



Assembly of Zn^{II} and Cd^{II} coordination polymers with different dimensionalities based on the semi-flexible 3-(1*H*-benzimidazol-2-yl)propanoic acid ligand

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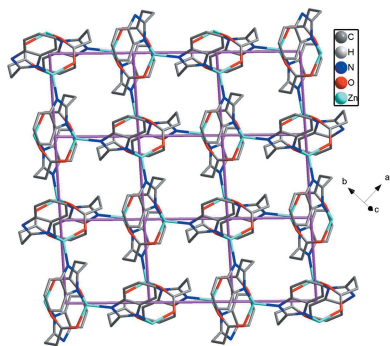
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Two new coordination polymers, namely, poly[[μ_3 -3-(1*H*-benzimidazol-2-yl)propanato]zinc(II)], [Zn(C₁₀H₈N₂O₂)]_n, (**1**), and poly[bis[μ_2 -3-(1*H*-benzimidazol-2-yl)propanato]cadmium(II)], [Cd(C₁₀H₈N₂O₂)₂]_n, (**2**) have been synthesized from 3-(1*H*-benzimidazol-2-yl)propanoic acid ligands through a mixed-ligand synthetic strategy under a solvothermal environment, and studied by single-crystal X-ray diffraction. Complex **1** crystallizes in the orthorhombic space group *Pbca* and features a two-dimensional structure formed by a binuclear Zn₂O₄ core. Complex **2**, however, crystallizes in the monoclinic space group *P2₁/c* and forms a one-dimensional chain structure. The Zn^{II} and Cd^{II} ions have different coordination numbers and the 3-(1*H*-benzimidazol-2-yl)propanoate ligands display different coordination modes. The structures reported here show the importance of the selection of metal ions and suitable ligands.

1. Chemical context

The structures of coordination polymers are strongly influenced by the organic ligands and metal ions and it is important to choose suitable ligands and metal ions under appropriate synthetic conditions to synthesize coordination complexes with interesting structures. The exploration of metal–organic frameworks (MOFs) have received much attention because of their intriguing architectures and wide range of potential applications in different fields (Castellanos *et al.*, 2016; Zhang *et al.*, 2016; Kumar *et al.*, 2015; Liu *et al.*, 2016; Müller-Buschbaum *et al.*, 2015; Duerinck & Denayer, 2015; Mohan *et al.*, 2015). The assembly of Zn^{II} (Jurcic *et al.*, 2015; Karmakar *et al.*, 2016*a,b*; Liang *et al.*, 2016; Wannapaiboon *et al.*, 2015; Ying *et al.*, 2015) and Cd^{II} (Xiao *et al.*, 2015; Wu *et al.*, 2011; Hu *et al.*, 2015; Cao *et al.*, 2014; Zhang *et al.*, 2015) ions with multidentate nitrogen-containing ligands has produced various MOFs with fascinating structures and luminescent properties. The selection of chelating or bridging organic linkers often favors a structure-specific assembly and the factors that govern the formation of such complexes are complicated and include not only the nature of the Zn^{II} and Cd^{II} ions and ligand structure but also anion-directed interactions as well as reaction conditions. In order to explore the coordination chemistry of this type of ligand, 3-(1*H*-benzimidazol-2-yl)propanoic acid (H₂BIP) was chosen in the present study to construct new coordination polymers. A two-



dimensional Zn^{II} polymer and a one-dimensional Cd^{II} coordination polymer have been obtained.

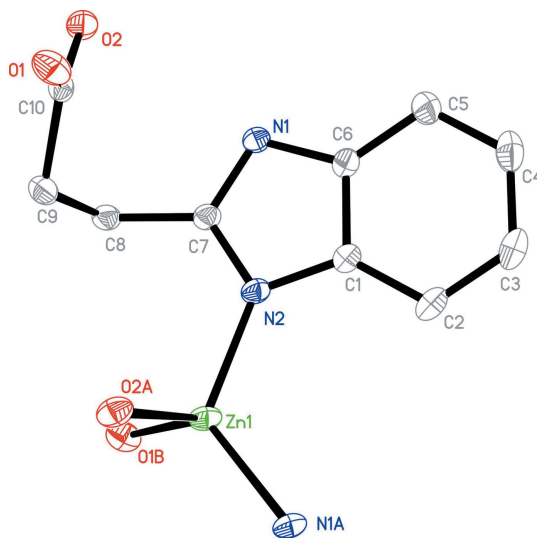
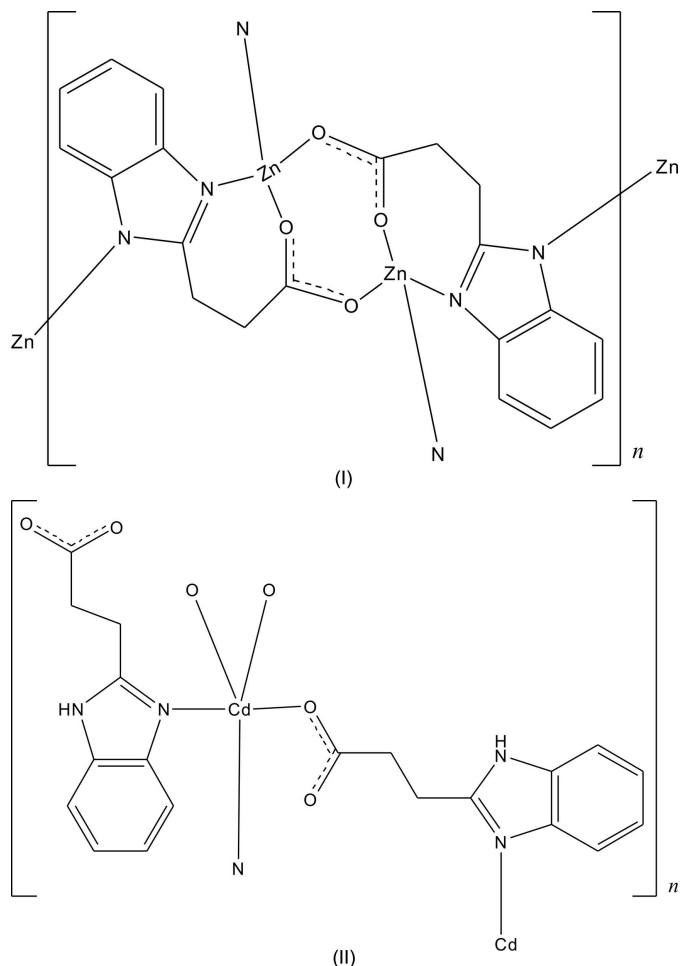


Figure 1

The asymmetric unit of **1**, with additional symmetry-related atoms. The displacement ellipsoids are drawn at the 30% probability level [symmetry codes: (A) $-x + \frac{3}{2}, y + \frac{1}{2}, z$; (B) $x - \frac{1}{2}, -y + \frac{1}{2}, -z$].

3-(1 λ^2 -benzoimidazol-2-yl)propanoate anion. All the Zn–N/O bond distances [Zn–O: 1.9563 (16)–2.0208 (17) and Zn–N: 1.9624 (18)–1.9661 (16) Å] and the bond angles around Zn1 [99.22 (6)–120.28 (7)°] fall into the normal range. Each 3-(1 λ^2 -benzoimidazol-2-yl)propanoate anion shows a tridentate chelating mode bridging three Zn^{II} ions with the Zn \cdots Zn distances of 4.066 (1), 5.870 (2) and 6.965 (2) Å. Zn1 and the symmetry-related Zn1 are bridged by O1 and O2 forming a binuclear Zn_2 cluster. Adjacent clusters are connected by a Zn–N bond of 1.9661 (16) Å to generate 2D square-grid (4,4) layers (Fig. 2).

2. Structural commentary

Complex **1** crystallizes in the orthorhombic crystal system in the centrosymmetric space group $Pbca$. The 3-(1*H*-benzoimidazol-2-yl)propanoic acid ligand deprotonates completely when bonding to Zn^{II} ions. The asymmetric unit of **1** consists of one Zn^{II} ion and one 3-(1 λ^2 -benzoimidazol-2-yl)propanoate anion. Geometric parameters are given in Table 1. As shown in Fig. 1, the Zn^{II} ion has a tetrahedral ZnO_2N_2 environment completed by N2 from one 3-(1 λ^2 -benzoimidazol-2-yl)propanoate anion, O2($-x + \frac{3}{2}, y + \frac{1}{2}, z$) and N1($-x + \frac{3}{2}, y + \frac{1}{2}, z$) from the second 3-(1 λ^2 -benzoimidazol-2-yl)propanoate anion and O1($x - \frac{1}{2}, -y + \frac{1}{2}, -z$) from the third

Table 1
Selected geometric parameters (Å, °) for **1**.

Zn1–O1 ⁱ	1.9563 (16)	Zn1–N2	1.9661 (16)
Zn1–N1 ⁱⁱ	1.9624 (18)	Zn1–O2 ⁱⁱ	2.0208 (17)
O1 ⁱ –Zn1–N1 ⁱⁱ	118.50 (7)	O1 ⁱ –Zn1–O2 ⁱⁱ	105.15 (6)
O1 ⁱ –Zn1–N2	106.84 (7)	N1 ⁱⁱ –Zn1–O2 ⁱⁱ	99.22 (6)
N1 ⁱⁱ –Zn1–N2	120.28 (7)	N2–Zn1–O2 ⁱⁱ	104.42 (6)

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

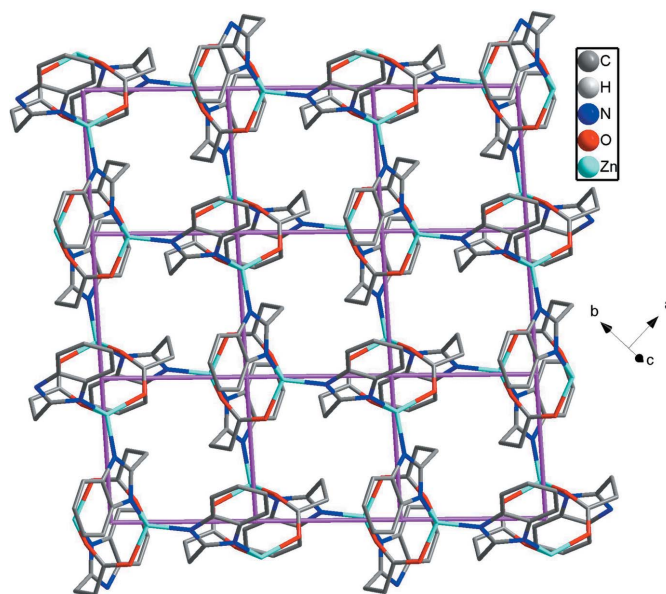


Figure 2

A perspective view of the 4-connected nodes in **1**.

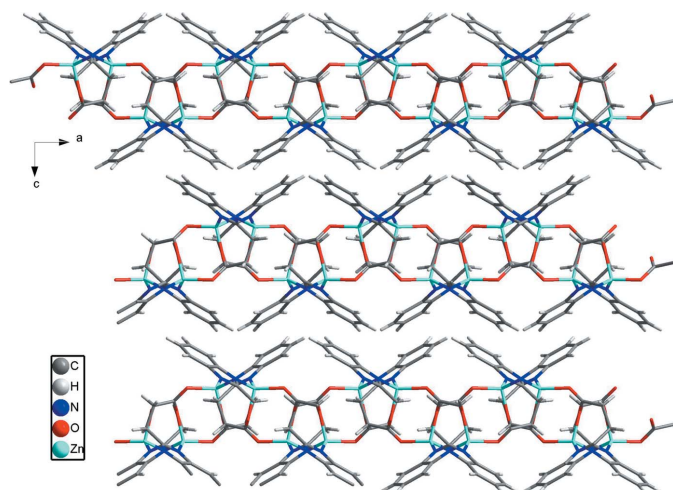


Figure 3
View of the three-dimensional framework of **1** formed by two-dimensional undulating sheets and van der Waals forces.

As there are no classical hydrogen bonds in **1**, these layers are packed by normal van der Waals forces into an extended 3D framework (Fig. 3).

Complex **2** crystallizes in the monoclinic crystal system in the centrosymmetric space group $P2_1/c$. The 3-(1*H*-benzimidazol-2-yl)propanoic acid ligands do not deprotonate completely when bonding to Cd^{II} ions. Geometric parameters are given in Table 2. As shown in Fig. 4, the Cd^{II} ion is five-coordinated by N3 from one 3-(1*H*-benzimidazol-2-yl)propanoate anion, N1($x, y - 1, z$) from the second 3-(1*H*-benzimidazol-2-yl)propanoate anion, O1 from the third and O3($-x, -y, -z + 1$) and O4($-x, -y, -z + 1$) from the fourth. All the Cd–N/O bond distances [Cd–O: 2.285 (2)–2.362 (2) and Cd–N: 2.262 (3)–2.271 (3) Å] and the bond angles around Cd1 [55.44 (9)–146.52 (9)°] fall into the normal range. A distance of 2.667 (2) Å between Cd1 and O2 indicates the existence of a weak interaction between them. Two HBIP[−] anions connects two Cd^{II} ions with one bidentate carboxylate and one N atom forming end-to-end binuclear Cd_2 cluster with

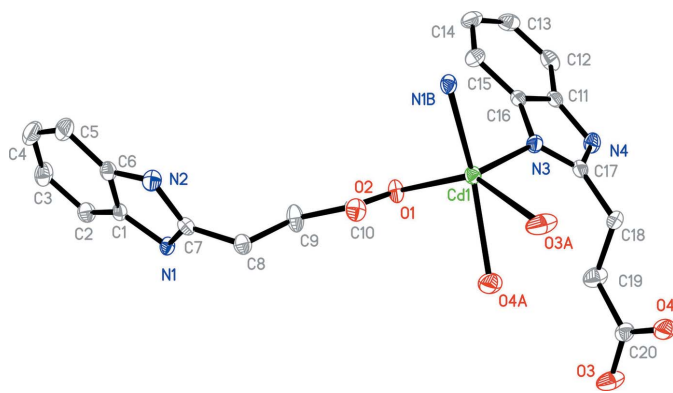


Figure 4
The asymmetric unit of **2**, with additional symmetry-related atoms. The displacement ellipsoids are drawn at the 30% probability level [symmetry codes: (A) $-x, -y, -z + 1$; (B) $x, y - 1, z$].

Table 2
Selected geometric parameters (Å, °) for **2**.

Cd1–N1 ⁱ	2.262 (3)	Cd1–O3 ⁱⁱⁱ	2.293 (2)
Cd1–N3	2.271 (3)	Cd1–O4 ⁱⁱ	2.362 (2)
Cd1–O1	2.285 (2)		
N1 ⁱ –Cd1–N3	103.73 (10)	O1–Cd1–O3 ⁱⁱⁱ	144.01 (9)
N1 ⁱ –Cd1–O1	106.08 (9)	N1 ⁱ –Cd1–O4 ⁱⁱ	146.52 (9)
N3–Cd1–O1	93.38 (9)	N3–Cd1–O4 ⁱⁱ	104.51 (10)
N1 ⁱ –Cd1–O3 ⁱⁱⁱ	100.41 (9)	O1–Cd1–O4 ⁱⁱ	89.85 (8)
N3–Cd1–O3 ⁱⁱⁱ	103.63 (10)	O3 ⁱⁱⁱ –Cd1–O4 ⁱⁱ	55.44 (9)

Symmetry codes: (i) $x, y - 1, z$; (ii) $-x, -y, -z + 1$.

Table 3
Hydrogen-bond geometry (Å, °) for **2**.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2–H2A \cdots O2 ⁱⁱⁱ	0.86	2.10	2.823 (4)	141
N4–H4A \cdots O1 ^{iv}	0.86	2.03	2.862 (4)	161

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

a distance of 7.274 (1) Å. The other two HBIP[−] anions act as bridges to join two neighboring binuclear Cd_2 clusters with one monodentate carboxylate and one N atom to generate 1D ladders along the b -axis direction (Fig. 5). In the crystal, N–H \cdots O hydrogen bonds (Table 3) and π – π interactions involving the imidazole rings and benzimidazole ring systems with centroid–centroid distances of 3.569 (2) and 3.838 (2) Å connect the 1D ladders along a - and c -axis directions into an extended 3D framework (Fig. 6). Although there are large potential voids within the 1D ladders (7.274×8.025 Å based on the distances of the Cd^{II} ions), they are interblocked by adjacent ladders.

3. Supramolecular features

The structures and the coordination modes of complexes **1** and **2** are quite different, which may be ascribed to a diverse metal coordination habit. The crystal structure of a Zn^{II} complex based on H_2BIP is reported for the first time. In a comparison with its counterparts based on similar benzimidazole carboxylic acids ligands, benzimidazole-2-butanoic acid (H_2BIB) and 2-(1*H*-benzimidazol-2-ylthio)acetic acid (H_2BITA), the

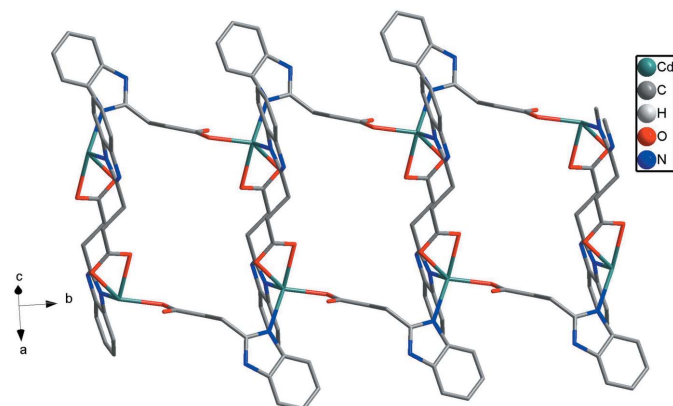


Figure 5
A view of the one-dimensional ladders in **2**.

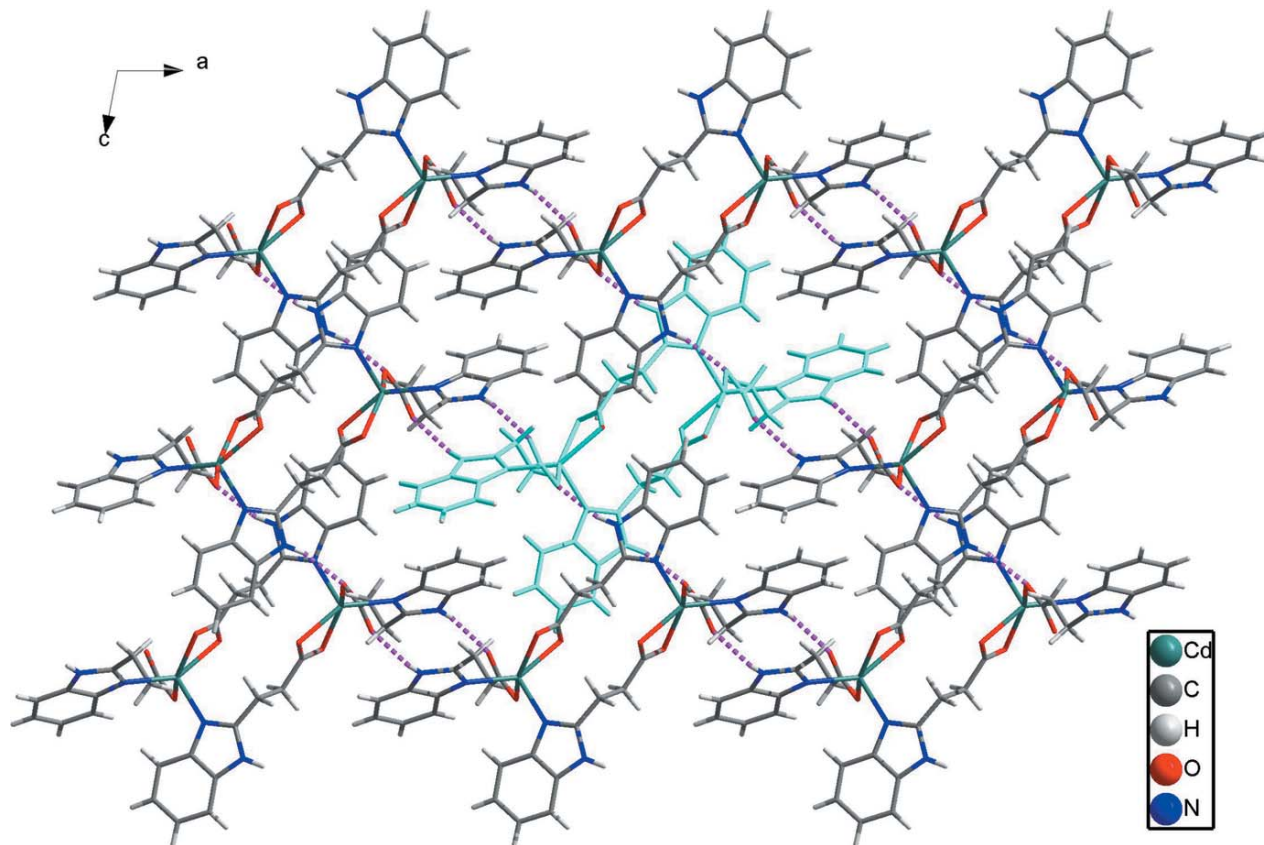


Figure 6

A perspective view of the three-dimensional frameworks in **2** formed by one-dimensional ladders and N–H···O hydrogen bonds (Table 3). The hydrogen bonds are shown as dashed lines.

same coordination modes are found for **1** ($\mu_3\text{-}\kappa\text{N},\text{O}:\kappa\text{O}':\kappa\text{N}'$ mode, $\mu_3\text{-BIP}^{2-}$) and $[\text{Zn}(\text{BIB})]_n$ ($\mu_3\text{-}\kappa\text{N},\text{O}:\kappa\text{O}':\kappa\text{N}'$ mode, $\mu_3\text{-BIP}^{2-}$; Zhang *et al.*, 2015) and different coordination modes are found for **1** and $[\text{Zn}_2(\text{HBITA})_4]\cdot(\text{DMF})_2\cdot(\text{H}_2\text{O})_2$ ($\mu_2\text{-}\kappa\text{N}:\kappa\text{O}$ mode, $\mu_2\text{-HBITA}^-$ and $\mu_1\text{-}\kappa\text{N},\text{O}$ mode, $\mu_1\text{-HBITA}^-$; Yu *et al.*, 2010), $[\text{Zn}_2(\text{HBITA})_4]_n$ ($\mu_2\text{-}\kappa\text{N}:\kappa\text{O}$ mode, $\mu_2\text{-HBITA}^-$; Yu *et al.*, 2010). Different dimensionalities, like 2D for **1**, 3D for $[\text{Zn}(\text{BIB})]_n$, 0D for $[\text{Zn}_2(\text{HBITA})_4]\cdot(\text{DMF})_2\cdot(\text{H}_2\text{O})_2$ and 2D for $[\text{Zn}_2(\text{HBITA})_4]_n$ are also found. Cd^{II} complexes based on H_2BIP have already been observed with the appropriate Et_3N reagent in a $\text{EtOH}/\text{H}_2\text{O}$ mixed solvent. By selection of the $\text{EtOH}/\text{H}_2\text{O}$ mixed solvent without any basic reagent, complex **2** was obtained with a relatively simple coordination mode ($\mu_2\text{-}\kappa\text{N}:\kappa\text{O},\text{O}'$ mode, $\mu_2\text{-HBIP}^-$) in comparison with diverse modes in $[\text{Cd}_5\text{Cl}_2(\text{HBIP})_4(\text{BIP})_2]\cdot 4\text{DMF}]_n$ ($\mu_2\text{-}\kappa\text{N},\text{O}:\kappa\text{O},\text{O}'$ mode, $\mu_2\text{-HBIP}^-$, $\mu_3\text{-}\kappa\text{N},\text{O}:\kappa\text{O},\text{O}':\kappa\text{N}'$ mode, $\mu_3\text{-BIP}^{2-}$, $\mu_3\text{-}\kappa\text{N},\text{O}:\kappa\text{O},\text{O}':\kappa\text{O}'$ mode, $\mu_3\text{-HBIP}^-$; Zheng *et al.*, 2012) and $[\text{Cd}_3(\text{HBIP})_2(\text{BIP})_2]_n$ ($\mu_3\text{-}\kappa\text{N},\text{O}:\kappa\text{O},\text{O}':\kappa\text{O}'$ mode, $\mu_3\text{-BIP}^{2-}$, $\mu_4\text{-}\kappa\text{N},\text{O}:\kappa\text{O}:\kappa\text{O}':\kappa\text{O}'$ mode, $\mu_4\text{-HBIP}^-$; Zheng *et al.*, 2012). In comparison with its counterpart based on similar benzimidazole carboxylic acids, H_2BIB , the same coordination modes are found for **2** and $[\text{Cd}(\text{HBIB})_2]_n\cdot(\text{H}_2\text{O})_n$ ($\mu_2\text{-}\kappa\text{N}:\kappa\text{O},\text{O}'$ mode, $\mu_2\text{-HBIB}^-$; Zhang *et al.*, 2015). Different dimensionalities, such as 1D for **2**, 2D for $[\text{Cd}_5\text{Cl}_2(\text{HBIP})_4(\text{BIP})_2]\cdot 4\text{DMF}]_n$, 1D for $[\text{Cd}_3(\text{HBIP})_2(\text{BIP})_2]_n$ and 2D for $[\text{Cd}(\text{HBIB})_2]_n\cdot(\text{H}_2\text{O})_n$ were

also found. The different coordination modes and dimensionalities show the important roles of spacer lengths and flexibilities of ligands. The crystal structures reported here and before show that ligands containing both flexible carboxylic and benzimidazole groups are suitable for the construction of coordination polymers with interesting structures, adopting diverse coordination modes. The significant effect of metal ions, spacer length and flexibility of ligands on the structural assemblies of such crystalline materials is critical to the assemblies of MOFs in some particular systems.

4. Database Survey

Complexes with benzimidazole-based carboxylic acid, for example, 1*H*-benzimidazole-2-carboxylic acid (Xia *et al.*, 2013; Qiao *et al.*, 2013; Małeckı & Maroń, 2012; Machura *et al.*, 2014; Fernández *et al.*, 2016) and 3-(1*H*-benzimidazole-2-yl) propanoic acid (Liu *et al.*, 2015) have been reported. A limited number of coordination polymers constructed from 3-(1*H*-benzimidazol-2-yl) propanoic acid (H_2BIP) have been reported including $[\text{Cd}_3(\text{HBIP})_2(\text{BIP})_2]_n$ and $[\text{Cd}_5\text{Cl}_2(\text{BIP})_4(\text{BIP})_2]_n$ (Zheng *et al.*, 2012). $[\text{Cd}_3(\text{HBIP})_2(\text{BIP})_2]_n$ presents a fascinating one-dimensional structure with helical character, made of four helical chains weaving together in two reverse orientations. $[\text{Cd}_5\text{Cl}_2(\text{BIP})_4(\text{BIP})_2]$ exhibits a distinct (4,4) network and infinite pentanuclear secondary building units.

Table 4
Experimental details.

	1	2
Crystal data		
Chemical formula	[Zn(C ₁₀ H ₈ N ₂ O ₂)]	[Cd(C ₁₀ H ₈ N ₂ O ₂) ₂]
<i>M_r</i>	253.55	490.79
Crystal system, space group	Orthorhombic, <i>Pbca</i>	Monoclinic, <i>P2₁/c</i>
Temperature (K)	296	293
<i>a</i> , <i>b</i> , <i>c</i> (Å)	8.956 (4), 10.697 (5), 20.331 (9)	13.6708 (6), 8.0253 (3), 17.3834 (7)
α , β , γ (°)	90, 90, 90	90, 100.972 (4), 90
<i>V</i> (Å ³)	1947.8 (15)	1872.31 (13)
<i>Z</i>	8	4
Radiation type	Mo <i>K</i> α	Mo <i>K</i> α
μ (mm ⁻¹)	2.50	1.20
Crystal size (mm)	0.28 × 0.25 × 0.21	0.28 × 0.25 × 0.19
Data collection		
Diffractometer	Bruker SMART CCD area-detector	Bruker SMART CCD area-detector
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2012)	Multi-scan (<i>SADABS</i> ; Bruker, 2012)
<i>T</i> _{min} , <i>T</i> _{max}	0.541, 0.622	0.923, 1.000
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	9832, 1725, 1525	6654, 3289, 2685
<i>R</i> _{int}	0.046	0.029
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.595	0.595
Refinement		
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.024, 0.063, 1.03	0.031, 0.064, 1.06
No. of reflections	1725	3289
No. of parameters	136	262
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.29, -0.56	0.33, -0.48

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXL2014* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009), *DIAMOND* (Brandenburg, 2008), *pubCIF* (Westrip, 2010) and *PLATON* (Spek, 2009).

5. Synthesis and crystallization

3-(1*H*-Benzimidazol-2-yl)propanoic acid (H₂BIP) was prepared by a literature method (Delval *et al.*, 2008). Other reagents and solvents used in the reactions were purchased from Aladdin-Chemical and used without purification.

5.1. Preparation of 1

H₂BIP (0.02 mmol, 0.038 g) and Zn(NO₃)₂·6H₂O (0.2 mmol, 0.060 g) were dissolved in EtOH/H₂O (1:1 *v/v*, 8 ml) mixed solvent. The mixture was sealed in a closed vessel and heated at 413 K for 72 h; the mixture was then cooled slowly to room temperature at a rate of 2 K h⁻¹. Many pale-yellow block-shaped crystals were collected.

5.2. Preparation of 2

H₂BIP (0.02 mmol, 0.038 g), Cd(CH₃COO)₂·2H₂O (0.2 mmol, 0.053 g) were dissolved in EtOH/H₂O (1:1 *v/v*, 8 ml) mixed solvent. The mixture was sealed in a closed vessel and heated at 413 K for 72 h; the mixture was then cooled slowly to room temperature at a rate of 2 K h⁻¹. Many brown prismatic crystals were collected.

5.3. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. H atoms on N atoms were found in the difference-Fourier map and were refined

isotropically while restraining the N–H distances to 0.86 Å. Other H atoms were generated geometrically and were allowed to ride on their parent atoms in the riding-model approximation, with C–H = 0.93 Å, *U*_{iso}(H) = 1.2*U*_{eq}(C)(aromatic) and C–H = 0.97 Å, *U*_{iso}(H) = 1.5*U*_{eq}(C) for methyl hydrogen atoms.

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References

- Brandenburg, K. (2008). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
 Bruker (2012). *APEX2*, *SADABS*, *SMART* and *SAINT*. Bruker AXS inc., Madison, Wisconsin, USA.
 Cao, T. T., Peng, Y. Q., Liu, T., Wang, S. N., Dou, J. M., Li, Y. W., Zhou, C. H., Li, D. C. & Bai, J. F. (2014). *CrystEngComm*, **16**, 10658–10673.

- Castellanos, S., Goulet-Hanssens, A., Zhao, F. L., Dikhtiarenko, A., Pustovarenko, A., Hecht, S., Gascon, J., Kapteijn, F. & Bléger, D. (2016). *Chem. Eur. J.* **22**, 746–752.
- Delval, F., Spyrtou, A., Verdán, S., Bernardinelli, G. & Williams, A. F. (2008). *New J. Chem.* **32**, 1394–1402.
- Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
- Duerinck, T. & Denayer, J. F. M. (2015). *Chem. Eng. Sci.* **124**, 179–187.
- Fernández, B., Gómez-Vílchez, A., Sánchez-González, C., Bayón, J., San Sebastián, E., Gómez-Ruiz, S., López-Chaves, C., Aranda, P., Llopis, J. & Rodríguez-Diéguez, A. (2016). *New J. Chem.* **40**, 5387–5393.
- Hu, Y. J., Yang, J., Liu, Y. Y., Song, S. Y. & Ma, J. F. (2015). *Cryst. Growth Des.* **15**, 3822–3831.
- Jurcic, M., Peveler, W. J., Savory, C. N., Scanlon, D. O., Kenyon, A. J. & Parkin, I. P. (2015). *J. Mater. Chem. A*, **3**, 6351–6359.
- Karmakar, A., Martins, L., Hazra, S., Guedes da Silva, M. F. C. & Pombeiro, A. J. L. (2016a). *Cryst. Growth Des.* **16**, 1837–1849.
- Karmakar, A., Rúbio, G., Guedes da Silva, M. F. C., Ribeiro, A. P. C. & Pombeiro, A. J. L. (2016b). *RSC Adv.* **6**, 89007–89018.
- Kumar, P., Deep, A. & Kim, K. H. (2015). *TrAC Trends Anal. Chem.* **73**, 39–53.
- Liang, F.-L., Ma, D.-Y. & Qin, L. (2016). *Acta Cryst.* **C72**, 373–378.
- Liu, X. B., Lin, H., Xiao, Z. Y., Fan, W. D., Huang, A., Wang, R. M., Zhang, L. L. & Sun, D. F. (2016). *Dalton Trans.* **45**, 3743–3749.
- Liu, Z., Zheng, S. & Feng, S. (2015). *Acta Cryst.* **E71**, m5–m6.
- Machura, B., Wolff, M., Benoist, E., Schachner, J. A., Mösch-Zanetti, N. C., Takao, K. & Ikeda, Y. (2014). *Polyhedron*, **69**, 205–218.
- Małecki, J. G. & Maroń, A. (2012). *Polyhedron*, **40**, 125–133.
- Mohan, B., Yoon, C., Jang, S. & Park, K. H. (2015). *ChemCatChem*, **7**, 405–412.
- Müller-Buschbaum, K., Beuerle, F. & Feldmann, C. (2015). *Micro-porous Mesoporous Mater.* **216**, 171–199.
- Qiao, C. F., Xia, Z. Q., Wei, Q., Zhou, C. S., Zhang, G. C., Chen, S. P. & Gao, S. L. (2013). *J. Coord. Chem.* **66**, 1202–1210.
- Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
- Wannapaiboon, S., Tu, M., Sumida, K., Khaletskaya, K., Furukawa, S., Kitagawa, S. & Fischer, R. A. (2015). *J. Mater. Chem. A*, **3**, 23385–23394.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
- Wu, H., Liu, H. Y., Yang, J., Liu, B., Ma, J. F., Liu, Y. Y. & Liu, Y. Y. (2011). *Cryst. Growth Des.* **11**, 2317–2324.
- Xia, Z. Q., Wei, Q., Yang, Q., Qiao, C. F., Chen, S. P., Xie, G., Zhang, G. C., Zhou, C. S. & Gao, S. L. (2013). *CrystEngComm*, **15**, 86–99.
- Xiao, Y. J., Liu, F. H., Zhao, L. & Su, Z. M. (2015). *Inorg. Chem. Commun.* **59**, 32–35.
- Ying, S.-M., Ru, J.-J. & Luo, W.-K. (2015). *Acta Cryst.* **C71**, 618–622.
- Yu, Q., Zeng, Y.-F., Zhao, J.-P., Yang, Q. & Bu, X.-H. (2010). *Cryst. Growth Des.* **10**, 1878–1884.
- Zhang, Y., Du, Z. & Luo, X. (2015). *Z. Anorg. Allg. Chem.* **641**, 2637–2640.
- Zhang, Z. Y., Yoshikawa, H. & Awaga, K. (2016). *Chem. Mater.* **28**, 1298–1303.
- Zheng, S. R., Cai, S. L., Tan, J. B., Fan, J. & Zhang, W.-G. (2012). *Inorg. Chem. Commun.* **21**, 100–103.

supporting information

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Assembly of Zn^{II} and Cd^{II} coordination polymers with different dimensionalities based on the semi-flexible 3-(1*H*-benzimidazol-2-yl)propanoic acid ligand

Xiao-Yan Li, Yong-Qiong Peng, Juan Li, Wei-Wei Fu, Yang Liu and Yu-Ming Li

Computing details

For both structures, data collection: *APEX2* (Bruker, 2012). Cell refinement: *SAINTE* (Bruker, 2012) for (1); *SMART* (Bruker, 2012) for (2). For both structures, data reduction: *SAINTE* (Bruker, 2012); program(s) used to solve structure: *SHELXL2014* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009); molecular graphics: *DIAMOND* (Brandenburg, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010) and *PLATON* (Spek, 2009).

Poly[[μ_3 -3-(1*H*-benzimidazol-2-yl)propionato]zinc(II)] (1)

Crystal data

[Zn(C₁₀H₈N₂O₂)]

$M_r = 253.55$

Orthorhombic, *Pbca*

$a = 8.956$ (4) Å

$b = 10.697$ (5) Å

$c = 20.331$ (9) Å

$V = 1947.8$ (15) Å³

$Z = 8$

$F(000) = 1024$

$D_x = 1.729$ Mg m⁻³

Mo *K*α radiation, $\lambda = 0.71073$ Å

Cell parameters from 5004 reflections

$\theta = 3.0$ – 27.6°

$\mu = 2.50$ mm⁻¹

$T = 296$ K

Block, yellow

$0.28 \times 0.25 \times 0.21$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

phi and ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2012)

$T_{\min} = 0.541$, $T_{\max} = 0.622$

9832 measured reflections

1725 independent reflections

1525 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.046$

$\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 2.0^\circ$

$h = -10 \rightarrow 10$

$k = -12 \rightarrow 11$

$l = -24 \rightarrow 24$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.024$

$wR(F^2) = 0.063$

$S = 1.03$

1725 reflections

136 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0338P)^2 + 0.8648P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.29$ e Å⁻³

$\Delta\rho_{\min} = -0.56$ e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.61499 (3)	0.44565 (2)	0.08133 (2)	0.02929 (11)
C1	0.8742 (2)	0.31428 (19)	0.14864 (9)	0.0272 (4)
C2	0.9402 (3)	0.4128 (2)	0.18261 (10)	0.0361 (5)
H2	0.8972	0.4919	0.1832	0.043*
C3	1.0712 (3)	0.3886 (2)	0.21531 (12)	0.0487 (6)
H3	1.1175	0.4528	0.2384	0.058*
C4	1.1366 (3)	0.2704 (3)	0.21484 (13)	0.0512 (6)
H4	1.2268	0.2584	0.2366	0.061*
C5	1.0711 (3)	0.1710 (2)	0.18305 (11)	0.0402 (5)
H5	1.1136	0.0917	0.1837	0.048*
C6	0.9381 (2)	0.19494 (18)	0.14985 (9)	0.0278 (4)
C7	0.7378 (2)	0.18898 (16)	0.08956 (9)	0.0273 (4)
C8	0.6243 (2)	0.1407 (2)	0.04189 (11)	0.0326 (5)
H8A	0.5329	0.1886	0.0464	0.039*
H8B	0.6018	0.0542	0.0523	0.039*
C9	0.6791 (2)	0.14918 (19)	−0.02923 (10)	0.0347 (5)
H9A	0.6001	0.1208	−0.0582	0.042*
H9B	0.6992	0.2361	−0.0396	0.042*
C10	0.8184 (2)	0.07312 (18)	−0.04282 (10)	0.0296 (4)
N1	0.84880 (17)	0.11670 (14)	0.11236 (9)	0.0289 (4)
N2	0.74575 (17)	0.30823 (13)	0.10974 (8)	0.0268 (4)
O1	0.91054 (16)	0.11866 (15)	−0.08295 (7)	0.0373 (4)
O2	0.83644 (16)	−0.03094 (12)	−0.01494 (7)	0.0332 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.03268 (17)	0.01695 (16)	0.03822 (18)	0.00017 (8)	0.00399 (10)	0.00205 (9)
C1	0.0323 (10)	0.0252 (10)	0.0240 (10)	−0.0034 (8)	0.0028 (8)	0.0001 (8)
C2	0.0459 (12)	0.0284 (11)	0.0341 (12)	−0.0065 (9)	0.0030 (10)	−0.0084 (9)
C3	0.0548 (14)	0.0475 (14)	0.0437 (13)	−0.0116 (12)	−0.0098 (12)	−0.0148 (12)
C4	0.0507 (14)	0.0570 (16)	0.0460 (14)	−0.0032 (12)	−0.0209 (11)	−0.0069 (13)
C5	0.0438 (12)	0.0384 (12)	0.0382 (12)	0.0045 (10)	−0.0119 (10)	−0.0008 (10)
C6	0.0329 (10)	0.0256 (10)	0.0250 (9)	−0.0030 (8)	−0.0006 (8)	0.0009 (8)
C7	0.0290 (10)	0.0207 (10)	0.0323 (10)	−0.0013 (8)	−0.0003 (8)	0.0000 (8)
C8	0.0283 (10)	0.0235 (10)	0.0459 (13)	0.0017 (8)	−0.0070 (9)	−0.0045 (9)
C9	0.0337 (11)	0.0287 (11)	0.0416 (12)	0.0044 (8)	−0.0113 (9)	−0.0002 (9)
C10	0.0326 (11)	0.0226 (10)	0.0336 (11)	−0.0011 (8)	−0.0119 (9)	−0.0037 (8)
N1	0.0332 (9)	0.0177 (8)	0.0360 (9)	0.0000 (7)	−0.0054 (7)	−0.0009 (7)

N2	0.0294 (9)	0.0193 (8)	0.0317 (9)	-0.0009 (7)	0.0013 (7)	-0.0006 (7)
O1	0.0330 (8)	0.0327 (9)	0.0461 (9)	0.0019 (6)	-0.0032 (6)	0.0111 (7)
O2	0.0423 (8)	0.0211 (7)	0.0360 (8)	0.0020 (6)	-0.0053 (6)	0.0013 (6)

Geometric parameters (Å, °)

Zn1—O1 ⁱ	1.9563 (16)	C6—N1	1.386 (3)
Zn1—N1 ⁱⁱ	1.9624 (18)	C7—N2	1.342 (2)
Zn1—N2	1.9661 (16)	C7—N1	1.342 (2)
Zn1—O2 ⁱⁱ	2.0208 (17)	C7—C8	1.496 (3)
C1—C2	1.392 (3)	C8—C9	1.530 (3)
C1—N2	1.398 (2)	C8—H8A	0.9700
C1—C6	1.399 (3)	C8—H8B	0.9700
C2—C3	1.374 (3)	C9—C10	1.515 (3)
C2—H2	0.9300	C9—H9A	0.9700
C3—C4	1.393 (4)	C9—H9B	0.9700
C3—H3	0.9300	C10—O1	1.259 (3)
C4—C5	1.375 (3)	C10—O2	1.260 (2)
C4—H4	0.9300	N1—Zn1 ⁱⁱⁱ	1.9624 (18)
C5—C6	1.393 (3)	O1—Zn1 ^{iv}	1.9563 (16)
C5—H5	0.9300	O2—Zn1 ⁱⁱⁱ	2.0207 (17)
O1 ⁱ —Zn1—N1 ⁱⁱ	118.50 (7)	N2—C7—C8	124.22 (17)
O1 ⁱ —Zn1—N2	106.84 (7)	N1—C7—C8	121.86 (16)
N1 ⁱⁱ —Zn1—N2	120.28 (7)	C7—C8—C9	111.96 (17)
O1 ⁱ —Zn1—O2 ⁱⁱ	105.15 (6)	C7—C8—H8A	109.2
N1 ⁱⁱ —Zn1—O2 ⁱⁱ	99.22 (6)	C9—C8—H8A	109.2
N2—Zn1—O2 ⁱⁱ	104.42 (6)	C7—C8—H8B	109.2
C2—C1—N2	131.70 (19)	C9—C8—H8B	109.2
C2—C1—C6	120.56 (19)	H8A—C8—H8B	107.9
N2—C1—C6	107.74 (16)	C10—C9—C8	113.88 (16)
C3—C2—C1	117.4 (2)	C10—C9—H9A	108.8
C3—C2—H2	121.3	C8—C9—H9A	108.8
C1—C2—H2	121.3	C10—C9—H9B	108.8
C2—C3—C4	121.8 (2)	C8—C9—H9B	108.8
C2—C3—H3	119.1	H9A—C9—H9B	107.7
C4—C3—H3	119.1	O1—C10—O2	123.33 (19)
C5—C4—C3	121.7 (2)	O1—C10—C9	116.77 (18)
C5—C4—H4	119.1	O2—C10—C9	119.89 (19)
C3—C4—H4	119.1	C7—N1—C6	105.65 (16)
C4—C5—C6	116.7 (2)	C7—N1—Zn1 ⁱⁱⁱ	123.27 (13)
C4—C5—H5	121.6	C6—N1—Zn1 ⁱⁱⁱ	130.11 (13)
C6—C5—H5	121.6	C7—N2—C1	105.11 (15)
N1—C6—C5	130.48 (19)	C7—N2—Zn1	126.10 (13)
N1—C6—C1	107.75 (17)	C1—N2—Zn1	128.46 (13)
C5—C6—C1	121.75 (18)	C10—O1—Zn1 ^{iv}	117.83 (13)
N2—C7—N1	113.75 (17)	C10—O2—Zn1 ⁱⁱⁱ	124.96 (13)

N2—C1—C2—C3	-178.1 (2)	N2—C7—N1—Zn1 ⁱⁱⁱ	-170.56 (13)
C6—C1—C2—C3	1.8 (3)	C8—C7—N1—Zn1 ⁱⁱⁱ	4.9 (3)
C1—C2—C3—C4	0.0 (4)	C5—C6—N1—C7	-177.4 (2)
C2—C3—C4—C5	-1.8 (4)	C1—C6—N1—C7	0.7 (2)
C3—C4—C5—C6	1.6 (4)	C5—C6—N1—Zn1 ⁱⁱⁱ	-8.6 (3)
C4—C5—C6—N1	178.1 (2)	C1—C6—N1—Zn1 ⁱⁱⁱ	169.47 (14)
C4—C5—C6—C1	0.2 (3)	N1—C7—N2—C1	0.6 (2)
C2—C1—C6—N1	179.73 (18)	C8—C7—N2—C1	-174.75 (18)
N2—C1—C6—N1	-0.4 (2)	N1—C7—N2—Zn1	174.49 (13)
C2—C1—C6—C5	-2.0 (3)	C8—C7—N2—Zn1	-0.8 (3)
N2—C1—C6—C5	177.93 (18)	C2—C1—N2—C7	179.8 (2)
N2—C7—C8—C9	90.4 (2)	C6—C1—N2—C7	-0.1 (2)
N1—C7—C8—C9	-84.6 (2)	C2—C1—N2—Zn1	6.1 (3)
C7—C8—C9—C10	61.3 (2)	C6—C1—N2—Zn1	-173.81 (13)
C8—C9—C10—O1	-144.39 (18)	O2—C10—O1—Zn1 ^{iv}	-19.8 (3)
C8—C9—C10—O2	36.4 (3)	C9—C10—O1—Zn1 ^{iv}	160.95 (13)
N2—C7—N1—C6	-0.8 (2)	O1—C10—O2—Zn1 ⁱⁱⁱ	108.7 (2)
C8—C7—N1—C6	174.63 (18)	C9—C10—O2—Zn1 ⁱⁱⁱ	-72.1 (2)

Symmetry codes: (i) $x-1/2, -y+1/2, -z$; (ii) $-x+3/2, y+1/2, z$; (iii) $-x+3/2, y-1/2, z$; (iv) $x+1/2, -y+1/2, -z$.

Poly[bis[μ_2 -3-(1*H*-benzimidazol-2-yl)propionato]cadmium(II)] (2)

Crystal data

[Cd(C₁₀H₈N₂O₂)₂]

$M_r = 490.79$

Monoclinic, $P2_1/c$

$a = 13.6708$ (6) Å

$b = 8.0253$ (3) Å

$c = 17.3834$ (7) Å

$\beta = 100.972$ (4)°

$V = 1872.31$ (13) Å³

$Z = 4$

$F(000) = 984$

$D_x = 1.741$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2660 reflections

$\theta = 3.0$ – 27.4 °

$\mu = 1.20$ mm⁻¹

$T = 293$ K

Prism, brown

$0.28 \times 0.25 \times 0.19$ mm

Data collection

Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

ϕ and ω scans

Absorption correction: multi-scan

(SADABS; Bruker, 2012)

$T_{\min} = 0.923$, $T_{\max} = 1.000$

6654 measured reflections

3289 independent reflections

2685 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.029$

$\theta_{\max} = 25.0$ °, $\theta_{\min} = 2.4$ °

$h = -16 \rightarrow 15$

$k = -9 \rightarrow 6$

$l = -20 \rightarrow 14$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.064$

$S = 1.06$

3289 reflections

262 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0234P)^2]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$

$$\Delta\rho_{\max} = 0.33 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.48 \text{ e } \text{\AA}^{-3}$$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.22103 (2)	0.06562 (3)	0.41588 (2)	0.02433 (9)
C1	0.4463 (3)	1.0429 (4)	0.37316 (19)	0.0254 (8)
C2	0.4459 (3)	1.1926 (4)	0.33279 (19)	0.0343 (9)
H2	0.3890	1.2587	0.3224	0.041*
C3	0.5321 (3)	1.2403 (5)	0.3087 (2)	0.0442 (11)
H3	0.5337	1.3410	0.2825	0.053*
C4	0.6164 (3)	1.1402 (5)	0.3229 (2)	0.0503 (11)
H4	0.6734	1.1750	0.3056	0.060*
C5	0.6179 (3)	0.9902 (5)	0.3622 (2)	0.0444 (10)
H5	0.6740	0.9224	0.3710	0.053*
C6	0.5323 (3)	0.9465 (4)	0.3874 (2)	0.0298 (8)
C7	0.4118 (3)	0.8209 (4)	0.43435 (18)	0.0263 (8)
C8	0.3603 (3)	0.6815 (4)	0.46664 (19)	0.0305 (8)
H8A	0.3197	0.7255	0.5020	0.037*
H8B	0.4094	0.6069	0.4962	0.037*
C9	0.2949 (3)	0.5857 (4)	0.4010 (2)	0.0404 (10)
H9A	0.3250	0.5925	0.3548	0.048*
H9B	0.2308	0.6413	0.3886	0.048*
C10	0.2768 (3)	0.4031 (4)	0.4167 (2)	0.0261 (8)
C11	0.0502 (3)	-0.0701 (4)	0.18100 (19)	0.0274 (8)
C12	0.0484 (3)	-0.0730 (4)	0.1006 (2)	0.0373 (9)
H12	-0.0082	-0.1041	0.0648	0.045*
C13	0.1354 (3)	-0.0273 (4)	0.0773 (2)	0.0390 (10)
H13	0.1371	-0.0271	0.0241	0.047*
C14	0.2200 (3)	0.0185 (5)	0.1299 (2)	0.0397 (10)
H14	0.2769	0.0493	0.1113	0.048*
C15	0.2218 (3)	0.0193 (4)	0.2096 (2)	0.0336 (9)
H15	0.2790	0.0490	0.2452	0.040*
C16	0.1354 (3)	-0.0256 (4)	0.23458 (19)	0.0237 (8)
C17	0.0228 (3)	-0.0925 (4)	0.30217 (19)	0.0272 (8)
C18	-0.0301 (3)	-0.1297 (4)	0.3673 (2)	0.0333 (9)
H18A	0.0190	-0.1575	0.4136	0.040*
H18B	-0.0717	-0.2271	0.3534	0.040*
C19	-0.0936 (3)	0.0092 (5)	0.3873 (2)	0.0433 (10)
H19A	-0.1486	0.0260	0.3436	0.052*
H19B	-0.0544	0.1107	0.3937	0.052*

C20	-0.1353 (3)	-0.0190 (5)	0.4602 (2)	0.0317 (9)
O1	0.21406 (17)	0.3287 (3)	0.36487 (13)	0.0316 (6)
O2	0.32390 (18)	0.3331 (3)	0.47586 (13)	0.0309 (6)
O3	-0.1888 (2)	0.0912 (3)	0.48158 (15)	0.0504 (8)
O4	-0.1163 (2)	-0.1496 (3)	0.49775 (14)	0.0448 (7)
N1	0.3712 (2)	0.9617 (3)	0.40401 (15)	0.0242 (7)
N2	0.5075 (2)	0.8066 (3)	0.42631 (16)	0.0313 (7)
H2A	0.5466	0.7247	0.4426	0.038*
N3	0.1154 (2)	-0.0401 (3)	0.31043 (16)	0.0277 (7)
N4	-0.0197 (2)	-0.1100 (3)	0.22566 (16)	0.0323 (7)
H4A	-0.0800	-0.1408	0.2079	0.039*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02465 (15)	0.02141 (14)	0.02708 (15)	0.00049 (12)	0.00527 (10)	0.00198 (12)
C1	0.026 (2)	0.0254 (19)	0.0239 (17)	-0.0039 (16)	0.0022 (15)	-0.0025 (17)
C2	0.037 (2)	0.029 (2)	0.037 (2)	-0.0006 (18)	0.0046 (17)	0.0021 (19)
C3	0.051 (3)	0.040 (2)	0.042 (2)	-0.015 (2)	0.010 (2)	0.009 (2)
C4	0.039 (3)	0.061 (3)	0.054 (3)	-0.016 (2)	0.015 (2)	0.002 (3)
C5	0.026 (2)	0.048 (2)	0.059 (3)	-0.005 (2)	0.005 (2)	-0.005 (2)
C6	0.027 (2)	0.032 (2)	0.0278 (19)	-0.0043 (17)	-0.0002 (16)	-0.0042 (18)
C7	0.029 (2)	0.0229 (18)	0.0250 (18)	0.0007 (16)	0.0010 (15)	-0.0038 (16)
C8	0.035 (2)	0.0219 (18)	0.034 (2)	0.0000 (17)	0.0061 (17)	0.0028 (17)
C9	0.044 (3)	0.0257 (19)	0.045 (2)	-0.0080 (18)	-0.0073 (19)	0.009 (2)
C10	0.022 (2)	0.0234 (18)	0.035 (2)	0.0023 (16)	0.0105 (16)	0.0010 (18)
C11	0.031 (2)	0.0212 (18)	0.0298 (19)	-0.0004 (17)	0.0061 (16)	-0.0025 (17)
C12	0.051 (3)	0.030 (2)	0.027 (2)	0.0007 (19)	-0.0016 (18)	-0.0008 (18)
C13	0.052 (3)	0.040 (2)	0.027 (2)	0.010 (2)	0.0142 (19)	0.0035 (19)
C14	0.037 (2)	0.045 (2)	0.042 (2)	0.005 (2)	0.0196 (19)	0.002 (2)
C15	0.027 (2)	0.040 (2)	0.034 (2)	0.0014 (18)	0.0064 (17)	0.0027 (19)
C16	0.025 (2)	0.0212 (18)	0.0250 (18)	0.0012 (15)	0.0043 (15)	-0.0018 (16)
C17	0.033 (2)	0.0193 (18)	0.0300 (19)	-0.0023 (16)	0.0080 (16)	-0.0010 (16)
C18	0.032 (2)	0.0331 (19)	0.038 (2)	-0.0099 (18)	0.0142 (17)	-0.0029 (19)
C19	0.047 (3)	0.047 (2)	0.039 (2)	0.013 (2)	0.016 (2)	0.015 (2)
C20	0.024 (2)	0.038 (2)	0.033 (2)	-0.0041 (18)	0.0044 (17)	-0.003 (2)
O1	0.0296 (15)	0.0226 (12)	0.0384 (14)	-0.0051 (11)	-0.0042 (11)	0.0023 (12)
O2	0.0314 (15)	0.0244 (13)	0.0347 (13)	0.0038 (11)	0.0008 (11)	0.0087 (12)
O3	0.055 (2)	0.0548 (17)	0.0489 (16)	0.0248 (15)	0.0285 (15)	0.0199 (15)
O4	0.063 (2)	0.0349 (15)	0.0430 (16)	0.0055 (14)	0.0273 (14)	0.0078 (14)
N1	0.0207 (16)	0.0187 (14)	0.0324 (16)	-0.0001 (12)	0.0034 (12)	0.0043 (13)
N2	0.0227 (17)	0.0265 (15)	0.0426 (17)	0.0053 (14)	0.0004 (14)	0.0050 (15)
N3	0.0290 (18)	0.0281 (16)	0.0269 (16)	-0.0065 (14)	0.0073 (13)	-0.0028 (14)
N4	0.0273 (18)	0.0346 (17)	0.0331 (17)	-0.0078 (14)	0.0012 (14)	-0.0014 (16)

Geometric parameters (Å, °)

Cd1—N1 ⁱ	2.262 (3)	C10—O1	1.269 (4)
Cd1—N3	2.271 (3)	C11—N4	1.378 (4)
Cd1—O1	2.285 (2)	C11—C12	1.393 (5)
Cd1—O3 ⁱⁱ	2.293 (2)	C11—C16	1.393 (4)
Cd1—O4 ⁱⁱ	2.362 (2)	C12—C13	1.377 (5)
Cd1—O2	2.667 (2)	C12—H12	0.9300
Cd1—C20 ⁱⁱⁱ	2.667 (4)	C13—C14	1.382 (5)
Cd1—C10	2.813 (3)	C13—H13	0.9300
C1—C6	1.389 (5)	C14—C15	1.382 (5)
C1—C2	1.391 (4)	C14—H14	0.9300
C1—N1	1.406 (4)	C15—C16	1.382 (5)
C2—C3	1.377 (5)	C15—H15	0.9300
C2—H2	0.9300	C16—N3	1.401 (4)
C3—C4	1.389 (5)	C17—N3	1.316 (4)
C3—H3	0.9300	C17—N4	1.354 (4)
C4—C5	1.382 (5)	C17—C18	1.485 (4)
C4—H4	0.9300	C18—C19	1.495 (5)
C5—C6	1.371 (5)	C18—H18A	0.9700
C5—H5	0.9300	C18—H18B	0.9700
C6—N2	1.386 (4)	C19—C20	1.503 (5)
C7—N1	1.323 (4)	C19—H19A	0.9700
C7—N2	1.346 (4)	C19—H19B	0.9700
C7—C8	1.487 (4)	C20—O4	1.236 (4)
C8—C9	1.518 (4)	C20—O3	1.249 (4)
C8—H8A	0.9700	C20—Cd1 ⁱⁱ	2.667 (4)
C8—H8B	0.9700	O3—Cd1 ⁱⁱ	2.293 (2)
C9—C10	1.520 (4)	O4—Cd1 ⁱⁱ	2.362 (2)
C9—H9A	0.9700	N1—Cd1 ⁱⁱⁱ	2.262 (3)
C9—H9B	0.9700	N2—H2A	0.8600
C10—O2	1.239 (4)	N4—H4A	0.8600
N1 ⁱ —Cd1—N3	103.73 (10)	O2—C10—O1	123.4 (3)
N1 ⁱ —Cd1—O1	106.08 (9)	O2—C10—C9	120.6 (3)
N3—Cd1—O1	93.38 (9)	O1—C10—C9	115.9 (3)
N1 ⁱ —Cd1—O3 ⁱⁱ	100.41 (9)	O2—C10—Cd1	70.45 (18)
N3—Cd1—O3 ⁱⁱ	103.63 (10)	O1—C10—Cd1	52.94 (15)
O1—Cd1—O3 ⁱⁱ	144.01 (9)	C9—C10—Cd1	168.8 (2)
N1 ⁱ —Cd1—O4 ⁱⁱ	146.52 (9)	N4—C11—C12	132.8 (3)
N3—Cd1—O4 ⁱⁱ	104.51 (10)	N4—C11—C16	105.3 (3)
O1—Cd1—O4 ⁱⁱ	89.85 (8)	C12—C11—C16	121.8 (3)
O3 ⁱⁱ —Cd1—O4 ⁱⁱ	55.44 (9)	C13—C12—C11	116.2 (4)
N1 ⁱ —Cd1—O2	84.96 (8)	C13—C12—H12	121.9
N3—Cd1—O2	145.40 (8)	C11—C12—H12	121.9
O1—Cd1—O2	52.26 (7)	C12—C13—C14	122.5 (4)
O3 ⁱⁱ —Cd1—O2	107.64 (9)	C12—C13—H13	118.8
O4 ⁱⁱ —Cd1—O2	81.96 (8)	C14—C13—H13	118.8

N1 ⁱ —Cd1—C20 ⁱⁱ	124.62 (11)	C15—C14—C13	121.2 (4)
N3—Cd1—C20 ⁱⁱ	106.84 (10)	C15—C14—H14	119.4
O1—Cd1—C20 ⁱⁱ	116.79 (10)	C13—C14—H14	119.4
O3 ⁱⁱ —Cd1—C20 ⁱⁱ	27.87 (10)	C16—C15—C14	117.4 (4)
O4 ⁱⁱ —Cd1—C20 ⁱⁱ	27.60 (9)	C16—C15—H15	121.3
O2—Cd1—C20 ⁱⁱ	94.44 (9)	C14—C15—H15	121.3
N1 ⁱ —Cd1—C10	96.06 (9)	C15—C16—C11	120.9 (3)
N3—Cd1—C10	119.59 (10)	C15—C16—N3	130.4 (3)
O1—Cd1—C10	26.30 (8)	C11—C16—N3	108.6 (3)
O3 ⁱⁱ —Cd1—C10	128.08 (10)	N3—C17—N4	111.4 (3)
O4 ⁱⁱ —Cd1—C10	85.33 (9)	N3—C17—C18	125.4 (3)
O2—Cd1—C10	25.96 (8)	N4—C17—C18	123.3 (3)
C20 ⁱⁱ —Cd1—C10	106.94 (11)	C17—C18—C19	114.6 (3)
C6—C1—C2	119.6 (3)	C17—C18—H18A	108.6
C6—C1—N1	109.1 (3)	C19—C18—H18A	108.6
C2—C1—N1	131.3 (3)	C17—C18—H18B	108.6
C3—C2—C1	118.2 (4)	C19—C18—H18B	108.6
C3—C2—H2	120.9	H18A—C18—H18B	107.6
C1—C2—H2	120.9	C18—C19—C20	114.4 (3)
C2—C3—C4	120.9 (4)	C18—C19—H19A	108.7
C2—C3—H3	119.5	C20—C19—H19A	108.7
C4—C3—H3	119.5	C18—C19—H19B	108.7
C5—C4—C3	121.7 (4)	C20—C19—H19B	108.7
C5—C4—H4	119.2	H19A—C19—H19B	107.6
C3—C4—H4	119.2	O4—C20—O3	121.3 (3)
C6—C5—C4	116.6 (4)	O4—C20—C19	119.9 (3)
C6—C5—H5	121.7	O3—C20—C19	118.8 (3)
C4—C5—H5	121.7	O4—C20—Cd1 ⁱⁱ	62.30 (19)
C5—C6—N2	131.8 (4)	O3—C20—Cd1 ⁱⁱ	59.13 (18)
C5—C6—C1	123.0 (4)	C19—C20—Cd1 ⁱⁱ	176.2 (3)
N2—C6—C1	105.2 (3)	C10—O1—Cd1	100.76 (19)
N1—C7—N2	111.9 (3)	C10—O2—Cd1	83.59 (19)
N1—C7—C8	126.8 (3)	C20—O3—Cd1 ⁱⁱ	93.0 (2)
N2—C7—C8	120.9 (3)	C20—O4—Cd1 ⁱⁱ	90.1 (2)
C7—C8—C9	110.5 (3)	C7—N1—C1	105.5 (3)
C7—C8—H8A	109.5	C7—N1—Cd1 ⁱⁱⁱ	126.7 (2)
C9—C8—H8A	109.5	C1—N1—Cd1 ⁱⁱⁱ	127.2 (2)
C7—C8—H8B	109.5	C7—N2—C6	108.3 (3)
C9—C8—H8B	109.5	C7—N2—H2A	125.9
H8A—C8—H8B	108.1	C6—N2—H2A	125.9
C8—C9—C10	116.5 (3)	C17—N3—C16	106.3 (3)
C8—C9—H9A	108.2	C17—N3—Cd1	131.2 (2)
C10—C9—H9A	108.2	C16—N3—Cd1	121.4 (2)
C8—C9—H9B	108.2	C17—N4—C11	108.4 (3)
C10—C9—H9B	108.2	C17—N4—H4A	125.8
H9A—C9—H9B	107.3	C11—N4—H4A	125.8

Symmetry codes: (i) $x, y-1, z$; (ii) $-x, -y, -z+1$; (iii) $x, y+1, z$.

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N2—H2 <i>A</i> \cdots O2 ^{iv}	0.86	2.10	2.823 (4)	141
N4—H4 <i>A</i> \cdots O1 ^v	0.86	2.03	2.862 (4)	161

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