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## Key indicators

Single-crystal X-ray study  
 $T = 295$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
 $R$  factor = 0.015  
 $wR$  factor = 0.039  
Data-to-parameter ratio = 16.2For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.A three-dimensional porous cadmium(II)  
coordination polymer: poly[[pyridine- $\kappa$ N]-  
cadmium(II)]- $\mu_3$ -imidazole-4,5-dicarboxylato-  
 $\kappa^6$ N,O:N',O':O',O'']

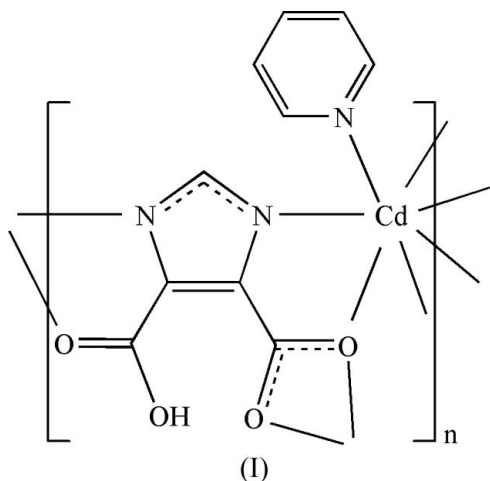
In the title coordination polymer,  $[\text{Cd}(\text{C}_5\text{H}_2\text{N}_2\text{O}_4)(\text{C}_5\text{H}_5\text{N})]_n$ , the  $\text{Cd}^{\text{II}}$  atom exists in a pentagonal-bipyramidal environment that has two N atoms and four O atoms from three different imidazole-4,5-dicarboxylate ligands, and an N atom from a pyridine molecule. The Cd atoms are linked by the imidazole-4,5-dicarboxylate ligands to give rise to a three-dimensional open framework with channels.

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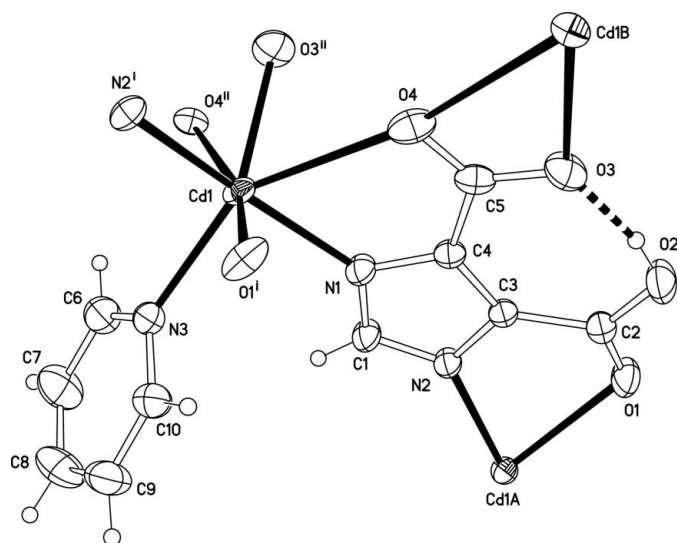
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## Comment

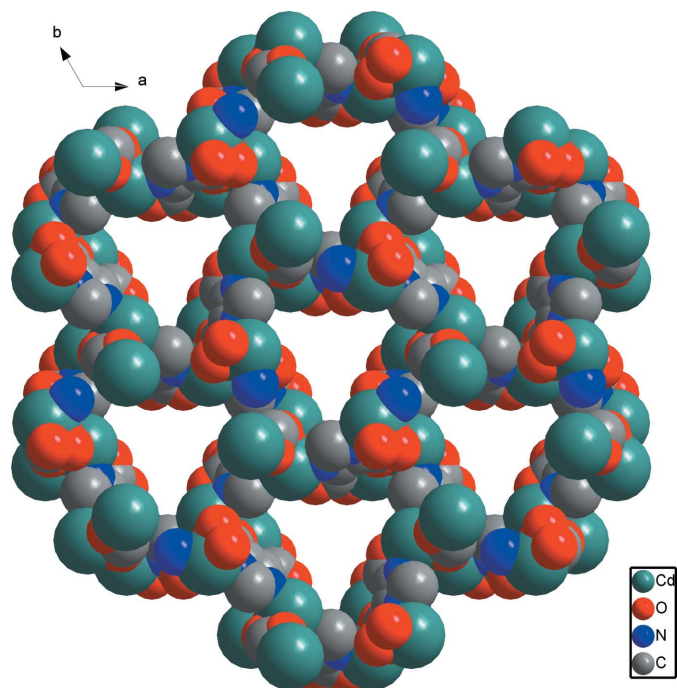
1*H*-Imidazole-4,5-dicarboxylic acid ( $\text{H}_3\text{IDC}$ ) binds to metals by using its carboxylate O and imidazole N atoms to form monodentate and/or multidentate  $M-\text{O}$  and  $M-\text{N}$  bonds. The acid can be successively deprotonated to furnish  $\text{H}_2\text{IDC}^-$ ,  $\text{HIDC}^{2-}$  and  $\text{IDC}^{3-}$  anions, these anions giving rise to a wide range of supramolecular architectures. To our knowledge, three transition metal complexes of Mn, Zn and Cd complexes with three-dimensional structures (Zhang *et al.*, 2006; Lu *et al.*, 2006) have been reported to date. In this paper, we report the title complex  $[\text{Cd}(\text{HIDC})(\text{pyridine})]_n$ , (I), which was synthesized hydrothermally from the reaction of cadmium dinitrate tetrahydrate, 1*H*-imidazole-4,5-dicarboxylic acid and pyridine.



The Cd atom is coordinated by an N atom from the pyridine molecule, and two N atoms and four O atoms from three different  $\text{HIDC}^{2-}$  groups. The coordination polyhedron is a pentagonal bipyramid whose equatorial plane is defined by atoms O4, O1<sup>i</sup>, O4<sup>ii</sup>, O3<sup>ii</sup> and N3 [symmetry codes: (i)  $-y + \frac{1}{3}$ ,  $-x + \frac{2}{3}$ ,  $z + \frac{1}{6}$ ; (ii)  $-x + y - \frac{1}{3}$ ,  $-x + \frac{1}{3}$ ,  $z + \frac{1}{3}$ ] [r.m.s. deviation = 0.17 (2) Å; deviation of the Cd atom from this plane is 0.34 (2) Å]. The axial positions are occupied by atoms N1 and N2<sup>i</sup> [angle of 161.78 (7)°]. The Cd—O4 and Cd—O4<sup>ii</sup> distances are considerably longer but lying within the range for the



**Figure 1** Part of the polymeric structure of the title complex, with displacement ellipsoids shown at the 30% probability level. [Symmetry codes: (i)  $-y + \frac{1}{3}, -x + \frac{2}{3}, z + \frac{1}{6}$ ; (ii)  $-x + y - \frac{1}{3}, -x + \frac{2}{3}, z + \frac{1}{3}$ ; (A)  $-y + \frac{2}{3}, -x + \frac{1}{3}, z - \frac{1}{6}$ ; (B)  $-y + \frac{1}{3}, x - y + \frac{2}{3}, z - \frac{1}{3}$ .]



**Figure 2** A view of the three-dimensional network, with the one-dimensional channels down the *c* axis (pyridine molecules and H atoms have been omitted).

normal Cd–carboxylate bond distances [2.209 (2)–2.879 (2) Å] reported for Cd<sup>II</sup> carboxylate coordination polymers (Clegg *et al.*, 1995).

The HIDC<sup>2-</sup> group bridges three Cd atoms to form two five-membered and one four-membered rings. The structure has an extended three-dimensional open framework with one-dimensional channels. Although the effective pore size is significantly diminished by the pyridine molecules, the volume

of each is 57 Å<sup>3</sup> (Fig. 2). As the architecture is somewhat similar to a molecular sieve, the compound represents a candidate for applications in adsorption, molecular recognition and host–guest chemistry.

### Experimental

Cadmium dinitrate tetrahydrate (3.08 g, 10 mmol), pyridine (1 ml) and 1*H*-imidazole-4,5-dicarboxylic acid (1.54 g, 10 mmol) were dissolved in water (25 ml). The mixture was sealed in a 50 ml Teflon-lined stainless steel bomb and held at 403 K for 5 d. The bomb was cooled naturally to room temperature, and colorless prismatic crystals were obtained after several days. C, H & N analysis, calculated for C<sub>10</sub>H<sub>7</sub>CdN<sub>3</sub>O<sub>4</sub>: C 34.75, H 2.04, N 12.16%; found: C 34.79, H 2.08, N 12.13%.

#### Crystal data

[Cd(C<sub>5</sub>H<sub>2</sub>N<sub>2</sub>O<sub>4</sub>)(C<sub>5</sub>H<sub>5</sub>N)]  
*M<sub>r</sub>* = 345.60  
 Trigonal, *R*3*c*  
*a* = 21.112 (3) Å  
*c* = 13.953 (3) Å  
*V* = 5385.9 (16) Å<sup>3</sup>  
*Z* = 18

*D<sub>x</sub>* = 1.918 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
*μ* = 1.83 mm<sup>-1</sup>  
*T* = 295 (2) K  
 Prism, colorless  
 0.37 × 0.25 × 0.19 mm

#### Data collection

Rigaku R-Axis RAPID  
 diffractometer  
*ω* scans  
 Absorption correction: multi-scan  
 (ABSCOR; Higashi, 1995)  
*T<sub>min</sub>* = 0.582, *T<sub>max</sub>* = 0.705

16748 measured reflections  
 2687 independent reflections  
 2595 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.015  
*θ<sub>max</sub>* = 27.5°

#### Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.015  
*wR*(*F*<sup>2</sup>) = 0.039  
*S* = 1.03  
 2687 reflections  
 166 parameters  
 H atoms treated by a mixture of  
 independent and constrained  
 refinement

*w* = 1/[σ<sup>2</sup>(*F<sub>o</sub>*<sup>2</sup>) + (0.0269*P*)<sup>2</sup>  
 + 1.8634*P*]  
 where *P* = (*F<sub>o</sub>*<sup>2</sup> + 2*F<sub>c</sub>*<sup>2</sup>)/3  
 (Δ/σ)<sub>max</sub> = 0.002  
 Δρ<sub>max</sub> = 0.37 e Å<sup>-3</sup>  
 Δρ<sub>min</sub> = -0.21 e Å<sup>-3</sup>  
 Absolute structure: Flack (1983),  
 1353 Friedel pairs  
 Flack parameter: -0.003 (19)

**Table 1**

Selected geometric parameters (Å, °).

Cd1–N1	2.2070 (17)	Cd1–O4 <sup>ii</sup>	2.709 (2)
Cd1–N2 <sup>i</sup>	2.2185 (17)	O1–C2	1.218 (3)
Cd1–N3	2.361 (2)	O2–C2	1.302 (3)
Cd1–O1 <sup>i</sup>	2.525 (2)	O3–C5	1.268 (3)
Cd1–O3 <sup>ii</sup>	2.3225 (17)	O4–C5	1.224 (3)
Cd1–O4	2.792 (2)		
N1–Cd1–N2 <sup>i</sup>	161.78 (7)		

Symmetry codes: (i)  $-y + \frac{1}{3}, -x + \frac{2}{3}, z + \frac{1}{6}$ ; (ii)  $-x + y - \frac{1}{3}, -x + \frac{1}{3}, z + \frac{1}{3}$ .

**Table 2**

Hydrogen-bond 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>
O2–H11...O3	0.84 (5)	1.69 (3)	2.518 (3)	168 (4)

H atoms on C atoms were placed in calculated positions, with C—H = 0.93 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ , and were refined in the riding-model approximation. The hydroxyl H atom was located in a difference Fourier map and refined with an O—H distance restraint of 0.85 (1) Å and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ .

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSK, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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