

Yang Qu,^{a,b} Zhao-Di Liu,^a
Min-Yu Tan^{a*} and Hai-Liang
Zhu^b

^aDepartment of Chemistry, Lanzhou University, Lanzhou 730000, People's Republic of China, and ^bDepartment of Chemistry, Fuyang Normal College, Fuyang Anhui 236041, People's Republic of China

Correspondence e-mail: minyu-tan@163.com

Key indicators

Single-crystal X-ray study
T = 298 K
Mean $\sigma(\text{C}-\text{C}) = 0.007 \text{ \AA}$
Disorder in main residue
R factor = 0.044
wR factor = 0.116
Data-to-parameter ratio = 14.3

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

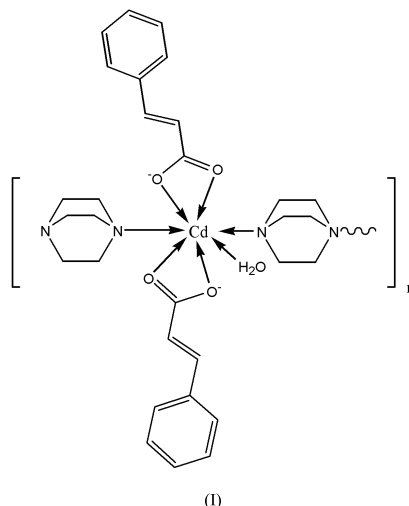
catena-Poly[[aquadicinnamatocadmium]- μ -1,4-diazabicyclo[2.2.2]octane]

The title compound, $[\text{Cd}(\text{C}_9\text{H}_8\text{O}_2)_2(\text{C}_6\text{H}_{12}\text{N}_2)(\text{H}_2\text{O})]_n$, forms a one-dimensional polymeric chain. Both cinnamate ligands are bidentate anions and the 1,4-diazabicyclo[2.2.2]octane (dabco) molecule acts as an end-to-end bridging ligand. The Cd atom, located at a position of site symmetry *m*, has a slightly distorted pentagonal bipyramidal coordination environment consisting of two N atoms of dabco ligands, four cinnamate O atoms and one water ligand, with the dabco N atoms in the axial positions. The chains are cross-linked by hydrogen bonds involving the coordinated water molecules, forming a two-dimensional network.

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Comment

Coordination polymers or metal-organic frameworks (MOFs) are of great current interest due to their potential electronic, magnetic, optical and catalytic applications (Batten & Robson, 1998). For example, triethylenediamine is a bidentate ligand that can coordinate to metal ions *via* two N atoms. It has a very versatile coordination behaviour, since it can form bridges between metallic centres, generating varied and sometimes surprising molecular architectures (Zhu *et al.*, 2003). In general, the factors influencing the formation of coordination polymers are still not well understood, in spite of the fact that the self-assembly of these architectures has been documented to be highly influenced by factors such as the nature of the metal ions (Carlucci *et al.*, 1995), templates (Tong, Ye *et al.*, 1998), and experimental conditions (Tong, Chen *et al.*, 1998). Much work is required to extend our knowledge of the relevant structural types and establish proper synthetic strategies leading to the desired types of materials.



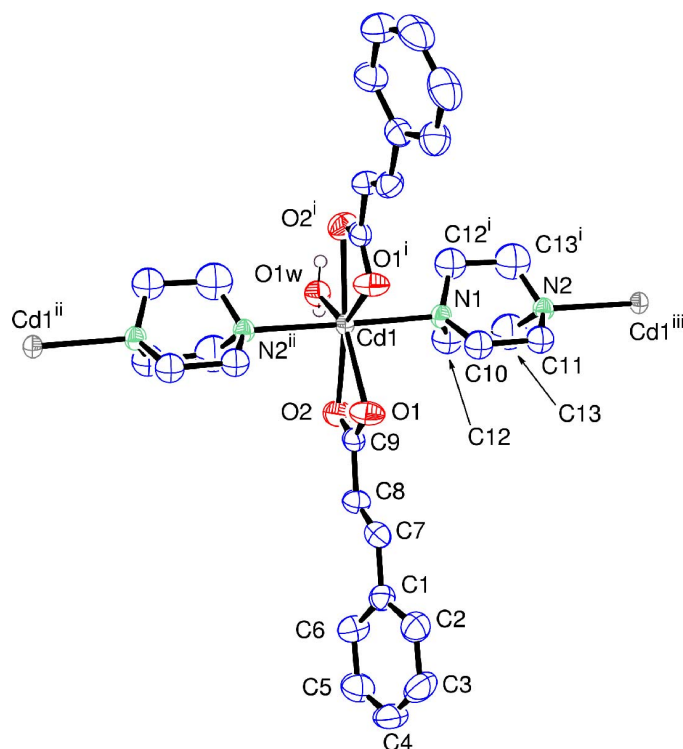


Figure 1

A fragment of the polymeric structure of (I). Displacement ellipsoids for non-H atoms are drawn at the 50% probability level and all H atoms except H1 and its symmetry equivalent (arbitrary spheres) are omitted for clarity. Only one orientation of the disordered dabco species is shown. Symmetry codes: (i) $x, \frac{1}{2} - y, z$; (ii) $x, y, z + 1$; (iii) $x, y, z - 1$.

Here we report the crystal structure of the title compound, (I), (Fig. 1) which is a new coordination polymer involving Cd^{2+} , cinnamate anions, and 1,4-diazabicyclo[2.2.2]octane (dabco) molecules. Selected geometrical data are presented in Table 1. The Cd atom (site symmetry m) is seven-coordinate in a somewhat distorted pentagonal bipyramidal environment. The pentagonal basal plane is defined by four O atoms from two cinnamate ligands and one aqua O atom (Table 1) with the dabco N atoms occupying the axial positions. The dabco molecule acts as a bridging ligand, linking Cd atoms in an end-to-end coordination mode [$\text{N1}-\text{Cd1}-\text{N2} = 176.76(17)^\circ$], generating almost linear chains, with a $\text{Cd} \cdots \text{Cd}$ separation of $7.483(6) \text{ \AA}$. The $\text{Cd1}-\text{N1}$ and $\text{Cd1}-\text{N2}$ bond lengths of $2.459(6)$ and $2.422(6) \text{ \AA}$, respectively, are consistent with those in related compounds. [$\text{Cd}-\text{N} = 2.437(2) \text{ \AA}$] (Tao *et al.*, 2003)

Compound (I) forms an infinite one-dimensional chain extending along the c axis. A three-dimensional network structure is formed *via* $\text{O}-\text{H} \cdots \text{O}$ interactions [$\text{O}-\text{H} \cdots \text{O} = 2.707(6) \text{ \AA}$] between the carboxylate O atoms and the coordinated water H atoms (Table 2).

Experimental

Cadmium cinnamate (1 mmol, 260 mg) and 1,4-diazabicyclo[2.2.2]octane (1 mmol, 112 mg) were dissolved in an aqueous ammonia solution (10 ml, 30%), and the mixture was stirred for about 20 min at room temperature. The resulting clear colourless solution was kept in

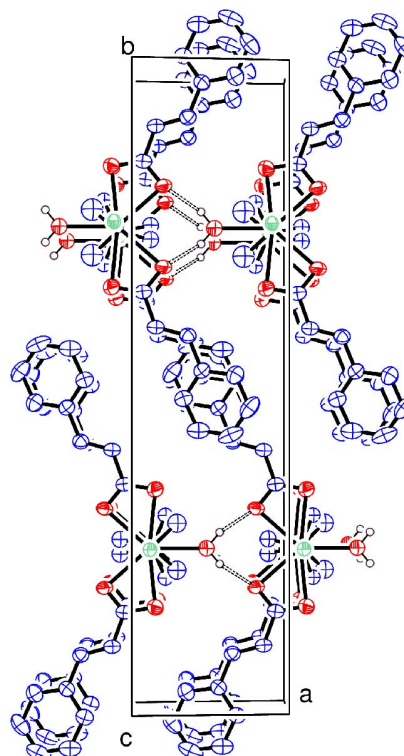


Figure 2

The unit-cell packing in (I), viewed down c , with hydrogen bonds shown as dashed lines. Only one orientation of the disordered dabco species is shown. H atoms other than those of water have been omitted.

air and, after slow evaporation of the solvent over a period of a week, large colourless crystals of (I) formed at the bottom of the vessel. The crystals were isolated, washed three times with water and dried in a vacuum desiccator using anhydrous CaCl_2 (yield = 57%). Elemental analysis found: C 53.60, H 5.26, N 5.18, Cd 20.90%; calculated for $\text{C}_{24}\text{H}_{27}\text{CdN}_2\text{O}_5$: C 53.79, H 5.08, N 5.23, Cd 20.98%.

Crystal data

$[\text{Cd}(\text{C}_9\text{H}_8\text{O}_2)_2(\text{C}_6\text{H}_{12}\text{N}_2)(\text{H}_2\text{O})]$
 $M_r = 536.88$
 Monoclinic, $P2_1/m$
 $a = 6.143(1) \text{ \AA}$
 $b = 25.340(5) \text{ \AA}$
 $c = 7.483(1) \text{ \AA}$
 $\beta = 97.58(3)^\circ$
 $V = 1154.7(3) \text{ \AA}^3$
 $Z = 2$

$D_x = 1.544 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 Cell parameters from 800 reflections
 $\theta = 2.4-26.0^\circ$
 $\mu = 0.98 \text{ mm}^{-1}$
 $T = 298(2) \text{ K}$
 Block, colourless
 $0.43 \times 0.34 \times 0.26 \text{ mm}$

Data collection

Bruker SMART CCD diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.708, T_{\max} = 0.774$
 5681 measured reflections

2113 independent reflections
 1943 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.044$
 $\theta_{\max} = 25.5^\circ$
 $h = -7 \rightarrow 7$
 $k = -30 \rightarrow 24$
 $l = -8 \rightarrow 9$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.116$
 $S = 1.10$
 2113 reflections
 148 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0653P)^2 + 0.4917P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.82 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.85 \text{ e \AA}^{-3}$

Table 1
Selected geometric parameters (Å, °).

Cd1—O1W	2.286 (4)	Cd1—N1	2.424 (5)
Cd1—O2	2.375 (4)	Cd1—N2 ⁱ	2.459 (5)
Cd1—O1	2.398 (3)		
O1W—Cd1—O2	84.31 (8)	O2—Cd1—N1	90.89 (9)
O2—Cd1—O2 ⁱⁱ	168.45 (16)	O1—Cd1—N1	89.88 (13)
O2—Cd1—O1 ⁱⁱ	137.13 (11)	O1W—Cd1—N2 ⁱ	88.05 (16)
O1W—Cd1—O1	138.56 (7)	O2—Cd1—N2 ⁱ	88.81 (9)
O2—Cd1—O1	54.29 (11)	O1—Cd1—N2 ⁱ	92.42 (13)
O1 ⁱⁱ —Cd1—O1	82.86 (15)	N1—Cd1—N2 ⁱ	176.93 (15)
O1W—Cd1—N1	88.88 (16)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1 ⁱⁱⁱ —O1 ⁱⁱⁱ	0.85	1.89	2.711 (5)	162

Symmetry code: (iii) $1 + x, y, z$.

The C atoms and their attached H atoms of the dabco molecule were modelled as disordered over two positions with symmetry-constrained equal occupancies. The H atoms bonded to C were placed in idealized locations and refined as riding on their carrier atoms [$d(C-H) = 0.93-0.97$ Å]. The water H atom was located in a

difference map and refined as riding in its as-found relative position. The constraint $U_{iso}(H) = 1.2U_{eq}(\text{carrier})$ was applied in all cases.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINTE* (Siemens, 1996); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

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