

Diaquabis(4-methylbenzoato- κ^2 O,O')-cadmium(II)

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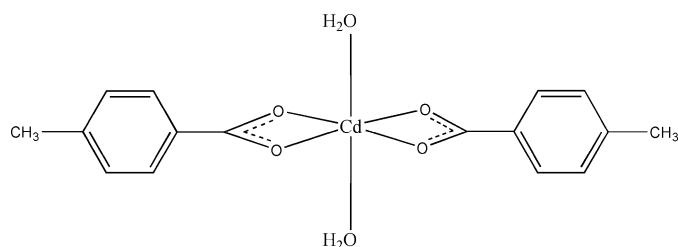
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.024; wR factor = 0.062; data-to-parameter ratio = 14.4.

In the title mononuclear complex, $[\text{Cd}(\text{C}_8\text{H}_7\text{O}_2)_2(\text{H}_2\text{O})_2]$, the Cd^{II} atom possesses crystallographically imposed C_2 site symmetry, and is coordinated by four O atoms from two 4-methylbenzoate ligands and two water molecules, displaying a distorted octahedral geometry. The molecules are assembled *via* intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen-bond interactions into a supramolecular architecture.

Related literature

For the crystal structure of 4-methylbenzoic acid, see: Song *et al.* (2007).



Experimental

Crystal data

$[\text{Cd}(\text{C}_8\text{H}_7\text{O}_2)_2(\text{H}_2\text{O})_2]$	$V = 1638.21(8) \text{ \AA}^3$
$M_r = 418.70$	$Z = 4$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 26.5836(8) \text{ \AA}$	$\mu = 1.36 \text{ mm}^{-1}$
$b = 5.3542(1) \text{ \AA}$	$T = 296(2) \text{ K}$
$c = 12.0625(3) \text{ \AA}$	$0.28 \times 0.26 \times 0.24 \text{ mm}$
$\beta = 107.414(3)^\circ$	

Data collection

Bruker APEXII diffractometer	7419 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1528 independent reflections
$T_{\text{min}} = 0.702$, $T_{\text{max}} = 0.736$	1462 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.026$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.024$	106 parameters
$wR(F^2) = 0.062$	H-atom parameters constrained
$S = 1.19$	$\Delta\rho_{\text{max}} = 0.30 \text{ e \AA}^{-3}$
1528 reflections	$\Delta\rho_{\text{min}} = -0.74 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1W}-\text{H2W}\cdots\text{O1}^{\text{i}}$	0.81	1.94	2.739 (2)	169
$\text{O1W}-\text{H1W}\cdots\text{O2}^{\text{ii}}$	0.80	1.97	2.757 (2)	170

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINTE* (Bruker, 2004); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Bruker, 2004); software used to prepare material for publication: *SHELXL97* and *XP*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2040).

References

- Bruker (2004). *APEX2*, *SAINTE* and *XP*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
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supplementary materials

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Diaquabis(4-methylbenzoato- κ^2O,O')cadmium(II)

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Comment

In the structural investigation of 4-methylbenzoate complexes, it has been found that the 4-methylbenzoic acid functions as a multidentate ligand (Song *et al.* 2007), with versatile binding and coordination modes. In this paper, we report the crystal structure of the title compound (Fig. 1), a new Cd complex obtained by the reaction of 4-methylbenzoic acid with cadmium chloride in alkaline aqueous solution.

As illustrated in Fig. 1, the Cd^{II} atom, possesses crystallographically imposed C₂ symmetry, which is coordinated by four O atoms from two 4-methylbenzoate ligands and two water molecules, and displaying a distorted octahedral geometry. Intermolecular O—H...O hydrogen bond interactions (Table 1) between the coordinated water molecules and the carboxyl O atoms of 4-methylbenzoate ligands stabilize the structural packing (Fig. 2).

Experimental

A mixture of cadmium chloride(183 mg, 1 mmol), 4-methylbenzoic acid (136 mg, 1 mmol), NaOH (60 mg, 1.5 mmol) and H₂O (12 ml) was placed in a 23 ml Teflon reactor, which was heated to 433 K for three days and then cooled to room temperature at a rate of 10 K h⁻¹. The crystals obtained were washed with water and dried in air.

Refinement

Carbon-bound H atoms were placed at calculated positions and were treated as riding on the parent C atoms with C—H = 0.93 Å, and with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$. Water H atoms were tentatively located in difference Fourier maps and were refined with distance restraints of O—H = 0.82 Å and H...H = 1.29 Å, each within a standard deviation of 0.01 Å and with $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{O})$.

Figures

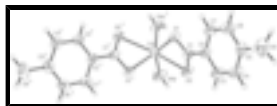


Fig. 1. The structure of the title compound, showing the atomic numbering scheme. Non-H atoms are shown with 30% probability displacement ellipsoids. [Symmetry code: (i) 2 - x, y, -z + 3/2.]

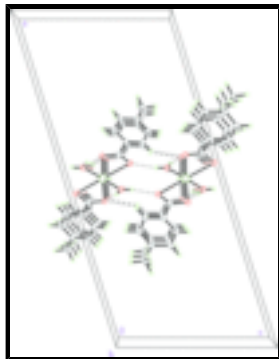


Fig. 2. A packing view of the title compound. The intermolecular hydrogen bonds are shown as dashed lines.

Diaquabis(4-methylbenzoato- κ^2O,O')cadmium(II)

Crystal data

[Cd(C₈H₇O₂)₂(H₂O)₂]

$M_r = 418.70$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 26.5836$ (8) Å

$b = 5.3542$ (1) Å

$c = 12.0625$ (3) Å

$\beta = 107.414$ (3)°

$V = 1638.21$ (8) Å³

$Z = 4$

$F_{000} = 840$

$D_x = 1.698$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 3600 reflections

$\theta = 1.4$ – 28°

$\mu = 1.36$ mm⁻¹

$T = 296$ (2) K

Block, colorless

$0.28 \times 0.26 \times 0.24$ mm

Data collection

Bruker APEXII
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 10 pixels mm⁻¹

$T = 296$ (2) K

φ and ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)

$T_{\min} = 0.702$, $T_{\max} = 0.736$

7419 measured reflections

1528 independent reflections

1462 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.026$

$\theta_{\max} = 25.5^\circ$

$\theta_{\min} = 1.6^\circ$

$h = -32 \rightarrow 32$

$k = -6 \rightarrow 6$

$l = -14 \rightarrow 14$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.024$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$wR(F^2) = 0.062$	$w = 1/[\sigma^2(F_o^2) + (0.0402P)^2 + 0.1795P]$
$S = 1.19$	where $P = (F_o^2 + 2F_c^2)/3$
1528 reflections	$(\Delta/\sigma)_{\max} < 0.001$
106 parameters	$\Delta\rho_{\max} = 0.30 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.74 \text{ e } \text{\AA}^{-3}$
	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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd	1.0000	0.07846 (3)	0.7500	0.03171 (11)
O1	0.93430 (7)	0.3608 (3)	0.71337 (13)	0.0357 (3)
O2	0.95598 (6)	0.2636 (3)	0.55703 (12)	0.0396 (4)
O1W	1.03133 (8)	-0.2139 (3)	0.66052 (13)	0.0501 (5)
H1W	1.0312	-0.2214	0.5943	0.075*
H2W	1.0438	-0.3428	0.6915	0.075*
C1	0.92908 (9)	0.3898 (4)	0.60582 (19)	0.0311 (5)
C2	0.89107 (10)	0.5837 (4)	0.5416 (2)	0.0324 (5)
C3	0.89229 (10)	0.6742 (5)	0.4358 (2)	0.0454 (6)
H3	0.9174	0.6137	0.4031	0.054*
C4	0.85694 (11)	0.8530 (6)	0.3773 (2)	0.0489 (6)
H4	0.8582	0.9083	0.3051	0.059*
C5	0.81971 (11)	0.9516 (5)	0.4240 (2)	0.0434 (6)
C6	0.81879 (12)	0.8613 (6)	0.5309 (3)	0.0565 (7)
H6	0.7938	0.9232	0.5638	0.068*
C7	0.85403 (10)	0.6813 (6)	0.5901 (2)	0.0477 (6)
H7	0.8529	0.6257	0.6623	0.057*
C8	0.78203 (12)	1.1528 (6)	0.3609 (3)	0.0601 (7)
H8A	0.7485	1.1303	0.3745	0.090*
H8B	0.7776	1.1418	0.2791	0.090*
H8C	0.7960	1.3138	0.3890	0.090*

Atomic displacement parameters (\AA^2)

U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
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supplementary materials

Cd	0.04502 (18)	0.02220 (15)	0.03014 (15)	0.000	0.01461 (11)	0.000
O1	0.0501 (10)	0.0346 (7)	0.0261 (8)	0.0036 (7)	0.0173 (7)	0.0045 (6)
O2	0.0552 (10)	0.0377 (8)	0.0283 (7)	0.0131 (7)	0.0162 (7)	0.0004 (6)
O1W	0.0907 (14)	0.0338 (9)	0.0352 (8)	0.0196 (9)	0.0329 (9)	0.0057 (7)
C1	0.0400 (12)	0.0263 (10)	0.0283 (11)	-0.0038 (9)	0.0122 (10)	-0.0043 (8)
C2	0.0378 (13)	0.0327 (13)	0.0272 (11)	0.0011 (8)	0.0103 (10)	-0.0027 (8)
C3	0.0589 (16)	0.0480 (14)	0.0371 (12)	0.0187 (12)	0.0264 (11)	0.0090 (11)
C4	0.0630 (17)	0.0490 (14)	0.0395 (13)	0.0171 (13)	0.0226 (12)	0.0120 (12)
C5	0.0429 (14)	0.0393 (13)	0.0417 (14)	0.0073 (10)	0.0029 (11)	-0.0040 (10)
C6	0.0528 (16)	0.0713 (17)	0.0522 (16)	0.0241 (14)	0.0261 (14)	0.0045 (14)
C7	0.0494 (14)	0.0644 (16)	0.0358 (12)	0.0155 (13)	0.0225 (11)	0.0068 (12)
C8	0.0557 (17)	0.0515 (15)	0.0629 (18)	0.0172 (15)	0.0021 (14)	0.0002 (15)

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

Cd—O1W	2.202 (2)	C3—H3	0.9300
Cd—O1	2.252 (2)	C4—C5	1.382 (4)
Cd—O2	2.478 (1)	C4—H4	0.9300
Cd—C1	2.719 (2)	C5—C6	1.383 (4)
O1—C1	1.272 (3)	C5—C8	1.512 (4)
O2—C1	1.251 (3)	C6—C7	1.384 (4)
O1W—H1W	0.7994	C6—H6	0.9300
O1W—H2W	0.8075	C7—H7	0.9300
C1—C2	1.493 (3)	C8—H8A	0.9600
C2—C3	1.375 (3)	C8—H8B	0.9600
C2—C7	1.389 (3)	C8—H8C	0.9600
C3—C4	1.379 (4)		
O1W—Cd—O1W ⁱ	89.36 (9)	O1—C1—Cd	55.3 (1)
O1W—Cd—O1 ⁱ	100.87 (7)	C2—C1—Cd	171.8 (2)
O1W—Cd—O1	140.02 (6)	C3—C2—C7	118.3 (2)
O1 ⁱ —Cd—O1	95.64 (9)	C3—C2—C1	121.8 (2)
O1W—Cd—O2 ⁱ	127.11 (6)	C7—C2—C1	119.9 (2)
O1—Cd—O2 ⁱ	92.08 (6)	C2—C3—C4	121.2 (2)
O1W—Cd—O2	88.02 (5)	C2—C3—H3	119.4
O1—Cd—O2	55.00 (5)	C4—C3—H3	119.4
O2 ⁱ —Cd—O2	132.83 (7)	C3—C4—C5	121.2 (2)
O1W—Cd—C1 ⁱ	117.25 (7)	C3—C4—H4	119.4
O1 ⁱ —Cd—C1 ⁱ	27.66 (6)	C5—C4—H4	119.4
O1—Cd—C1 ⁱ	93.58 (6)	C4—C5—C6	117.4 (2)
O2 ⁱ —Cd—C1 ⁱ	27.36 (6)	C4—C5—C8	120.9 (3)
O2—Cd—C1 ⁱ	113.43 (6)	C6—C5—C8	121.6 (3)
O1W—Cd—C1	114.45 (6)	C5—C6—C7	121.7 (2)
O1—Cd—C1	27.66 (6)	C5—C6—H6	119.1
O2—Cd—C1	27.36 (6)	C7—C6—H6	119.1
C1 ⁱ —Cd—C1	104.39 (9)	C6—C7—C2	120.0 (2)
C1—O1—Cd	97.09 (13)	C6—C7—H7	120.0

C1—O2—Cd	87.13 (13)	C2—C7—H7	120.0
Cd—O1W—H1W	129.6	C5—C8—H8A	109.5
Cd—O1W—H2W	123.0	C5—C8—H8B	109.5
H1W—O1W—H2W	107.3	H8A—C8—H8B	109.5
O2—C1—O1	120.7 (2)	C5—C8—H8C	109.5
O2—C1—C2	121.6 (2)	H8A—C8—H8C	109.5
O1—C1—C2	117.7 (2)	H8B—C8—H8C	109.5
O2—C1—Cd	65.5 (2)		
O1W—Cd—O1—C1	-27.42 (18)	C1 ⁱ —Cd—C1—O2	113.42 (14)
O1W ⁱ —Cd—O1—C1	-129.62 (13)	O1W—Cd—C1—O1	161.03 (13)
O1 ⁱ —Cd—O1—C1	86.96 (13)	O1W ⁱ —Cd—C1—O1	58.30 (15)
O2 ⁱ —Cd—O1—C1	141.99 (13)	O1 ⁱ —Cd—C1—O1	-95.31 (15)
O2—Cd—O1—C1	-1.63 (12)	O2 ⁱ —Cd—C1—O1	-42.12 (15)
C1 ⁱ —Cd—O1—C1	114.64 (14)	O2—Cd—C1—O1	177.1 (2)
O1W—Cd—O2—C1	165.40 (14)	C1 ⁱ —Cd—C1—O1	-69.48 (13)
O1W ⁱ —Cd—O2—C1	77.70 (14)	O2—C1—C2—C3	-15.4 (4)
O1 ⁱ —Cd—O2—C1	-93.79 (13)	O1—C1—C2—C3	162.9 (2)
O1—Cd—O2—C1	1.64 (12)	O2—C1—C2—C7	166.1 (2)
O2 ⁱ —Cd—O2—C1	-52.29 (12)	O1—C1—C2—C7	-15.6 (3)
C1 ⁱ —Cd—O2—C1	-75.63 (17)	C7—C2—C3—C4	-1.6 (4)
Cd—O2—C1—O1	-2.8 (2)	C1—C2—C3—C4	179.9 (2)
Cd—O2—C1—C2	175.45 (19)	C2—C3—C4—C5	1.4 (5)
Cd—O1—C1—O2	3.1 (2)	C3—C4—C5—C6	-0.9 (5)
Cd—O1—C1—C2	-175.22 (17)	C3—C4—C5—C8	178.3 (3)
O1W—Cd—C1—O2	-16.06 (15)	C4—C5—C6—C7	0.8 (5)
O1W ⁱ —Cd—C1—O2	-118.79 (13)	C8—C5—C6—C7	-178.5 (3)
O1 ⁱ —Cd—C1—O2	87.59 (13)	C5—C6—C7—C2	-1.0 (5)
O1—Cd—C1—O2	-177.1 (2)	C3—C2—C7—C6	1.4 (4)
O2 ⁱ —Cd—C1—O2	140.78 (11)	C1—C2—C7—C6	179.9 (3)

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

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

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1W—H2W \cdots O1 ⁱⁱ	0.81	1.94	2.739 (2)	169
O1W—H1W \cdots O2 ⁱⁱⁱ	0.80	1.97	2.757 (2)	170

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

Fig. 1

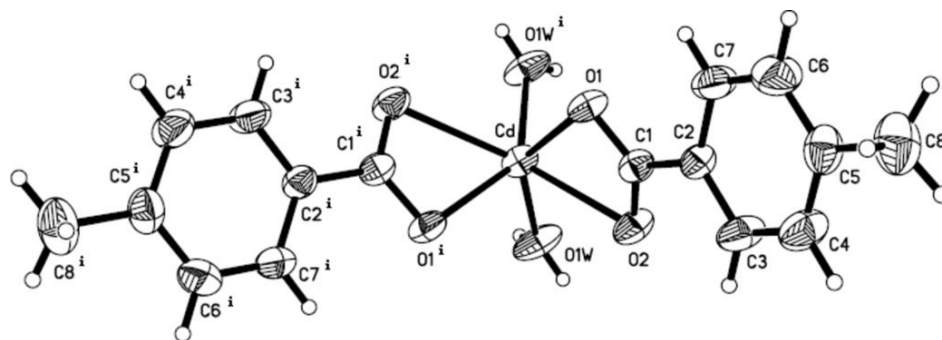


Fig. 2

