

## The coordination polymer poly[bis- $[\mu_2$ -2-(2,2'-bi-1*H*-imidazol-1-yl)-acetato]cadmium]

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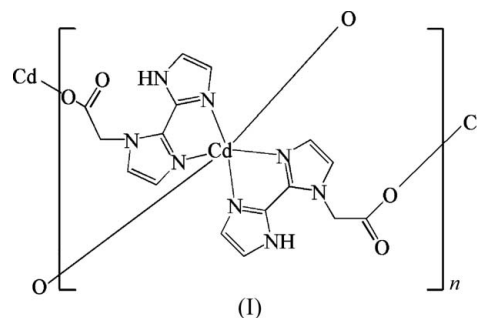
The title compound,  $[\text{Cd}(\text{C}_8\text{H}_7\text{N}_4\text{O}_2)_2]_n$ , crystallizes in the centrosymmetric triclinic space group  $P\bar{1}$  with an asymmetric unit consisting of a bivalent  $\text{Cd}^{\text{II}}$  atom and two 2-(2,2'-bi-1*H*-imidazol-1-yl)acetate ( $\text{BDAC}^-$ ) anions. Two inversion-related  $\text{BDAC}^-$  ligands are oppositely arranged and bind two  $\text{Cd}^{\text{II}}$  ions to form a  $[\text{Cd}_2(\text{BDAC})_2]$  rhomboid subunit which is bridged by another  $\text{BDAC}^-$  ligand to form an infinite ladder along the *a* direction containing parallelogram grids. The three-dimensional supramolecular architecture is formed by hydrogen bonds and  $\text{C}-\text{H}\cdots\pi$  and  $\pi-\pi$  interactions.

### Comment

The design and synthesis of coordination polymers is an attractive area of research not only because of the diverse topologies and intriguing structures of these compounds but also because of their potential applications in optics, magnetism, gas storage, ion exchange and catalysis (Eddaoudi *et al.*, 2001; Kitagawa *et al.*, 2004; Ferey *et al.*, 2005; Roy *et al.*, 2009). From the viewpoint of crystal engineering, the most effective and facile approach to coordination polymers is to utilize an applicable ligand to link metal ions to give an infinite framework, and the multipyridine and multicarboxylate spacers are good candidates for the construction of novel metal-organic compounds (Braverman *et al.*, 2007; Chen *et al.*, 2009; Liang *et al.*, 2009; Wang *et al.*, 2011).

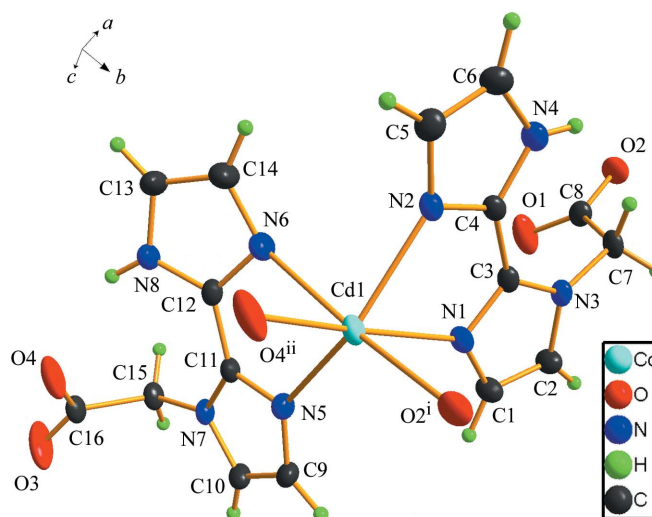
2-(2,2'-Bi-1*H*-imidazol-1-yl)acetic acid (HBDAC) is a typical example of a multidentate N- and O-donor ligand and, to the best of our knowledge, has not been explored to date. First, HBDAC is a flexible ligand with N- and O-donors on opposite sides, enabling the ligand to act as a linear bridge; second, the deprotonated  $\text{BDAC}^-$  ligand contains two bridging moieties which can lead to a variety of connection modes with metal centres, providing abundant structural motifs; third, it can act not only as a hydrogen-bond donor but also as an acceptor, which makes it a wonderful candidate for the construction of supramolecular networks. Here, we have

selected HBDAC as an organic linker, generating the title  $\text{Cd}^{\text{II}}$  coordination polymer, poly[[ $\mu_2$ -2-(2,2'-bi-1*H*-imidazol-1-yl)-acetato]cadmium], (I), the crystal structure of which we now report.

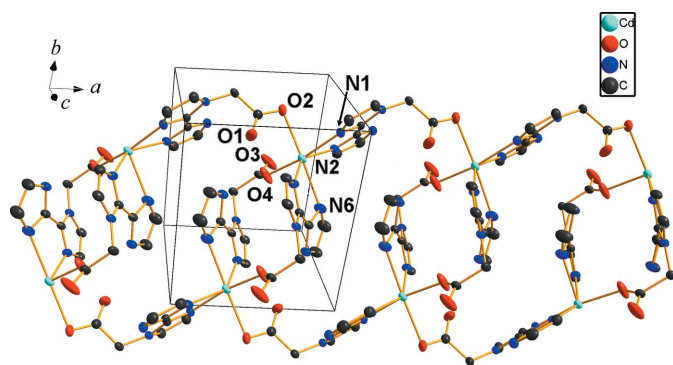


Compound (I) crystallizes in the centrosymmetric triclinic space group  $P\bar{1}$  with an asymmetric unit comprising a bivalent  $\text{Cd}^{\text{II}}$  atom and two  $\text{BDAC}^-$  anions ( $\text{BDAC-A}$  contains atoms N1–N4/O1/O2/C1–C8 and  $\text{BDAC-B}$  contains atoms N5–N8/O3/O4/C9–C16) (Fig. 1). The coordination environment at cadmium is best considered as a distorted  $\{\text{CdN}_4\text{O}_2\}$  octahedron formed by four N atoms (N1, N2, N5 and N6) from two different chelating  $\text{BDAC}^-$  ligands and two *cis*-O atoms [O2<sup>i</sup> and O4<sup>ii</sup>; symmetry codes: (i)  $x - 1, y, z$ ; (ii)  $-x + 1, -y + 1, -z + 2$ ] from two other  $\text{BDAC}^-$  ligands. The Cd–O bond lengths are 2.224 (3) and 2.443 (3) Å, while the Cd–N bond lengths vary greatly from 2.329 (3) to 2.503 (3) Å. The average Cd–O and Cd–N distances in (I) are comparable to those in reported Cd-based compounds (Liu *et al.*, 2008; Farnum *et al.*, 2011). It is worth noting that all  $\text{BDAC}^-$  ligands linked to two  $\text{Cd}^{\text{II}}$  ions adopt an exobidentate chelating/bridging coordination mode.

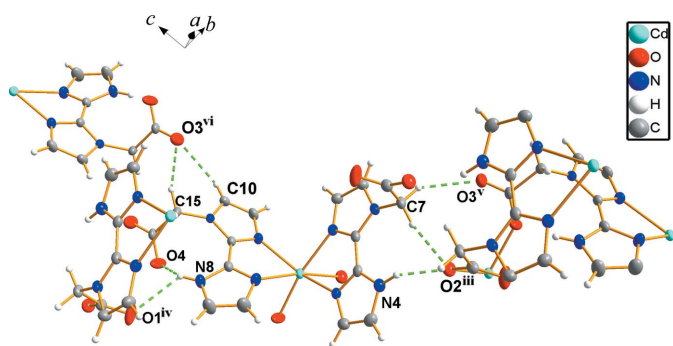
Two inversion-related  $\text{BDAC-B}$  ligands are oppositely arranged and bind two  $\text{Cd}^{\text{II}}$  ions to form a  $[\text{Cd}_2(\text{BDAC-B})_2]$


**Figure 1**

A view of the local coordination environment of the  $\text{Cd}^{\text{II}}$  cation in (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. [Symmetry codes: (i)  $x - 1, y, z$ ; (ii)  $-x + 1, -y + 1, -z + 2$ .]



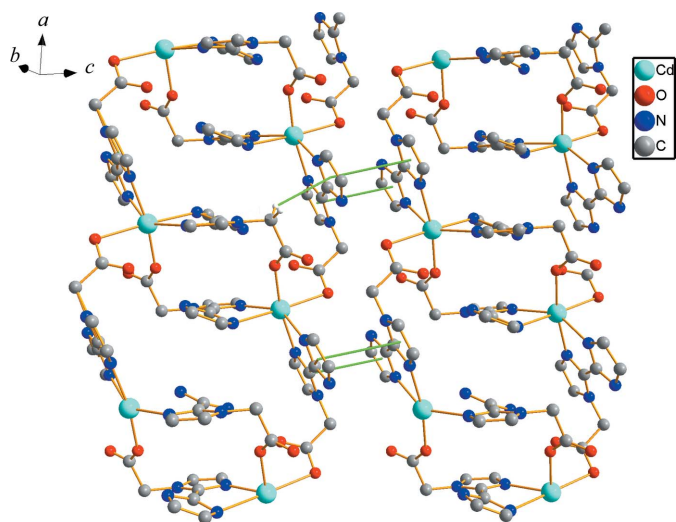
**Figure 2**  
A single  $[\text{Cd}(\text{BDAC})]_n$  chain in (I).



**Figure 3**  
A perspective view of the three-dimensional supramolecular architecture of (I), incorporating  $\text{C}-\text{H}\cdots\text{O}$  and  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds. The symmetry codes are as in Table 1.

rhomboid subunit (16-membered macrocycle). The  $\text{Cd}\cdots\text{Cd}$  through-space distances across the dinuclear unit are 7.017 Å. The rhomboid  $[\text{Cd}_2(\text{BDAC}-B)_2]$  subunit is further bridged by BDAC-*A* ligands to form an infinite ladder (Fig. 2) containing a parallelogram grid (dimensions =  $7.97 \times 12.92$  Å based on  $\text{Cd}\cdots\text{Cd}$  distances) arranged parallel to the *a* direction. The  $\text{Cd}\cdots\text{Cd}$  contact distances through the crystallographically distinct BDAC<sup>−</sup> ligands are 8.1262 (14) and 7.0170 (8) Å. These differences are provided by conformational variances within the distinct BDAC<sup>−</sup> ligands. In BDAC-*A*, the carboxylate group is twisted by 81.92 (13)° relative to the plane of the imidazole ring; the related torsion angle in BDAC-*B* is 68.74 (12)°.

There are extensive inter- and intramolecular hydrogen bonds of the  $\text{N}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\text{O}$  types connecting the one-dimensional chains of (I). Hydrogen bonds are found between N8 and O1/O4 with donor-acceptor distances of 3.049 (4) and 2.794 (4) Å, respectively. Carbonyl atom O2 acts as an acceptor in two hydrogen-bonding interactions; one involves alkyl atom C7 of a neighbouring complex, with an  $\text{O}\cdots\text{C}$  distance of 3.231 (5) Å, while the second (stronger) hydrogen bond is directed to atom N4, with an  $\text{O}\cdots\text{N}$  distance of 2.792 (4) Å, forming eight-membered rings which extend the structure to form a two-dimensional sheet. Furthermore, carbonyl atom O3 acts as an acceptor in three further hydrogen-bonding interactions, involving alkyl atoms C7, C10



**Figure 4**  
A projection of (I) showing  $\text{C}-\text{H}\cdots\pi$  and  $\pi-\pi$  interactions.

and C15, with  $\text{O}\cdots\text{C}$  distances of 3.299 (5), 3.317 (5) and 3.461 (5) Å, respectively, forming six-membered rings which further extend the structure into a three-dimensional network (Fig. 3). It is interesting that the packing in the unit cell is also stabilized by weak  $\pi-\pi$  interactions. The centroid of the N1/C1/C2/N3/C3 ring,  $\text{Cg}_1$ , is involved in a weak  $\pi-\pi$  interaction with the centroid of the N2/C4/N4/C6/C5 ring,  $\text{Cg}_2$ , at  $(-x + 2, -y + 1, -z + 2)$ , the distance between the interleaved ligands being 3.613 (2) Å. In addition, a  $\text{C}-\text{H}\cdots\pi$  interaction (Fig. 4) is observed between the C15—H15*B* group and the centroid of the N2/C4/N4/C6/C5 ring,  $\text{Cg}_3$ , with  $\text{C15}\cdots\text{Cg}_3^{\text{iv}} = 3.593$  (4) Å,  $\text{H15B}\cdots\text{Cg}_3^{\text{iv}} = 2.89$  Å and  $\text{C3}-\text{H15B}\cdots\text{Cg}_3^{\text{iv}} = 130^\circ$  [symmetry code: (iv)  $-x + 2, -y + 1, -z + 2$ ].

## Experimental

A mixture of  $\text{Cd}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$  (34.6 mg, 0.1 mmol), HBDAC (19.2 mg, 0.1 mmol) and KOH (11.2 mg, 0.2 mmol) in  $\text{H}_2\text{O}$  (10 ml) was sealed in a 16 ml Teflon-lined stainless steel container and heated at 463 K for 72 h. After cooling to room temperature, colourless block-shaped crystals of (I) were collected by filtration and washed with water and ethanol several times (yield 33.1%, based on HBDAC). Elemental analysis calculated for  $\text{C}_{16}\text{H}_{14}\text{CdN}_8\text{O}_4$ : C 38.84, H 2.85, N 22.65%; found: C 38.72, H 2.87, N 22.56%.

### Crystal data

$[\text{Cd}(\text{C}_8\text{H}_7\text{N}_4\text{O}_2)_2]$	$\gamma = 83.055$ (3)°
$M_r = 494.76$	$V = 868.5$ (3) Å <sup>3</sup>
Triclinic, $P\bar{1}$	$Z = 2$
$a = 8.1262$ (14) Å	Mo $K\alpha$ radiation
$b = 10.5663$ (19) Å	$\mu = 1.30$ mm <sup>−1</sup>
$c = 10.8076$ (19) Å	$T = 273$ K
$\alpha = 73.150$ (3)°	$0.19 \times 0.17 \times 0.15$ mm
$\beta = 78.568$ (3)°	

### Data collection

Bruker SMART CCD area-detector diffractometer	4352 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2000)	3072 independent reflections
$T_{\text{min}} = 0.781, T_{\text{max}} = 0.822$	2637 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.041$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$	262 parameters
$wR(F^2) = 0.065$	H-atom parameters constrained
$S = 0.97$	$\Delta\rho_{\max} = 0.54 \text{ e } \text{\AA}^{-3}$
3013 reflections	$\Delta\rho_{\min} = -0.39 \text{ e } \text{\AA}^{-3}$

All N- and C-bound H atoms were placed in calculated positions and refined using a riding model, with N—H = 0.86 Å, C—H = 0.93 (imidazole) or 0.97 Å (methylene) and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N,C})$ .

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: WQ3007). Services for accessing these data are described at the back of the journal.

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**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N4—H4 $\cdots$ O2 <sup>iii</sup>	0.86	2.01	2.792 (4)	150
C7—H7B $\cdots$ O2 <sup>iii</sup>	0.97	2.28	3.231 (5)	166
N8—H8 $\cdots$ O4	0.86	2.11	2.794 (4)	136
N8—H8 $\cdots$ O1 <sup>iv</sup>	0.86	2.46	3.049 (4)	126
C7—H7A $\cdots$ O3 <sup>v</sup>	0.97	2.48	3.299 (5)	142
C10—H10 $\cdots$ O3 <sup>vi</sup>	0.93	2.56	3.317 (5)	139
C15—H15A $\cdots$ O3 <sup>vi</sup>	0.97	2.57	3.461 (5)	153

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

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