Acta Crystallographica Section E
**Structure Reports
Online**
ISSN 1600-5368

A two-dimensional cadmium(II) coordination polymer with unusual 4.8^2 topology: poly[aqua(μ_3-1*H*-imidazole-4,5-dicarboxylato)cadmium(II)]

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Received 13 March 2007
Accepted 2 April 2007

Key indicators

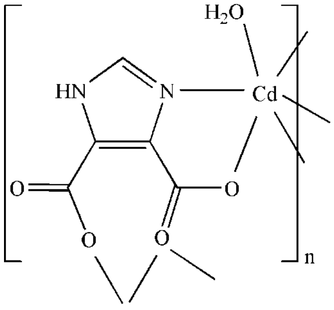
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.017
wR factor = 0.043
Data-to-parameter ratio = 12.3

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

In the title coordination polymer, $[Cd(C_5H_2N_2O_4)(H_2O)]_n$, the Cd^{II} atom is six-coordinated by one N atom and four O atoms from three individual imidazole-4,5-dicarboxylate (HIDC^{2-}) anions and the O atom of a water molecule. The HIDC^{2-} anion serves as a bridging ligand to link the Cd^{II} atoms into a two-dimensional network.

Comment

The anion of 1*H*-imidazole-4,5-dicarboxylic acid (H_3IDC) exemplifies a bridging multi-dentate ligand that is used in the formation of supramolecular complexes. The acid can be successively deprotonated to furnish H_2IDC^-, HIDC^{2-} and IDC^{3-} anions, these anions giving rise to a wide range of supramolecular architectures (Zhang *et al.*, 2005, 2006; Lu *et al.*, 2006). We report here the crystal structure of the title two-dimensional Cd^{II} coordination polymer $[Cd(HIDC)(H_2O)]_n$, (I), which contains a rare two-dimensional 4.8^2 net.



(I)

As shown in Fig. 1, the asymmetric unit of complex (I) comprises one Cd^{II} atom, one HIDC^{2-} dianion and one coordinated water molecule (Fig. 1). Each Cd^{II} ion is six-coordinated by one N atom [Cd—N = 2.2383 (18) Å] and four O atoms [Cd—O = 2.2865 (15)–2.4294 (16) Å] from three HIDC^{2-} ligands, and the O atom of a water molecule [Cd—O1w = 2.3073 (18) Å]. The coordination geometry around the Cd^{II} atom can be best described as distorted trigonal-prismatic (Fig. 2).

It is interesting to note that each HIDC^{2-} anion serves as a bridging ligand to link Cd^{II} atoms into a two-dimensional network structure (Fig. 3). In terms of topology, reducing the Cd^{II} centers as three-connected nodes, while the HIDC^{2-} ligands are viewed as linkers, this layer can be represented topologically as a 4.8^2 net (Fig. 4). The sheet of 4.8^2 topology consists of three-connected nodes shared by one tetragon and two octagons. Such a net was predicted by Wells (1977) but previously rarely observed for coordination frameworks

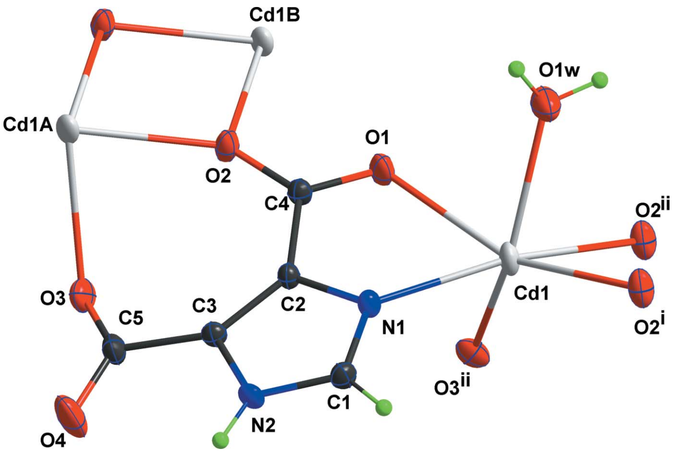


Figure 1
The asymmetric unit of the title complex, extended to show the complete coordination of Cd and the surroundings of the organic ligand, with displacement ellipsoids drawn at the 30% probability level. [Symmetry codes: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$. (A) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$; (B) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.]

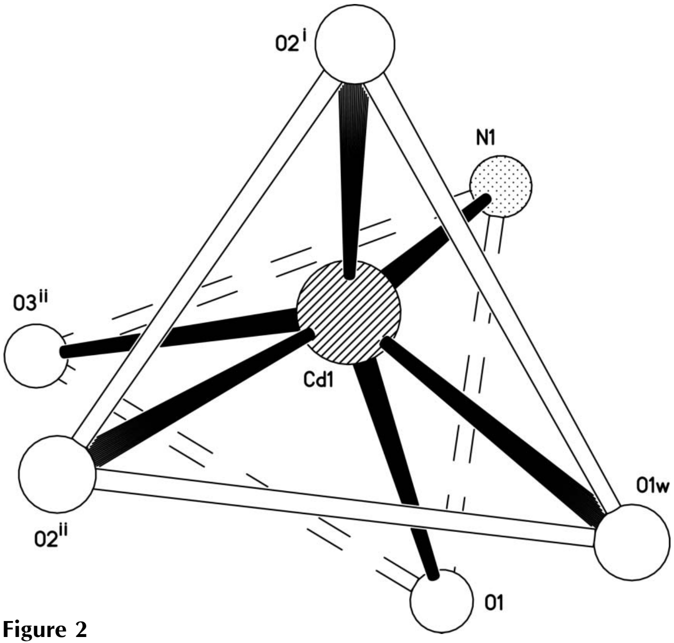


Figure 2
The coordination polydedron of the Cd^{II} atom.

(Long *et al.*, 2000; Kang *et al.*, 2005). In the two-dimensional network, strong π–π stacking interactions are observed between adjacent parallel imidazole rings (symmetry relationship: $-x+1, -y+1, -z+1$), with a centroid–centroid separation of 3.3618 (6) Å. Furthermore, a three-dimensional supramolecular network is constructed *via* hydrogen-bonding interactions, involving the water molecules, the uncoordinated imidazole N atom, and carboxylate O atoms of HIDC^{2-} ligands (Table 2).

Experimental

Cadmium dinitrate tetrahydrate (3.08 g, 10 mmol), 1*H*-imidazole-4,5-dicarboxylic acid (1.54 g, 10 mmol) and NaOH (0.4 g, 10 mmol) were dissolved in an aqueous solution (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 then allowed to cool naturally to room temperature, and colorless prismatic crystals of (I) were obtained after several days. Analysis calculated for $C_5H_4CdN_2O_5$: C 21.11, H 1.42, N 9.85%; found: C 21.15, H 1.46, N 9.83%.

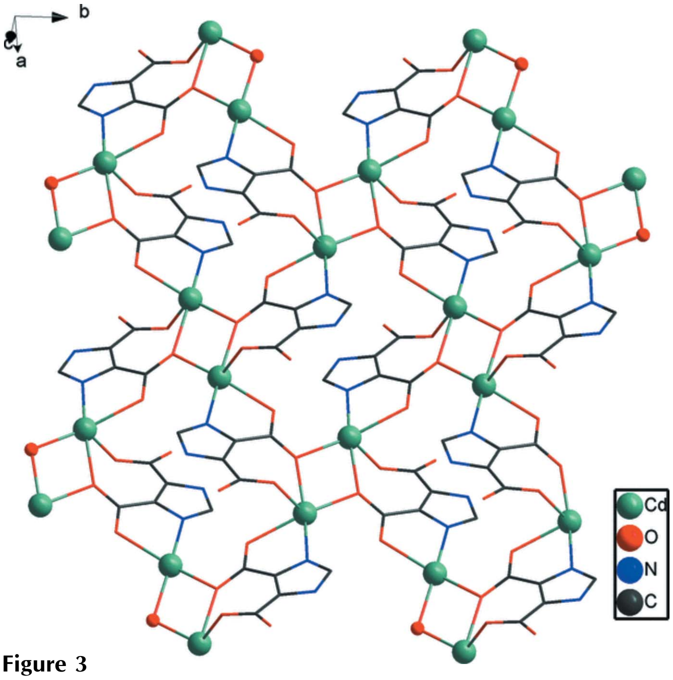


Figure 3
The two-dimensional network structure of (I). For clarity, water molecules and H atoms have been omitted.

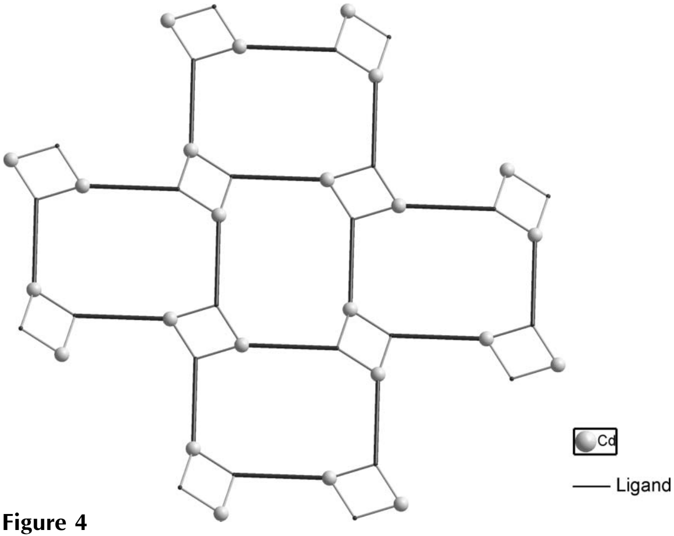


Figure 4
Schematic representation of the 4.8^2 topology of (I).

Crystal data

$[Cd(C_5H_2N_2O_4)(H_2O)]$
$M_r = 284.50$
Monoclinic, $P2_1/n$
$a = 6.5915$ (13) Å
$b = 9.950$ (2) Å
$c = 10.546$ (2) Å
$\beta = 105.73$ (3)°
$V = 665.8$ (2) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 3.27$ mm^{-1}
$T = 295$ (2) K
0.35 × 0.24 × 0.16 mm

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Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995) $T_{\min} = 0.401$, $T_{\max} = 0.594$
6292 measured reflections
1521 independent reflections
1464 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.017$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.017$
$wR(F^2) = 0.043$
$S = 1.07$
1521 reflections
124 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max} = 0.55$ e Å^{-3}
$\Delta\rho_{\min} = -0.44$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.2383 (18)	Cd1—O2$^{\rm ii}$	2.3122 (17)
Cd1—O2$^{\rm i}$	2.2865 (15)	Cd1—O3$^{\rm ii}$	2.3649 (16)
Cd1—O1*W*	2.3073 (18)	Cd1—O1	2.4294 (16)
N1—Cd1—O2$^{\rm i}$	116.35 (6)	O1*W*—Cd1—O3$^{\rm ii}$	141.09 (6)
N1—Cd1—O1*W*	111.29 (7)	O2$^{\rm ii}$—Cd1—O3$^{\rm ii}$	77.53 (6)
O2$^{\rm i}$—Cd1—O1*W*	81.49 (7)	N1—Cd1—O1	70.45 (6)
N1—Cd1—O2$^{\rm ii}$	164.91 (6)	O2$^{\rm i}$—Cd1—O1	159.05 (6)
O2$^{\rm i}$—Cd1—O2$^{\rm ii}$	71.60 (6)	O1*W*—Cd1—O1	77.65 (6)
O1*W*—Cd1—O2$^{\rm ii}$	81.94 (6)	O2$^{\rm ii}$—Cd1—O1	106.95 (6)
N1—Cd1—O3$^{\rm ii}$	87.44 (6)	O3$^{\rm ii}$—Cd1—O1	77.27 (6)
O2$^{\rm i}$—Cd1—O3$^{\rm ii}$	121.49 (6)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O4$^{\rm iii}$	0.85 (1)	1.85 (1)	2.696 (3)	173 (3)
O1*W*—H1*W*2···O3$^{\rm iv}$	0.85 (1)	2.07 (2)	2.877 (3)	158 (3)
N2—H2···O3$^{\rm v}$	0.86	1.92	2.776 (2)	171

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

H atoms on C and N atoms were placed in calculated positions, with C—H = 0.93 Å, N—H = 0.86 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$(C,N), and were refined in the riding-model approximation. Water H atoms were located in a difference Fourier map and refined with O—H and H···H distance restraints of 0.85 (1) and 1.39 (1) Å, respectively, and $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}$(O).

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 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*.

The authors thank the Heilongjiang Province Natural Science Foundation (No. B200501), the Scientific Fund of Remarkable Teachers of Heilongjiang Province (1054 G036) and Heilongjiang University for supporting this study.

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