	0.0189 (10)	-0.0009 (10)

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C1	0.0404 (12)	0.0269 (10)	0.0293 (11)	0.0039 (9)	0.0110 (10)	0.0010 (9)
C8	0.045 (2)	0.0317 (17)	0.051 (2)	0.000	0.0109 (16)	0.000
C2	0.0379 (12)	0.0304 (11)	0.0301 (11)	-0.0009 (9)	0.0135 (9)	0.0015 (9)
C6	0.0445 (13)	0.0378 (12)	0.0338 (12)	-0.0033 (10)	0.0179 (11)	-0.0055 (10)
C3	0.0488 (14)	0.0483 (14)	0.0398 (13)	-0.0055 (12)	0.0246 (12)	-0.0078 (11)
C4	0.0447 (14)	0.0506 (14)	0.0483 (14)	-0.0037 (12)	0.0285 (12)	-0.0033 (12)

Geometric parameters (\AA , $^\circ$)

Zn1—O1	1.9582 (18)	C7—C2	1.386 (3)
Zn1—O1 ⁱ	1.9582 (18)	C7—C6	1.387 (3)
Zn1—O4	1.975 (2)	C7—H7	0.9300
Zn1—O4 ⁱ	1.975 (2)	C1—C2	1.487 (3)
O3—C5	1.377 (3)	C8—O3 ⁱⁱ	1.404 (2)
O3—C8	1.404 (2)	C8—H8A	0.9700
O4—H2	0.88 (4)	C8—H8B	0.9700
O4—H1	0.74 (3)	C2—C3	1.396 (3)
O2—C1	1.239 (3)	C6—H6	0.9300
O1—C1	1.292 (3)	C3—C4	1.366 (3)
C5—C4	1.380 (3)	C3—H3	0.9300
C5—C6	1.392 (3)	C4—H4	0.9300
O1—Zn1—O1 ⁱ	102.26 (11)	O1—C1—C2	115.52 (19)
O1—Zn1—O4	99.87 (9)	O3—C8—O3 ⁱⁱ	112.0 (3)
O1 ⁱ —Zn1—O4	132.40 (8)	O3—C8—H8A	109.2
O1—Zn1—O4 ⁱ	132.40 (8)	O3 ⁱⁱ —C8—H8A	109.2
O1 ⁱ —Zn1—O4 ⁱ	99.87 (9)	O3—C8—H8B	109.2
O4—Zn1—O4 ⁱ	95.27 (13)	O3 ⁱⁱ —C8—H8B	109.2
C5—O3—C8	119.93 (16)	H8A—C8—H8B	107.9
Zn1—O4—H2	130 (2)	C7—C2—C3	118.3 (2)
Zn1—O4—H1	119 (2)	C7—C2—C1	122.2 (2)
H2—O4—H1	111 (3)	C3—C2—C1	119.5 (2)
C1—O1—Zn1	109.52 (14)	C7—C6—C5	118.8 (2)
O3—C5—C4	113.8 (2)	C7—C6—H6	120.6
O3—C5—C6	126.0 (2)	C5—C6—H6	120.6
C4—C5—C6	120.2 (2)	C4—C3—C2	120.8 (2)
C2—C7—C6	121.5 (2)	C4—C3—H3	119.6
C2—C7—H7	119.3	C2—C3—H3	119.6
C6—C7—H7	119.3	C3—C4—C5	120.4 (2)
O2—C1—O1	121.1 (2)	C3—C4—H4	119.8
O2—C1—C2	123.4 (2)	C5—C4—H4	119.8
O1 ⁱ —Zn1—O1—C1	86.84 (14)	O1—C1—C2—C7	158.0 (2)
O4—Zn1—O1—C1	-135.58 (15)	O2—C1—C2—C3	159.3 (2)
O4 ⁱ —Zn1—O1—C1	-29.01 (18)	O1—C1—C2—C3	-21.1 (3)
C8—O3—C5—C4	-176.2 (2)	C2—C7—C6—C5	1.0 (3)
C8—O3—C5—C6	3.1 (3)	O3—C5—C6—C7	179.5 (2)
Zn1—O1—C1—O2	-1.0 (3)	C4—C5—C6—C7	-1.2 (3)

Zn1—O1—C1—C2	179.28 (14)	C7—C2—C3—C4	0.9 (4)
C5—O3—C8—O3 ⁱⁱ	64.94 (16)	C1—C2—C3—C4	-180.0 (2)
C6—C7—C2—C3	-0.9 (3)	C2—C3—C4—C5	-1.2 (4)
C6—C7—C2—C1	-179.9 (2)	O3—C5—C4—C3	-179.3 (2)
O2—C1—C2—C7	-21.7 (3)	C6—C5—C4—C3	1.3 (4)

Symmetry codes: (i) $-x, y, -z+1/2$; (ii) $-x+1, y, -z+3/2$.

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O4—H1 \cdots O1 ⁱⁱⁱ	0.74 (3)	2.13 (3)	2.851 (3)	167 (3)
O4—H2 \cdots O2 ^{iv}	0.88 (4)	1.78 (4)	2.657 (3)	177 (4)
C8—H8A \cdots Cg3 ^v	0.97	2.97	3.741 (3)	137
C8—H8B \cdots Cg3 ^{vi}	0.97	2.97	3.741 (3)	137

Symmetry codes: (iii) $x, y-1, z$; (iv) $x, -y, z-1/2$; (v) $x, y+1, z$; (vi) $-x+1, y+1, -z+3/2$.

Fig. 2

