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Poly[[bis(1*H*-benzimidazole-κN^3)-cadmium(II)]-μ-aqua-μ-succinato-$\kappa^2 O^1$:O^4]

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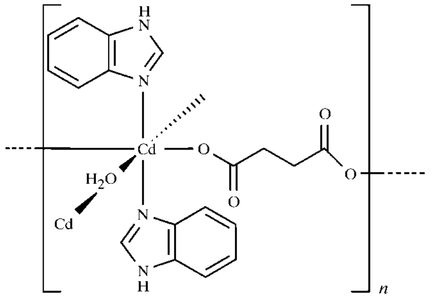
The title compound, $[\mathrm{Cd}(\mathrm{C_4H_4O_4})(\mathrm{C_7H_6N_2})_2(\mathrm{H_2O})]_n$, is a three-dimensional polymeric complex. The $\mathrm{Cd^{II}}$ atom is located on an inversion centre and assumes an elongated octahedral coordination geometry, with a long Cd—O distance of 2.5381 (5) Å to the coordinated bridging water molecule. The succinate dianion, located on another inversion centre, bridges adjacent Cd atoms to form succinate-bridged polymeric chains. The coordinated water molecule is located on a twofold axis and links adjacent succinate-bridged chains to form a water-bridged polymeric chain.

Comment

In carboxylate-bridged metal complexes, a variety of bridging modes, such as μ_2, μ_3 and μ_4, have been found (Ng, 1998; Rastsvetaeva *et al.*, 1996; Ng & Kumar Das, 1993). Some recent structure determinations have shown that the coordination mode of the carboxylate anion is related to hydrogen bonding between the carboxylate and imidazole ligands (Liu *et al.*, 2003). In order to study the effect of this hydrogen bonding between carboxylate and neighbouring ligands on the coordination mode of the carboxylate, a series of metal complexes with both dicarboxylate and benzimidazole ligands has been prepared in our laboratory. The title compound, (I), is one of these and its crystal stucture is presented here.

The structure of (I) is shown in Fig. 1. This $\mathrm{Cd^{II}}$ complex is polymeric, with the repeat unit containing a $\mathrm{Cd^{II}}$ atom, a water molecule, a succinate dianion and two benzimidazole molecules. The Cd atom is located on an inversion centre. The coordination geometry is an elongated octahedron formed by succinate dianions, benzimidazole ligands and water molecules, with a normal Cd—O1 bond length of 2.2421 (13) Å and a longer Cd—O3 bond distance (discussed below).

The succinate dianion is located on an inversion centre. The planar carbon skeleton is approximately perpendicular to the carboxyl group, the two planes forming a dihedral angle of 78.56 (17)°. Each succinate dianion bridges two adjacent Cd atoms *via* both terminal carboxyl groups, forming the succinate-bridged polymeric chain shown in Fig. 1. The carboxyl group coordinates to the Cd atom in a monodentate fashion and the uncoordinated carboxyl atom O2 is hydrogen bonded to the neighbouring coordinated water molecule (Fig. 1) and benzimidazole ligand (Fig. 2 and Table 2).



(I)

The coordinated water atom O3 is located on a twofold axis and links adjacent succinate-bridged chains to form water-bridged polymeric chains along the [001] direction (Fig. 2). The two succinate-bridged chains linked by the water molecule extend along the [$\overline{1}$10] and [110] directions, separated by 4.8912 (10) Å, which is half the *c* length. Thus, these polymeric chains are nearly perpendicular to each other and form the three-dimensional polymeric structure (Fig. 3). O—H···O and N—H···O hydrogen bonds (Table 2) stabilize the three-dimensional polymeric structure of (I).

The Cd—O3 bond distance of 2.5381 (5) Å is significantly longer than the Cd—O(water) bonds found in analogous reported structures, for example, 2.373 (3) Å in poly[μ-nicotinato-μ-bromo-monoaquacadmium] (Zhang *et al.*, 1996) and 2.364–2.279 Å in diaquasuccinatocadmium(II) hemihydrate (Griffith *et al.*, 1982). However, it is comparable to the Cd—O(μ_2-$\mathrm{H_2O}$) bond distances found in some μ_2-aqua-cadmium(II) complexes, for example, 2.537 Å in *catena*[bis(μ_2-aqua)hexakis(μ_2-cyano)aquadicadmium(II)dicopper(I)] (Nishikiori, 1996) and 2.619 Å in di-μ-aqua-bis[1,1,1-triaqua-μ-(*o*-phenylenediamine-*N*,*N*,*N*′,*N*′-tetraacetato)dicadmium(II)] octahydrate (Nakasuka *et al.*, 1986). The Cd—O3—$\mathrm{Cd^{ii}}$ bond angle in (I) is 148.96 (8)°, which is much larger than the values of 113.8 and 104.8°, respectively, in the μ_2-aqua-cadmium(II) complexes cited above [symmetry code: (ii) $1 - x, y, \frac{1}{2} - z$]. However, the Cd—O($\mu_2$-$\mathrm{H_2O}$) bond distances are essentially the same in these complexes. This fact may suggest an electrostatic bonding interaction between the Cd atom and the bridging water molecule.

The benzimidazole ligand displays normal geometry in (I). A π–π stacking interaction is usually found in the structures of metal complexes with benzimidazole ligands, but no π–π stacking between the benzimidazole rings was observed in the present three-dimensional polymeric structure.

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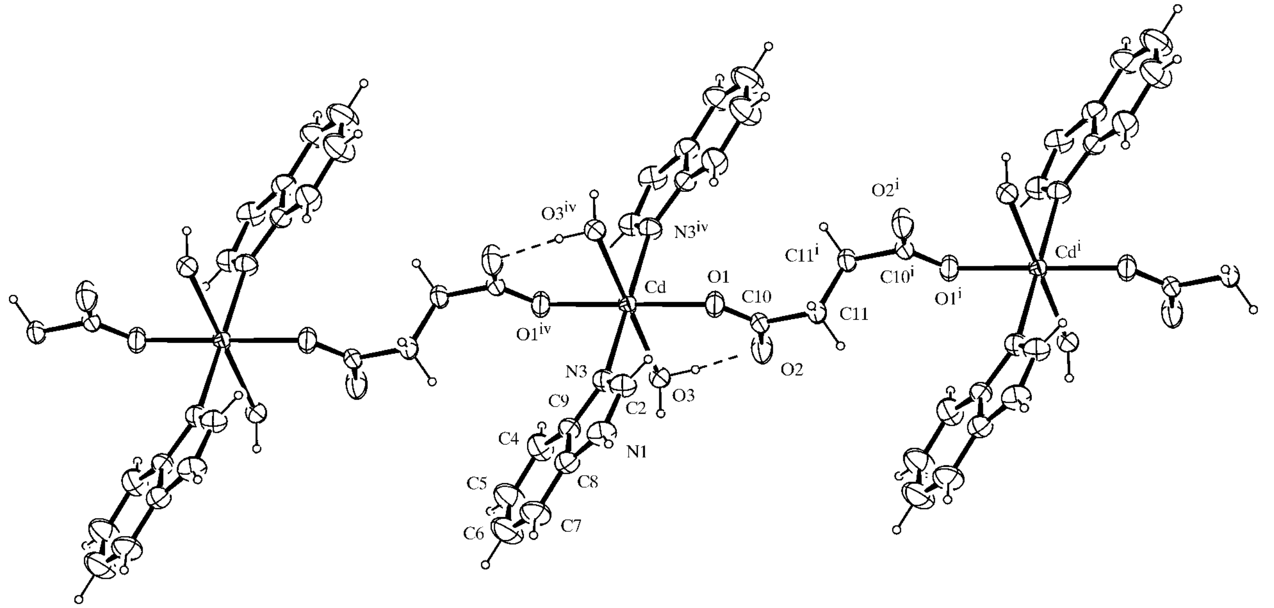

Figure 1

The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level [symmetry codes: (i) $\frac{1}{2} - x, \frac{1}{2} - y, 1 - z$; (iv) $1 - x, -y, 1 - z$].

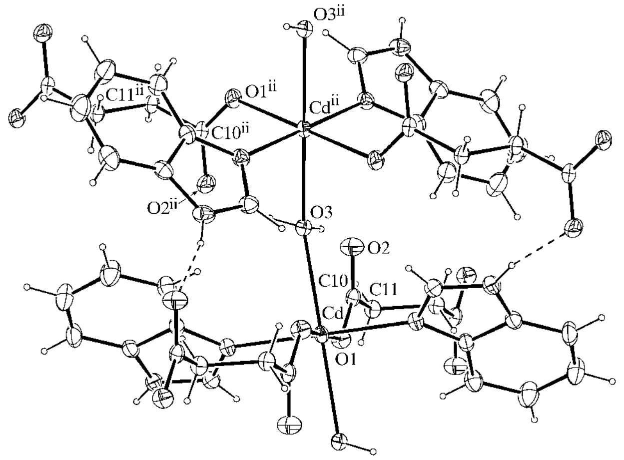

Figure 2

Illustration of the coordinated water atom O3 linking neighbouring succinate-bridged chains of complex (I) [symmetry code: (ii) $1 - x, y, \frac{1}{2} - z$].

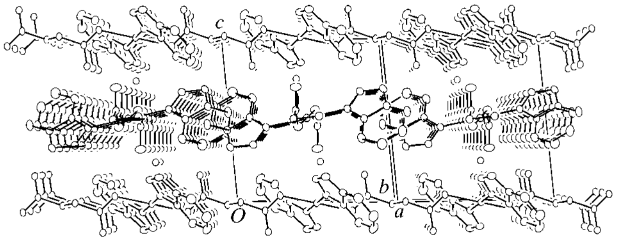

Figure 3

The molecular packing in (I), showing the succinate-bridged chains extending along different directions. Bonds involving the coordinated water atom (O3) have been omitted for clarity.

Experimental

$CdCl_2 \cdot 2H_2O$ (0.11 g, 0.5 mmol) was added to an aqueous solution (20 ml) of succinic acid (0.06 g, 0.5 mmol) and NaOH (0.04 g, 1 mmol). After refluxing the mixture for 1 h, an aqueous solution (10 ml) of benzimidazole (0.12 g, 1 mmol) was added. The solution was refluxed for a further 3 h and then filtered. After cooling to room temperature, the solution was filtered once more. Single crystals of (I) were obtained from the filtrate after 40 d.

Crystal data

$[Cd(C_4H_4O_4)(C_7H_6N_2)_2(H_2O)]$
$M_r = 482.76$
Monoclinic, $C2/c$
$a = 13.1406\ (11)$ Å
$b = 14.0664\ (12)$ Å
$c = 9.7823\ (10)$ Å
$\beta = 97.415\ (19)°$
$V = 1793.0\ (3)$ Å^3
$Z = 4$
$D_x = 1.788$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6608 reflections
$\theta = 2.8$–$26.0°$
$\mu = 1.26$ mm^{-1}
$T = 295\ (2)$ K
Prism, colourless
$0.32 \times 0.24 \times 0.16$ mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.660$, $T_{max} = 0.818$
8568 measured reflections
2061 independent reflections
1922 reflections with $I > 2\sigma(I)$
$R_{int} = 0.015$
$\theta_{max} = 27.5°$
$h = -17 \rightarrow 17$
$k = -18 \rightarrow 18$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.072$
$S = 1.34$
2061 reflections
130 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 0.6321P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.64$ e Å^{-3}
$\Delta\rho_{min} = -0.56$ e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997)
Extinction coefficient: 0.0097 (6)

Table 1
Selected geometric parameters (Å, °).

Cd—O1	2.2421 (13)	C10—C11	1.518 (2)
Cd—N3	2.2936 (15)	C11—C11^{i}	1.532 (3)
Cd—O3	2.5381 (5)		
O1—Cd—N3	86.69 (5)	C10—O1—Cd	123.99 (12)
O1—Cd—O3	91.96 (5)	Cd^{ii}—O3—Cd	148.96 (8)
N3—Cd—O3	87.78 (5)		

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

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$\cdots$O2^{iii}	0.86	1.96	2.799 (2)	166
O3—H3$\cdots$O2	0.88	1.82	2.688 (2)	168

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

Methylene and water H atoms were located in difference Fourier maps and included in the structure-factor calculations in fixed positions, with $U_{\rm iso}$(H) = 0.05 Å^2. The H atoms of the benzimidazole ligands were placed in calculated positions, with C—H = 0.93 Å and N—H = 0.86 Å, and included in the final cycles of refinement using a riding model, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$ of the carrier atom.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: OB1153). Services for accessing these data are described at the back of the journal.

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