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Key indicators

Single-crystal X-ray study
T = 293 K
Mean $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$
R factor = 0.024
wR factor = 0.052
Data-to-parameter ratio = 16.5

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

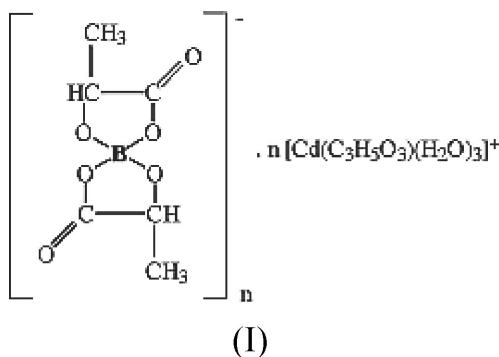
Poly[[triacquacadmium(II)- μ_3 -lactato] dilactato-boron(1-)]

In the title compound, $\{[\text{Cd}(\text{C}_3\text{H}_5\text{O}_3)(\text{H}_2\text{O})_3](\text{C}_6\text{H}_8\text{BO}_6)\}_n$, the Cd atom is seven-coordinate. The Cd—O distances range from 2.290 (3) to 2.518 (2) Å. The structure is stabilized by a network of O—H...O and C—H...O hydrogen bonds involving the H atoms of the lactate in the cation and the O atoms of the borodilactate anion.

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Comment

Non-linear optical (NLO) materials play a vital role in advancing laser technology and opto-electronic applications, such as optical computing, optical data storage and optical communication. It has been reported that semi-organic NLO materials combine the large non-linearity of organics and the favourable crystal growth properties of inorganic salts (Jiang & Fang, 1999; Jiang *et al.*, 2001). The crystal structures of ammonium and lithium borodilactates, which are NLO materials, have been reported by Angeli Mary *et al.* (2002) and Dhanuskodi *et al.* (2002), respectively. We have prepared the title compound, (I), which crystallizes in the orthorhombic space group $P2_12_12_1$ with $Z = 4$.



In (I), the Cd atom is chelated by two lactates, one of which chelates through the carboxylate and hydroxyl groups, while the other chelates through only the carboxylate group. The other three coordination sites are occupied by water molecules. As shown in Fig. 2, the lactate monoanion links three water-coordinated Cd ions into a three-dimensional network structure. The B atom forms two covalent bonds with O3 and O6 and extended B—O bonds to O2 and O5 (Table 1). The O—B—O bond angles around boron indicate a distorted tetrahedral environment. Similar bond lengths and deviations from the tetrahedral values of bond angles around boron have been reported in the literature (Angeli Mary *et al.*, 2002). The dihedral angle between the planes of the two lactate groups of the borodilactate anion is 84.8 (2)°. This value is comparable with that of 88.3 (10)° in ammonium borodilactate (Angeli Mary *et al.*, 2002). The structure is stabilized by a network of

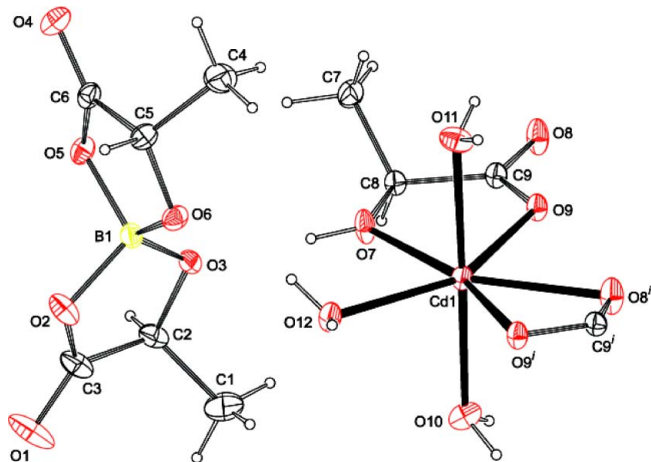


Figure 1

A view of the asymmetric unit of (I), with an extra carboxylate group to complete the Cd coordination, showing the atom-numbering scheme and 10% probability displacement ellipsoids. The symmetry code is as in Table 1.

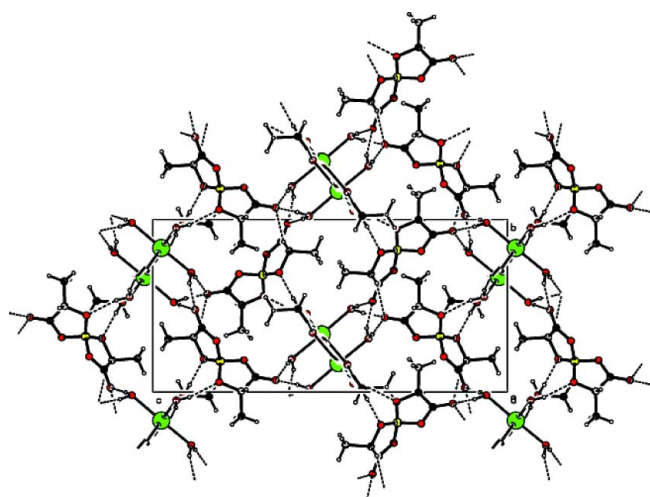


Figure 2

A view, along the *a* axis, of the packing of (I), with the hydrogen bonds shown as dashed lines.

O—H...O and C—H...O hydrogen bonds. Details of the hydrogen-bond contacts are given in Table 2.

Experimental

Boric acid (0.005 mol) and L-lactic acid (0.01 mol) were dissolved in doubly distilled water. Cadmium carbonate (0.0025 mol) was then added. The solution was stirred well using a magnetic stirrer. The mixture was evaporated to dryness at room temperature by continued heating at 333 K to avoid possible decomposition [m.p. 421 (1) K]. FT-IR (KBr, cm^{-1}): $\nu = 440$ (C=O out of plane bending), 630 (C=O in plane bending), 918 (BO_4 asymmetric stretching), 958 (B—O stretching), 1117 (C—H in plane bending), 1283 (C—C stretching), 1729 (C=O stretching), 3108 (C—H stretching). To grow single crystals of (I), the synthesized salt was dissolved in doubly distilled water and the solution was saturated at room temperature, filtered and allowed to evaporate slowly. Single crystals were obtained after one month.

Crystal data

$[\text{Cd}(\text{C}_3\text{H}_5\text{O}_3)(\text{H}_2\text{O})_3](\text{C}_6\text{H}_8\text{BO}_6)$
 $M_r = 442.46$
 Orthorhombic, $P2_12_12_1$
 $a = 8.424$ (5) Å
 $b = 10.184$ (5) Å
 $c = 20.943$ (5) Å
 $V = 1796.7$ (14) Å³
 $Z = 4$
 $D_x = 1.636$ Mg m⁻³

Mo $K\alpha$ radiation
 Cell parameters from 21 782 reflections
 $\theta = 1.9\text{--}27.1^\circ$
 $\mu = 1.27$ mm⁻¹
 $T = 293$ K
 Block, colourless
 $0.44 \times 0.39 \times 0.29$ mm

Data collection

Stoe IPDS-II diffractometer
 ω scans
 Absorption correction: by integration (*X-RED32*; Stoe & Cie, 2002)
 $T_{\text{min}} = 0.605$, $T_{\text{max}} = 0.710$
 23 149 measured reflections

3908 independent reflections
 3314 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.048$
 $\theta_{\text{max}} = 27.2^\circ$
 $h = -10 \rightarrow 10$
 $k = -13 \rightarrow 13$
 $l = -26 \rightarrow 26$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.024$
 $wR(F^2) = 0.052$
 $S = 0.93$
 3908 reflections
 237 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0308P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.42$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.33$ e Å⁻³
 Extinction correction: *SHELXL97*
 Extinction coefficient: 0.0266 (7)
 Absolute structure: Flack (1983), with 1622 Friedel pairs
 Flack parameter = -0.01 (2)

Table 1

Selected geometric parameters (Å, °).

Cd1—O7	2.334 (3)	Cd1—O9 ⁱ	2.518 (2)
Cd1—O9	2.311 (2)	O2—B1	1.498 (5)
Cd1—O10	2.297 (3)	O3—B1	1.436 (4)
Cd1—O11	2.290 (3)	O5—B1	1.499 (4)
Cd1—O12	2.256 (3)	O6—B1	1.426 (5)
Cd1—O8 ⁱ	2.351 (3)		
O7—Cd1—O9	67.64 (8)	O9 ⁱ —Cd1—O10	94.23 (10)
O7—Cd1—O10	89.73 (11)	O11—Cd1—O12	91.32 (12)
O7—Cd1—O11	89.22 (11)	O8 ⁱ —Cd1—O11	90.91 (10)
O7—Cd1—O12	80.33 (10)	O9 ⁱ —Cd1—O11	86.54 (11)
O7—Cd1—O8 ⁱ	146.64 (9)	O8 ⁱ —Cd1—O12	133.01 (9)
O7—Cd1—O9 ⁱ	160.35 (8)	O9 ⁱ —Cd1—O12	80.60 (8)
O9—Cd1—O10	94.21 (12)	O8 ⁱ —Cd1—O9 ⁱ	52.72 (8)
O9—Cd1—O11	86.03 (12)	O2—B1—O6	113.3 (3)
O9—Cd1—O12	147.87 (9)	O3—B1—O6	114.8 (3)
O8 ⁱ —Cd1—O9	79.09 (8)	O5—B1—O6	104.3 (3)
O9—Cd1—O9 ⁱ	131.03 (7)	O3—B1—O5	111.9 (3)
O10—Cd1—O11	178.75 (11)	O2—B1—O3	104.4 (3)
O10—Cd1—O12	87.83 (12)	O2—B1—O5	108.2 (3)
O8 ⁱ —Cd1—O10	90.35 (10)		

Symmetry code: (i) $x - \frac{1}{2}, \frac{3}{2} - y, 1 - z$.

Table 2

Hydrogen-bonding geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O7—H7...O3	0.84 (4)	1.85 (4)	2.665 (4)	167 (4)
O10—H101...O4 ⁱⁱⁱ	0.83 (4)	1.99 (6)	2.770 (5)	157 (7)
O10—H102...O1 ⁱⁱⁱ	0.81 (4)	2.00 (4)	2.808 (6)	177 (4)
O11—H111...O1 ^{iv}	0.83 (4)	1.98 (4)	2.780 (5)	162 (4)
O11—H112...O4 ^v	0.75 (4)	2.13 (4)	2.873 (5)	171 (5)
O12—H121...O6	0.81 (6)	1.98 (6)	2.768 (4)	164 (5)
O12—H122...O8 ^{vi}	0.87 (5)	1.82 (5)	2.677 (4)	169 (4)
C2—H2...O4 ^{vii}	0.98	2.59	3.536 (5)	162

Symmetry codes: (ii) $\frac{1}{2} - x, 2 - y, \frac{1}{2} + z$; (iii) $\frac{1}{2} + x, \frac{3}{2} - y, 1 - z$; (iv) $x, 1 + y, z$; (v) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$; (vi) $x - 1, y, z$; (vii) $1 - x, y - \frac{1}{2}, \frac{1}{2} - z$.

The H atom of the OH group of the lactate in the Cd complex and the H atoms of the water molecules were found in difference Fourier maps and refined isotropically. The other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms. The $U_{\text{iso}}(\text{H})$ values were constrained to be 1.2 (1.5 for methyl group) times U_{eq} of the carrier atoms.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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