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Poly[*diaqua*(μ_3 -succinato)cadmium(II)]

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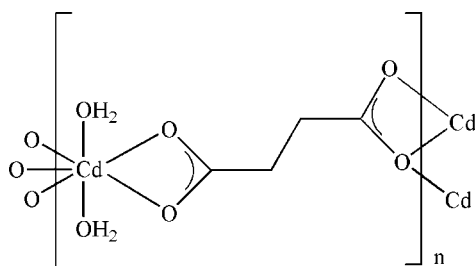
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.023; wR factor = 0.053; data-to-parameter ratio = 12.1.

The title compound, $[\text{Cd}(\text{C}_4\text{H}_4\text{O}_4)(\text{H}_2\text{O})_2]_n$, has been synthesized under hydrothermal conditions. The asymmetric unit consists of one Cd^{2+} cation, one succinate anion and two aqua ligands. The Cd atoms present a distorted pentagonal bipyramidal coordination and are bridged into layers parallel to (01) by succinate ligands.

Related literature

For different bridging modes in succinato complexes, see: Ng (1998); Rastsvetaeva *et al.* (1996); Brusau *et al.* (2000); He *et al.* (2006); He *et al.* (2007). For geometrical comparisons with related compounds, see Huo *et al.* (2005); Zhuo *et al.* (2006).



Experimental

Crystal data

$[\text{Cd}(\text{C}_4\text{H}_4\text{O}_4)(\text{H}_2\text{O})_2]$
 $M_r = 264.51$
Monoclinic, $P2_1/c$

$a = 7.7130$ (15) Å
 $b = 12.231$ (2) Å
 $c = 8.0560$ (16) Å

$\beta = 94.71$ (3) $^\circ$
 $V = 757.4$ (2) Å³
 $Z = 4$
Mo $K\alpha$ radiation

$\mu = 2.87$ mm⁻¹
 $T = 293$ K
 $0.40 \times 0.30 \times 0.21$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (SADABS; Bruker, 1998)
 $T_{\min} = 0.35$, $T_{\max} = 0.55$

6371 measured reflections
1409 independent reflections
1335 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.028$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.023$
 $wR(F^2) = 0.053$
 $S = 1.05$
1409 reflections
116 parameters
6 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.40$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.68$ e Å⁻³

Table 1

Selected bond lengths (Å).

Cd1—O4 ⁱ	2.255 (2)	Cd1—O5	2.329 (3)
Cd1—O2	2.284 (2)	Cd1—O1	2.389 (2)
Cd1—O6	2.302 (3)	Cd1—O3 ⁱ	2.690 (2)
Cd1—O4 ⁱⁱ	2.316 (2)		

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

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; 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: BG2243).

References

- Bruker (1998). SMART, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
Brusau, E. V., Pedregosa, J. C. G., Narda, E., Echeverria, G. & Punte, G. (2000). *J. Solid State Chem.* **153**, 1–8.
He, Y.-K., Wang, X.-F., Zhang, L.-T., Han, Z.-B. & Ng, S. W. (2007). *Acta Cryst.* **E63**, m3019.
He, Q., Zi, J.-F. & Zhang, F.-J. (2006). *Acta Cryst.* **E62**, m1266–m1267.
Huo, L.-H., Gao, S. & Ng, S. W. (2005). *Acta Cryst.* **E61**, m2357–m2358.
Ng, S. W. (1998). *Acta Cryst.* **C54**, 745–750.
Rastsvetaeva, R. K., Pushcharovsky, D. Yu., Furmanova, N. G. & Sharp, H. (1996). *Z. Kristallogr.* **211**, 808–810.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Zhuo, X., Pan, Z.-R., Wang, Z.-W., Li, Y.-Z. & Zheng, H.-G. (2006). *Chin. J. Inorg. Chem.* **22**, 1847–1851.

supplementary materials

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Comment

The succinate dianion has been used as a bridging ligand in the preparation of multinuclear metal complexes. A variety of bridging modes have been found (Ng, 1998; Rastsvetaeva *et al.*, 1996; Brusau *et al.*, 2000; He *et al.*, 2006; He *et al.*, 2007). We report herein the synthesis and crystal structure of a new succinate complex [Cd(C₄H₄O₄)(H₂O)₂] (I).

The asymmetric unit consists of one Cd²⁺ cation, one succinate anion and two aqua ligands (Fig. 1). The Cd atom is coordinated by seven O atoms of three succinate anions and two aqua ligand, forming a distorted pentagonal bipyramidal coordination geometry (Table 1), with Cd—O bond lengths which agree well with those observed in analogous complexes (Huo *et al.*, 2005; Zhuo *et al.*, 2006). Cd atoms are bridged by succinate ligands into a two-dimensional layer (Fig. 2).

Experimental

Cd(NO₃)₂·4H₂O (0.5 mmol, 0.154 g), succinic acid (0.5 mmol, 0.059 g), sodium hydroxide (1 mmol, 0.04 g) and water (12 ml) were placed in a 23-ml Teflon-lined Parr bomb. The bomb was heated at 453 K for 3 d. The colourless block-shaped crystals were filtered off and washed with water and acetone (yield 45%, based on Cd).

Refinement

Water H atoms were located in a difference Fourier map and refined with restrained O—H (0.85 (1) Å) and free $U_{\text{iso}}(\text{H})$. H atoms on C atom were positioned geometrically and refined using a riding model, with C—H = 0.97 Å.

Figures

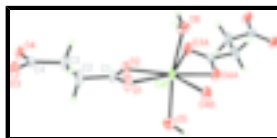


Fig. 1. A view of the molecular structure of (I) with the atom-numbering scheme and 30% displacement ellipsoids. Atoms with the suffix A and B are generated by the symmetry operations $x + 1, -y + 3/2, z + 1/2$ and $-x + 2, -y + 1, -z + 2$, respectively.

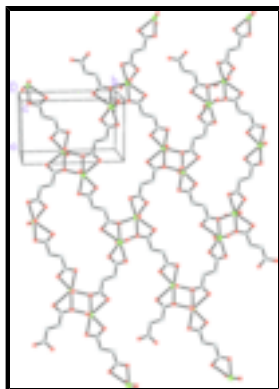


Fig. 2. The 2-D layer structure of compound (I) (H atoms of methylenes are omitted for clarity).

Poly[*diaqua*(μ_3 -succinato)cadmium(II)]

Crystal data

[Cd(C₄H₄O₄)(H₂O)₂]

$M_r = 264.51$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 7.7130$ (15) Å

$b = 12.231$ (2) Å

$c = 8.0560$ (16) Å

$\beta = 94.71$ (3)°

$V = 757.4$ (2) Å³

$Z = 4$

$F_{000} = 512.0$

$D_x = 2.32$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 2567 reflections

$\theta = 2.6$ – 25.5 °

$\mu = 2.87$ mm⁻¹

$T = 293$ K

Block, colorless

$0.40 \times 0.30 \times 0.21$ mm

Data collection

Bruker SMART CD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293$ K

φ and ω scans

Absorption correction: multi-scan (SADABS; Bruker, 1998)

$T_{\min} = 0.35$, $T_{\max} = 0.55$

6371 measured reflections

1409 independent reflections

1335 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.028$

$\theta_{\max} = 25.5$ °

$\theta_{\min} = 3.0$ °

$h = -9 \rightarrow 9$

$k = -14 \rightarrow 14$

$l = -9 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.023$

$wR(F^2) = 0.053$

Secondary atom site location: difference Fourier map

Hydrogen site location: constr

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0207P)^2 + 1.5P]$

$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
1409 reflections	$(\Delta/\sigma)_{\max} < 0.001$
116 parameters	$\Delta\rho_{\max} = 0.40 \text{ e } \text{\AA}^{-3}$
6 restraints	$\Delta\rho_{\min} = -0.68 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.17614 (3)	0.587427 (19)	0.08353 (3)	0.02570 (10)
C1	0.4820 (4)	0.6353 (3)	0.2526 (4)	0.0274 (7)
C2	0.6501 (5)	0.6626 (3)	0.3501 (6)	0.0454 (10)
H2A	0.6471	0.6327	0.4613	0.055*
H2B	0.7436	0.6262	0.2983	0.055*
C3	0.6922 (4)	0.7799 (3)	0.3648 (5)	0.0349 (9)
H3A	0.6046	0.8150	0.4262	0.042*
H3B	0.6840	0.8113	0.2538	0.042*
C4	0.8675 (4)	0.8072 (3)	0.4482 (4)	0.0252 (7)
O1	0.4603 (3)	0.5387 (2)	0.2005 (3)	0.0367 (6)
O2	0.3664 (3)	0.70570 (19)	0.2216 (3)	0.0352 (6)
O3	0.9815 (3)	0.7385 (2)	0.4838 (3)	0.0399 (6)
O4	0.8946 (3)	0.90780 (18)	0.4832 (3)	0.0307 (6)
O5	0.0710 (4)	0.5424 (2)	0.3376 (3)	0.0402 (6)
H5A	-0.012 (5)	0.499 (3)	0.325 (6)	0.072 (18)*
H5B	0.047 (5)	0.598 (2)	0.392 (5)	0.056 (15)*
O6	0.2576 (3)	0.5909 (2)	-0.1850 (3)	0.0332 (6)
H6A	0.348 (4)	0.553 (3)	-0.197 (5)	0.044 (12)*
H6B	0.278 (5)	0.6562 (17)	-0.213 (5)	0.051 (13)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.01635 (14)	0.02632 (15)	0.03318 (16)	-0.00248 (9)	-0.00550 (10)	-0.00305 (10)
C1	0.0181 (16)	0.0294 (18)	0.0342 (18)	-0.0041 (14)	-0.0016 (14)	-0.0046 (15)

supplementary materials

C2	0.032 (2)	0.034 (2)	0.065 (3)	-0.0035 (17)	-0.0250 (19)	0.0000 (19)
C3	0.0231 (18)	0.0299 (19)	0.049 (2)	-0.0034 (15)	-0.0132 (16)	-0.0034 (16)
C4	0.0213 (16)	0.0263 (18)	0.0278 (18)	-0.0025 (14)	-0.0003 (13)	-0.0029 (14)
O1	0.0220 (12)	0.0292 (14)	0.0572 (17)	0.0006 (10)	-0.0056 (11)	-0.0134 (12)
O2	0.0245 (13)	0.0274 (13)	0.0512 (16)	0.0008 (10)	-0.0117 (11)	-0.0102 (11)
O3	0.0264 (13)	0.0286 (13)	0.0619 (18)	0.0039 (11)	-0.0132 (12)	-0.0085 (12)
O4	0.0229 (12)	0.0228 (12)	0.0448 (15)	-0.0029 (9)	-0.0078 (11)	-0.0017 (10)
O5	0.0414 (16)	0.0419 (17)	0.0377 (16)	0.0015 (14)	0.0054 (12)	-0.0026 (13)
O6	0.0306 (14)	0.0266 (14)	0.0432 (15)	0.0036 (11)	0.0070 (11)	0.0052 (11)

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

Cd1—O4 ⁱ	2.255 (2)	C2—H2A	0.9700
Cd1—O2	2.284 (2)	C2—H2B	0.9700
Cd1—O6	2.302 (3)	C3—C4	1.498 (4)
Cd1—O4 ⁱⁱ	2.316 (2)	C3—H3A	0.9700
Cd1—O5	2.329 (3)	C3—H3B	0.9700
Cd1—O1	2.389 (2)	C4—O3	1.233 (4)
Cd1—O3 ⁱ	2.690 (2)	C4—O4	1.275 (4)
C1—O2	1.250 (4)	O5—H5B	0.84 (3)
C1—O1	1.260 (4)	O5—H5A	0.84 (3)
C1—C2	1.498 (5)	O6—H6A	0.85 (3)
C2—C3	1.474 (5)	O6—H6B	0.85 (3)
O4 ⁱ —Cd1—O2	136.02 (8)	C1—C2—H2B	108.3
O4 ⁱ —Cd1—O6	89.54 (10)	H2A—C2—H2B	107.4
O2—Cd1—O6	103.41 (10)	C2—C3—C4	116.0 (3)
O4 ⁱ —Cd1—O4 ⁱⁱ	74.92 (9)	C2—C3—H3A	108.3
O2—Cd1—O4 ⁱⁱ	147.52 (8)	C4—C3—H3A	108.3
O6—Cd1—O4 ⁱⁱ	82.91 (9)	C2—C3—H3B	108.3
O4 ⁱ —Cd1—O5	85.77 (10)	C4—C3—H3B	108.3
O2—Cd1—O5	88.74 (10)	H3A—C3—H3B	107.4
O6—Cd1—O5	166.39 (10)	O3—C4—O4	120.4 (3)
O4 ⁱⁱ —Cd1—O5	83.54 (10)	O3—C4—C3	123.5 (3)
O4 ⁱ —Cd1—O1	166.71 (8)	O4—C4—C3	116.1 (3)
O2—Cd1—O1	55.52 (8)	C1—O1—Cd1	89.42 (19)
O6—Cd1—O1	93.60 (10)	C1—O2—Cd1	94.6 (2)
O4 ⁱⁱ —Cd1—O1	92.64 (8)	C4—O4—Cd1 ⁱⁱⁱ	103.8 (2)
O5—Cd1—O1	88.23 (10)	C4—O4—Cd1 ^{iv}	146.3 (2)
O2—C1—O1	120.4 (3)	Cd1 ⁱⁱⁱ —O4—Cd1 ^{iv}	105.08 (9)
O2—C1—C2	121.6 (3)	Cd1—O5—H5B	112 (3)
O1—C1—C2	118.0 (3)	Cd1—O5—H5A	111 (3)
C3—C2—C1	115.8 (3)	H5B—O5—H5A	112 (3)
C3—C2—H2A	108.3	Cd1—O6—H6A	113 (3)
C1—C2—H2A	108.3	Cd1—O6—H6B	110 (3)
C3—C2—H2B	108.3	H6A—O6—H6B	108 (3)
O2—C1—C2—C3	-16.9 (6)	O1—C1—O2—Cd1	2.1 (4)

O1—C1—C2—C3	162.3 (4)	C2—C1—O2—Cd1	-178.7 (3)
C1—C2—C3—C4	-174.5 (3)	O4 ⁱ —Cd1—O2—C1	170.1 (2)
C2—C3—C4—O3	9.5 (6)	O6—Cd1—O2—C1	-86.3 (2)
C2—C3—C4—O4	-170.0 (4)	O4 ⁱⁱ —Cd1—O2—C1	11.7 (3)
O2—C1—O1—Cd1	-2.0 (3)	O5—Cd1—O2—C1	87.5 (2)
C2—C1—O1—Cd1	178.7 (3)	O1—Cd1—O2—C1	-1.2 (2)
O4 ⁱ —Cd1—O1—C1	-151.7 (4)	O3—C4—O4—Cd1 ⁱⁱⁱ	5.3 (4)
O2—Cd1—O1—C1	1.2 (2)	C3—C4—O4—Cd1 ⁱⁱⁱ	-175.2 (3)
O6—Cd1—O1—C1	105.0 (2)	O3—C4—O4—Cd1 ^{iv}	153.9 (3)
O4 ⁱⁱ —Cd1—O1—C1	-172.0 (2)	C3—C4—O4—Cd1 ^{iv}	-26.5 (6)
O5—Cd1—O1—C1	-88.5 (2)		

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

Fig. 1

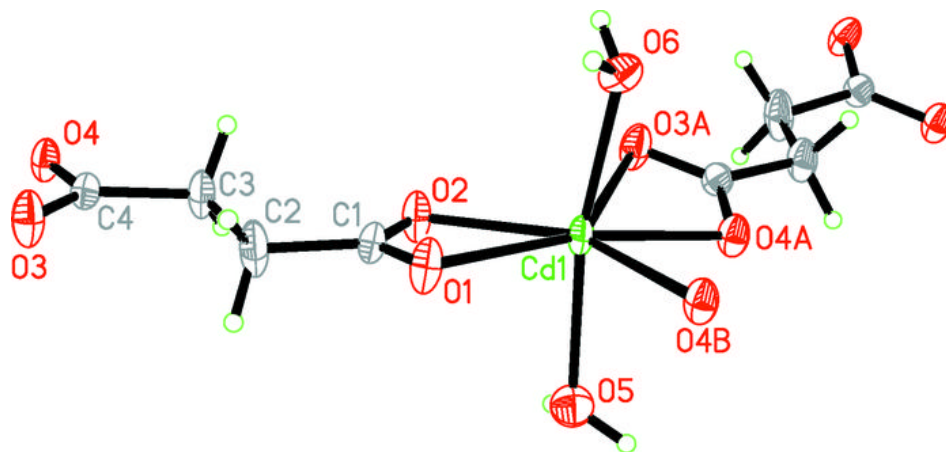


Fig. 2

