Diaquabis(cyclohexanecarboxylato)zinc(II) monohydrate

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In the title compound, $[Zn(C_7H_{11}O_2)_2(H_2O)_2]\cdot H_2O$, the Zn^{II} atom (site symmetry $\bar{1}$) is four-coordinated by two O atoms from the cyclohexanecarboxylate anions and two O atoms from the water molecules, forming a slightly distorted square-planar coordination. The O atom of the uncoordinated water molecule lies on a crystallographic twofold rotation axis. In the crystal, the components are linked by O—H⋯O hydrogen bonds, forming a three-dimensional network.

Related literature

For background, see: Cheng *et al.* (2006). For reference structural data, see: Allen *et al.* (1987).
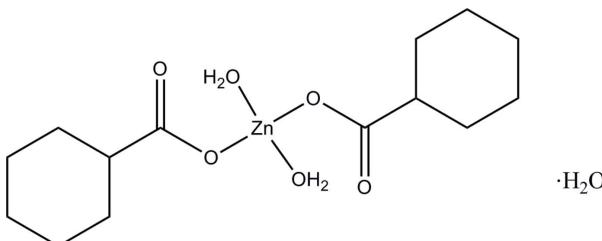
Experimental

Crystal data
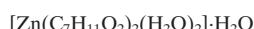
$[Zn(C_7H_{11}O_2)_2(H_2O)_2]\cdot H_2O$
$M_r = 373.75$
Monoclinic, $P2/c$
$a = 15.9045$ (16) Å
$b = 4.9295$ (6) Å
$c = 11.5335$ (16) Å
$\beta = 91.585$ (6)°

$V = 903.89$ (19) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 1.39$ mm^{-1}
$T = 296$ K
$0.28 \times 0.25 \times 0.22$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.698$, $T_{max} = 0.750$
4764 measured reflections

1752 independent reflections
1436 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
200 standard reflections every 3 reflections intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.158$
$S = 1.07$
1752 reflections
114 parameters
4 restraints

H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 1.00$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—O2	1.961 (3)	Zn1—O3	1.977 (4)

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O7—H7⋯O1	0.834 (10)	1.99 (3)	2.699 (4)	142 (5)
O3—H3D⋯O1^i	0.846 (10)	2.53 (7)	3.132 (6)	129 (8)
O3—H3C⋯O7^{ii}	0.853 (10)	2.17 (2)	2.997 (5)	164 (6)

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5057).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
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supporting information

Diaquabis(cyclohexanecarboxylato)zinc(II) monohydrate

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S1. Comment

There has been much research interest in acid metal complexes due to their molecular architectures and biological activities (e.g. Cheng *et al.*, 2006). In this work, we report here the crystal structure of the title compound, (I). In (I), all bond lengths are within normal ranges (Allen *et al.*, 1987) (Fig. 1). The Zn^{II} atom is four-coordinated by two O atoms from the cyclohexanecarboxylate and two O atoms from the water molecules, forming a slightly distorted square-planar coordination (Table 1). In the crystal, O—H⋯O hydrogen bonds (Table 2) link the components.

S2. Experimental

A mixture of cyclohexanecarboxylic acid (256 mg, 2 mmol) and ZnNO$_3$.6H$_2$O (1 mmol, 297 mg) in methanol (10 ml) was stirred for 2 h. After keeping the filtrate in air for 6 d, colourless blocks of (I) were formed.

S3. Refinement

The O-bound H atoms were located in a difference map and their positions were refined with the restraint O—H = 0.82 (1)Å. The other H atoms were positioned geometrically (C—H = 0.97–0.98Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(carrier).
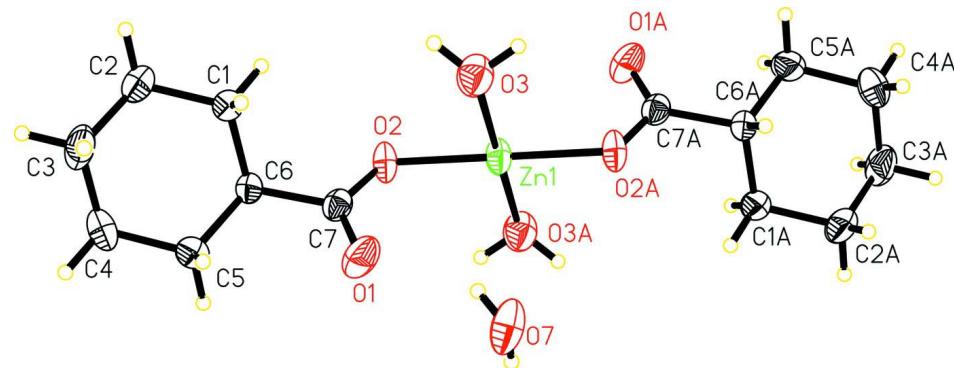
Figure 1

The molecular structure of (I) showing 30% probability displacement ellipsoids. Atoms with the suffix A are generated by the symmetry code (1–x, 1–y, –z).

Diaquabis(cyclohexanecarboxylato)zinc(II) monohydrate

Crystal data

[Zn(C$_7$H$_{11}$O$_2$)$_2$(H$_2$O)$_2$]·H$_2$O
M_r = 373.75
Monoclinic, *P*2/*c*

Hall symbol: -P 2yc
a = 15.9045 (16) Å
b = 4.9295 (6) Å

$c = 11.5335$ (16) Å
$\beta = 91.585$ (6)°
$V = 903.89$ (19) Å^3
$Z = 2$
$F(000) = 396$
$D_x = 1.373$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 25 reflections
$\theta = 9$–12°
$\mu = 1.39$ mm^{-1}
$T = 296$ K
Block, colorless
$0.28 \times 0.25 \times 0.22$ mm

Data collection

Enraf–Nonius CAD-4
  diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan
  (North *et al.*, 1968)
$T_{min} = 0.698$, $T_{max} = 0.750$
4764 measured reflections

1752 independent reflections
1436 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.6°$
$h = -18\rightarrow19$
$k = -6\rightarrow6$
$l = -12\rightarrow14$
200 standard reflections every 3 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.158$
$S = 1.07$
1752 reflections
114 parameters
4 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
$w = 1/[\sigma^2(F_o^2) + (0.0809P)^2 + 1.216P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 1.00$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}

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 (Å^2)

	x	y	z	$U_{iso}*/U_{eq}$
C1	0.2156 (3)	0.3294 (12)	−0.0060 (4)	0.0586 (12)
H1A	0.2463	0.2824	−0.0747	0.070*
H1B	0.2126	0.5256	−0.0017	0.070*
C2	0.1273 (3)	0.2162 (13)	−0.0177 (4)	0.0711 (14)
H2A	0.0988	0.2966	−0.0847	0.085*
H2B	0.1301	0.0218	−0.0300	0.085*
C3	0.0779 (3)	0.2734 (13)	0.0889 (5)	0.0743 (15)
H3A	0.0709	0.4676	0.0980	0.089*

H3B	0.0226	0.1917	0.0810	0.089*
C4	0.1236 (3)	0.1592 (16)	0.1934 (5)	0.0832 (18)
H4A	0.1264	−0.0367	0.1864	0.100*
H4B	0.0925	0.2017	0.2622	0.100*
C5	0.2124 (3)	0.2720 (13)	0.2071 (4)	0.0661 (14)
H5A	0.2095	0.4653	0.2221	0.079*
H5B	0.2405	0.1867	0.2733	0.079*
C6	0.2630 (2)	0.2234 (9)	0.0999 (3)	0.0427 (9)
H6	0.2708	0.0274	0.0908	0.051*
C7	0.3485 (2)	0.3560 (8)	0.1063 (4)	0.0455 (9)
H7	0.475 (3)	0.722 (8)	0.205 (3)	0.058 (14)*
O1	0.3660 (3)	0.5302 (7)	0.1802 (4)	0.0755 (11)
O2	0.39946 (17)	0.2822 (6)	0.0283 (3)	0.0549 (8)
O3	0.4282 (3)	0.7551 (8)	−0.0904 (4)	0.0718 (10)
O7	0.5000	0.8302 (10)	0.2500	0.0775 (16)
Zn1	0.5000	0.5000	0.0000	0.0492 (3)
H3D	0.384 (3)	0.71 (2)	−0.127 (5)	0.18 (5)*
H3C	0.457 (3)	0.852 (11)	−0.136 (4)	0.076 (18)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.045 (2)	0.085 (4)	0.046 (2)	−0.007 (2)	−0.0019 (18)	0.005 (2)
C2	0.048 (3)	0.097 (4)	0.067 (3)	−0.012 (3)	−0.011 (2)	−0.006 (3)
C3	0.037 (2)	0.094 (4)	0.092 (4)	−0.003 (2)	0.000 (2)	−0.010 (3)
C4	0.057 (3)	0.120 (5)	0.075 (3)	−0.017 (3)	0.026 (3)	0.004 (4)
C5	0.053 (3)	0.101 (4)	0.045 (2)	−0.002 (3)	0.005 (2)	0.002 (2)
C6	0.0374 (19)	0.046 (2)	0.045 (2)	−0.0065 (16)	0.0017 (16)	−0.0002 (17)
C7	0.041 (2)	0.041 (2)	0.054 (2)	−0.0016 (17)	−0.0066 (18)	0.0067 (19)
O1	0.065 (2)	0.074 (3)	0.086 (3)	−0.0155 (18)	−0.0144 (19)	−0.0217 (19)
O2	0.0323 (14)	0.0504 (17)	0.083 (2)	−0.0060 (12)	0.0125 (14)	0.0045 (15)
O3	0.060 (2)	0.066 (2)	0.089 (3)	−0.0020 (18)	−0.004 (2)	0.012 (2)
O7	0.047 (3)	0.041 (3)	0.143 (5)	0.000	−0.008 (3)	0.000
Zn1	0.0317 (4)	0.0478 (4)	0.0684 (5)	−0.0007 (3)	0.0066 (3)	0.0097 (3)

Geometric parameters (Å, º)

C1—C6	1.511 (6)	C5—H5A	0.9700
C1—C2	1.513 (6)	C5—H5B	0.9700
C1—H1A	0.9700	C6—C7	1.509 (5)
C1—H1B	0.9700	C6—H6	0.9800
C2—C3	1.503 (7)	C7—O1	1.236 (5)
C2—H2A	0.9700	C7—O2	1.281 (5)
C2—H2B	0.9700	Zn1—O2	1.961 (3)
C3—C4	1.500 (8)	Zn1—O3	1.977 (4)
C3—H3A	0.9700	O3—H3D	0.846 (10)
C3—H3B	0.9700	O3—H3C	0.853 (10)
C4—C5	1.521 (7)	O7—H7	0.834 (10)

C4—H4A	0.9700	Zn1—O2ⁱ	1.961 (3)
C4—H4B	0.9700	Zn1—O3ⁱ	1.977 (4)
C5—C6	1.513 (6)		
C6—C1—C2	112.6 (4)	C6—C5—H5A	109.3
C6—C1—H1A	109.1	C4—C5—H5A	109.3
C2—C1—H1A	109.1	C6—C5—H5B	109.3
C6—C1—H1B	109.1	C4—C5—H5B	109.3
C2—C1—H1B	109.1	H5A—C5—H5B	107.9
H1A—C1—H1B	107.8	C7—C6—C1	108.6 (3)
C3—C2—C1	111.3 (4)	C7—C6—C5	113.0 (4)
C3—C2—H2A	109.4	C1—C6—C5	110.0 (4)
C1—C2—H2A	109.4	C7—C6—H6	108.4
C3—C2—H2B	109.4	C1—C6—H6	108.4
C1—C2—H2B	109.4	C5—C6—H6	108.4
H2A—C2—H2B	108.0	O1—C7—O2	123.1 (4)
C4—C3—C2	109.5 (4)	O1—C7—C6	121.4 (4)
C4—C3—H3A	109.8	O2—C7—C6	115.5 (4)
C2—C3—H3A	109.8	C7—O2—Zn1	119.8 (3)
C4—C3—H3B	109.8	Zn1—O3—H3D	123 (6)
C2—C3—H3B	109.8	Zn1—O3—H3C	112 (4)
H3A—C3—H3B	108.2	H3D—O3—H3C	107.5 (17)
C3—C4—C5	112.0 (5)	O2—Zn1—O2ⁱ	180.0
C3—C4—H4A	109.2	O2—Zn1—O3	88.54 (15)
C5—C4—H4A	109.2	O2ⁱ—Zn1—O3	91.46 (15)
C3—C4—H4B	109.2	O2—Zn1—O3ⁱ	91.46 (15)
C5—C4—H4B	109.2	O2ⁱ—Zn1—O3ⁱ	88.54 (15)
H4A—C4—H4B	107.9	O3—Zn1—O3ⁱ	180.0
C6—C5—C4	111.7 (4)		
C6—C1—C2—C3	56.4 (6)	C5—C6—C7—O1	−14.3 (6)
C1—C2—C3—C4	−56.7 (7)	C1—C6—C7—O2	−69.8 (5)
C2—C3—C4—C5	57.1 (7)	C5—C6—C7—O2	167.9 (4)
C3—C4—C5—C6	−56.2 (7)	O1—C7—O2—Zn1	−13.6 (6)
C2—C1—C6—C7	−177.8 (4)	C6—C7—O2—Zn1	164.1 (3)
C2—C1—C6—C5	−53.7 (6)	C7—O2—Zn1—O2ⁱ	115 (24)
C4—C5—C6—C7	174.6 (5)	C7—O2—Zn1—O3	−79.1 (3)
C4—C5—C6—C1	53.1 (6)	C7—O2—Zn1—O3ⁱ	100.9 (3)
C1—C6—C7—O1	107.9 (5)		

Symmetry code: (i) −x+1, −y+1, −z.

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7···O1	0.83 (1)	1.99 (3)	2.699 (4)	142 (5)

O3—H3*D*···O1ⁱⁱ	0.85 (1)	2.53 (7)	3.132 (6)	129 (8)
O3—H3*C*···O7ⁱⁱⁱ	0.85 (1)	2.17 (2)	2.997 (5)	164 (6)

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