

## ***catena*-Poly[[diaquacadmium(II)]- $\mu$ -5-carboxylimidazole-4-carboxylato- $\kappa^4 N^1, O^5: O^4, N^3$ ]**

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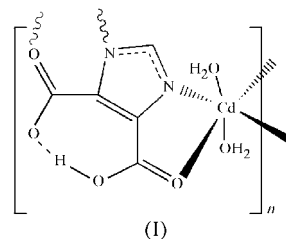
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A new cadmium coordination polymer,  $[\text{Cd}(\text{C}_5\text{H}_3\text{N}_2\text{O}_4)(\text{H}_2\text{O})_2]_n$ , possesses a one-dimensional zigzag chain structure built from  $\text{Cd}^{\text{II}}$  centers bridged sequentially by pairs of O and N atoms of the 5-carboxylimidazole-4-carboxylate ligand. The  $\text{Cd}^{\text{II}}$  center is in a distorted octahedral geometry, being coordinated by two O atoms from two coordinated water molecules  $[\text{Cd}-\text{O} = 2.322(7)$  and  $2.364(7)$  Å], and by two N atoms  $[\text{Cd}-\text{N} = 2.222(6)$  and  $2.232(6)$  Å] and two carboxyl O atoms  $[\text{Cd}-\text{O} = 2.383(6)$  and  $2.414(6)$  Å] from two 5-carboxylimidazole-4-carboxylate ligands.

### Comment

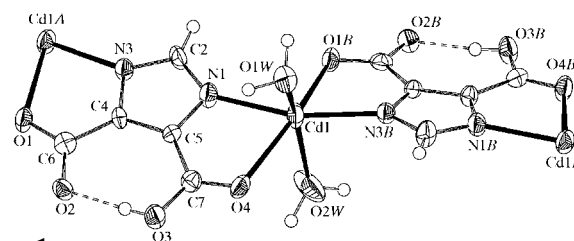
Coordination polymers built from  $d^{10}$  metals, such as cadmium(II), and rigid aromatic carboxylates have attracted considerable attention in recent years because they not only exhibit interesting structures but also possess photoluminescence properties (Evans *et al.*, 1999; Evans & Lin, 2000; Liu *et al.*, 2002; Tong *et al.*, 1999). A series of cadmium(II) carboxylates have been described recently (Dai *et al.*, 2002; Ganesan & Natarajan, 2004; Wang, Qin *et al.*, 2004). Although a discrete dimer, *viz.* *trans*-diaquabis(1*H*-imidazole-4,5-dicarboxylato)cadmium(II),  $[\text{Cd}(\text{C}_5\text{H}_3\text{N}_2\text{O}_4)_2(\text{H}_2\text{O})_2]$ , with the Cd atom on an inversion center, has been reported (Zhang, Fang *et al.*, 2004), to our knowledge, there is no reported polymer constructed from  $\text{Cd}^{\text{II}}$  and the 4,5-imidazoledicarboxylic acid ligand. This ligand has not been well documented in the design of functional coordination polymers (Caudle *et al.*, 1997; Huang *et al.*, 2001; Ma *et al.*, 2003; Rajendiran *et al.*, 2003; Wang, Gao *et al.*, 2004; Zhang, Huang *et al.*, 2004). However, it has two structural features that led to our research interest. The ligand has potential coordination sites involving both N atoms of the imidazole ring and all the carboxyl O atoms. The flexible multifunctional coordination sites give a high likelihood for generation of structures of different dimensions. In addition, this ligand possesses three removable H atoms and can be successively

deprotonated to generate the  $\text{C}_5\text{H}_3\text{N}_2\text{O}_4^-$ ,  $\text{C}_5\text{H}_2\text{N}_2\text{O}_4^{2-}$  and  $\text{C}_5\text{HN}_2\text{O}_4^{3-}$  ions, depending on the pH level, resulting in various acidity-dependent coordination modes. We report here the synthesis and structure of a new cadmium complex, (I). This is the first reported one-dimensional cadmium complex containing the 5-carboxylimidazole-4-carboxylate ligand as a linkage unit.

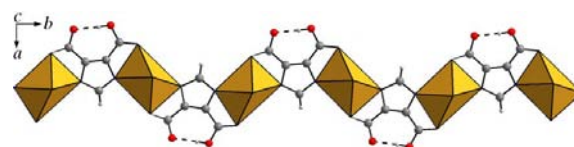


Our X-ray diffraction study shows (Fig. 1) that the asymmetric unit contains one  $\text{Cd}^{2+}$  cation, one 5-carboxylimidazole-4-carboxylate anion and two water molecules. The  $\text{Cd}^{\text{II}}$  center is in a distorted octahedral geometry, being coordinated by two O atoms from two coordinated water molecules, and by two N and two O atoms from two *b*-glide-related 5-carboxylimidazole-4-carboxylate ligands; the principal dimensions are given in Table 1. Each 5-carboxylimidazole-4-carboxylate anion is quasi-planar and connects successive  $\text{Cd}^{\text{II}}$  ions in a bis-bidentate mode, forming five-membered Cd/N/C/C/O rings. One N atom and one carboxylic acid group in the ligand are deprotonated, and there is an intramolecular O—H...O hydrogen bond (Fig. 1 and Table 2). The 5-carboxylimidazole-4-carboxylate ligands link neighboring  $\text{Cd}^{\text{II}}$  centers *via* a *b*-glide operation to form a one-dimensional zigzag chain composed of fused five-membered rings running along the *b*-axis direction, as shown in Fig. 2.

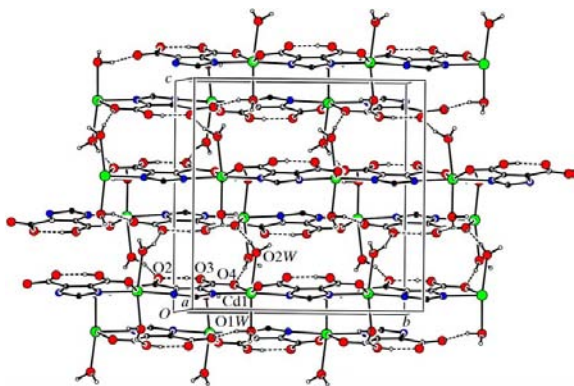
In the crystal structure, adjacent chains are held together by hydrogen bonds (Table 2) between water molecules and all four unique carboxy O atoms, thus generating a three-dimensional network. Fig. 3 shows a series of chains linked by hydrogen bonds involving one O—H bond from each of the water molecules (O1W—H11 and O2W—H22), thus gener-



**Figure 1**  
 A view of the coordination environment of the Cd atom. Anisotropic displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (A)  $\frac{1}{2} - x, -\frac{1}{2} + y, z$ ; (B)  $\frac{1}{2} - x, \frac{1}{2} + y, z$ .]



**Figure 2**  
 A view showing the one-dimensional chain structure extending in the *b* direction.



**Figure 3**  
A view along the *a*-axis direction, showing part of the three-dimensional network with chains linked into sheets by O—H...O hydrogen bonds.

ating a sheet in the *bc* plane. The remaining water OH groups then link these sheets into a three-dimensional network.

## Experimental

The title compound was synthesized by reacting Cd(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O (1 mmol), aqueous ammonia solution (0.1 ml, 25 wt%) and imidazole-4,5-dicarboxylic acid (1 mmol) in water (10.0 ml). The autoclave was heated at 443 K for 7 d. Upon cooling to room temperature, the desired product appeared as long yellow prisms in 43% yield.

### Crystal data

[Cd(C <sub>5</sub> H <sub>2</sub> N <sub>2</sub> O <sub>4</sub> )(H <sub>2</sub> O) <sub>2</sub> ]	Mo K $\alpha$ radiation
$M_r = 302.52$	Cell parameters from 165 reflections
Orthorhombic, <i>Pbcn</i>	$\theta = 2.5\text{--}25.1^\circ$
$a = 10.3280$ (12) Å	$\mu = 2.43$ mm <sup>-1</sup>
$b = 13.2177$ (14) Å	$T = 293$ (2) K
$c = 13.1813$ (16) Å	Prism, yellow
$V = 1799.4$ (4) Å <sup>3</sup>	$0.18 \times 0.12 \times 0.10$ mm
$Z = 8$	
$D_x = 2.233$ Mg m <sup>-3</sup>	

### Data collection

Siemens SMART CCD diffractometer	1587 independent reflections
$\varphi$ and $\omega$ scans	1149 reflections with $I > 2\sigma(I)$
Absorption correction: empirical (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.053$
$T_{\text{min}} = 0.711$ , $T_{\text{max}} = 0.784$	$\theta_{\text{max}} = 25.1^\circ$
4833 measured reflections	$h = -8 \rightarrow 12$
	$k = -13 \rightarrow 15$
	$l = -15 \rightarrow 11$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0428P)^2 + 9.3728P]$
$R[F^2 > 2\sigma(F^2)] = 0.051$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.120$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.18$	$\Delta\rho_{\text{max}} = 1.06$ e Å <sup>-3</sup>
1587 reflections	$\Delta\rho_{\text{min}} = -0.75$ e Å <sup>-3</sup>
128 parameters	
H-atom parameters constrained	

**Table 1**

Selected geometric parameters (Å, °).

Cd1—N1	2.232 (6)	Cd1—O2W	2.322 (7)
Cd1—N3 <sup>i</sup>	2.222 (6)	Cd1—O1 <sup>i</sup>	2.414 (6)
Cd1—O1W	2.364 (7)	Cd1—O4	2.383 (6)
N1—Cd1—N3 <sup>i</sup>	163.8 (2)	O4—Cd1—O1 <sup>i</sup>	155.04 (19)
O1W—Cd1—O2W	153.9 (3)		

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

**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>
O3—H3...O2	0.82	1.64	2.461 (7)	174
O1W—H11...O1 <sup>ii</sup>	0.95	1.88	2.806 (8)	165
O1W—H12...O3 <sup>iii</sup>	0.95	2.10	2.879 (8)	138
O2W—H21...O2 <sup>iv</sup>	0.95	1.90	2.769 (9)	151
O2W—H22...O4 <sup>v</sup>	0.95	1.85	2.790 (9)	172

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

H atoms were located in difference Fourier maps and were subsequently allowed for as riding atoms, with a C—H distance of 0.93 Å, a carboxyl O—H distance of 0.82 Å and water O—H distances of 0.95 Å, and with  $U_{\text{iso}}(\text{H})$  values of  $1.2U_{\text{eq}}(\text{C}, \text{carboxyl O})$  and 0.08 Å<sup>2</sup> (for water H atoms).

Data collection: SMART (Bruker, 1999); cell refinement: SMART; data reduction: SAINT (Bruker, 1999); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1997); software used to prepare material for publication: SHELXTL and PLATON (Spek, 2003).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: FG1767). Services for accessing these data are described at the back of the journal.

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