

**catena-Poly[[dinitratocadmium(II)]-  
 bis[ $\mu$ -bis(2-methyl-1*H*-imidazol-1-yl)-  
 methane- $\kappa^2N^3:N^{3'}$ ]]**

**Chuan-Ming Jin,\* Cai-Yuan Chen, Wei-Dong Wang and  
 Ling-Yan Wu**

Hubei Key Laboratory of Bioanalytical Techniques, Department of Chemistry and  
 Environmental Engineering, Hubei Normal University, Huangshi 435002, People's  
 Republic of China

Correspondence e-mail: cmjin@email.hbnu.edu.cn

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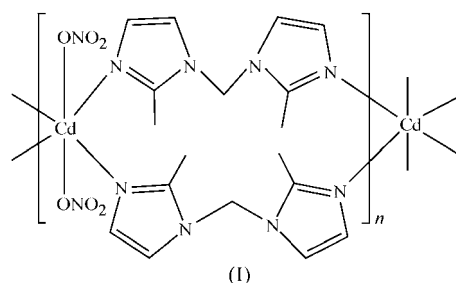
The title compound,  $[Cd(NO_3)_2(C_5H_{12}N_4)_2]_n$ , has a one-dimensional double-bridged chain polymer structure with a 16-membered macrometallacyclic tetragonal structural motif. The  $Cd^{II}$  ion occupies a crystallographic inversion centre and is coordinated by four equatorial N atoms from four distinct bis(2-methylimidazol-1-yl)methane ligands and two apical nitrate O atoms to form a slightly distorted octahedral coordination geometry.

**Comment**

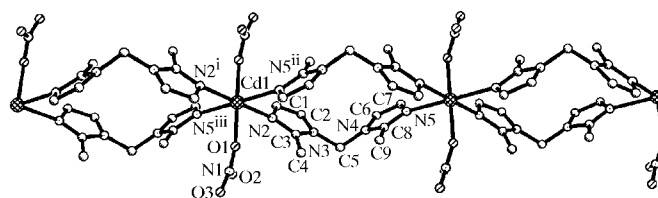
Coordination polymers have attracted a great deal of attention because of their intriguing structural properties and potential applications in magnetism, electrical conductivity, ion exchange, separation and catalysis (Carlucci *et al.*, 2003; Moulton & Zaworotko, 2001). Studies in this field have been focused on the design and construction of novel coordination frameworks and on the examination of the relationships between their structures and properties. Many coordination polymers with diverse architectures, such as linear or zigzag chains, helices, honeycombs, square grids, ladders, brick walls and interwoven diamondoids, have been developed extensively (Bünzli & Piguet, 2002; Sharma & Rogers, 1999). More recently, flexible components, both ligands and metals, have been employed as versatile building blocks for coordination polymer construction, allowing access to topologies that are often unattainable using more rigid components (Jung *et al.*, 2002). Bis(2-methylimidazol-1-yl)methane (2-mBIM) is a bis-imidazole ligand containing a connecting flexible methylene linker. We have reported an interesting infinite one-dimensional catenane polymer formed by the addition of a solution of 2-mBIM to  $AgNO_3$  (Jin *et al.*, 2006). We report here the interesting solid-state structure of a novel one-dimensional double-bridged chain polymer structure, (I), with a 16-

membered macrometallacyclic tetragonal structural motif, formed by the addition of a solution of 2-mBIM to  $Cd(NO_3)_2$ .

As revealed by single-crystal X-ray diffraction analysis, each  $Cd^{II}$  cation occupies a crystallographic inversion centre and is coordinated by four N atoms from four distinct 2-mBIM ligands and two O atoms from two nitrate anions to form a slightly distorted octahedral geometry about the cadmium center. The four N-donor atoms of the 2-mBIM ligands lie in the equatorial plane and the two coordinated nitrate anions in the apical positions (Fig. 1). Selected N—Cd—N and N—Cd—O bond angles are given in Table 1. The Cd1—N2 and Cd1—N5<sup>ii</sup> distances (see Table 1 for values and symmetry code) are within the range expected for such ligating bonds (Kasai *et al.*, 2000). It is noteworthy that the nitrate anion, a monodentate ligand, has a Cd1—O1 distance that is slightly shorter than those reported for similar structures (Wang *et al.*, 2000). The Cd1···O2 and Cd1···O3 distances are 3.319 (1) and 4.374 (2) Å, respectively.



Each pair of neighboring  $Cd^{II}$  centers is bridged by two 2-mBIM ligands to form a 16-membered macrometallacyclic tetragonal structural motif with a Cd···Cd separation of 9.654 Å. Each 2-mBIM ligand is coordinated to two  $Cd^{II}$  cations and acts as a bridge ligand to form a one-dimensional double-bridged chain polymer structure that runs along the  $[01\bar{1}]$  direction. The conformation of the 2-mBIM ligand in (I) is considerably different from that of free 2-mBIM (Jin & Gong, 2005), since the two methyl groups at the 2-position of the coordinated ligand point in the same direction (see Fig. 1). Each pair of 2-mBIM ligands in the same 16-membered metallacycle is centrosymmetric. The dihedral angle between the two imidazole rings of the same 2-mBIM ligand is 59.6°. Significant  $\pi$ — $\pi$  contacts [the shortest N···N distance is 3.707 (2) Å] and weak C—H···O interactions between adjacent one-dimensional double-bridged chain polymers are



**Figure 1**  
 The structure of (I), showing the atom numbering. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i)  $-x + 1, -y, -z + 2$ ; (ii)  $x, y - 1, z + 1$ ; (iii)  $-x + 1, -y + 1, -z + 1$ .]

present. Although similar one-dimensional double-bridged chain polymer structures have been documented for bipyridine ligands (Dong *et al.*, 2000), coordination polymer structures containing  $\text{Cd}(\text{NO}_3)_2$  and imidazole ligands are still quite rare.

## Experimental

A methanol solution (5 ml) of 2-mBIM (88 mg, 0.5 mmol) was diffused slowly into an aqueous solution (5 ml) of  $\text{Cd}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$  (154 mg, 0.5 mmol) in a test tube. Colorless crystals of (I) were formed at the solvent interface after two weeks in 84% yield.

### Crystal data

$[\text{Cd}(\text{NO}_3)_2(\text{C}_9\text{H}_{12}\text{N}_4)_2]$	$\gamma = 69.787 (2)^\circ$
$M_r = 588.87$	$V = 568.51 (11) \text{ \AA}^3$
Triclinic, $P\bar{1}$	$Z = 1$
$a = 7.9252 (9) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 9.2783 (10) \text{ \AA}$	$\mu = 1.02 \text{ mm}^{-1}$
$c = 9.4118 (10) \text{ \AA}$	$T = 298 (2) \text{ K}$
$\alpha = 62.192 (2)^\circ$	$0.32 \times 0.26 \times 0.24 \text{ mm}$
$\beta = 73.725 (2)^\circ$	

### Data collection

Bruker SMART APEX CCD area-detector diffractometer	5982 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	2229 independent reflections
$T_{\min} = 0.74$ , $T_{\max} = 0.78$	2168 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.060$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$	162 parameters
$wR(F^2) = 0.068$	H-atom parameters constrained
$S = 1.07$	$\Delta\rho_{\text{max}} = 0.77 \text{ e \AA}^{-3}$
2229 reflections	$\Delta\rho_{\text{min}} = -0.44 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Cd1—N2	2.338 (2)	Cd1—O1	2.404 (2)
Cd1—N5 <sup>ii</sup>	2.383 (2)		
N2 <sup>i</sup> —Cd1—N5 <sup>ii</sup>	85.17 (8)	N2—Cd1—O1	95.91 (7)
N2—Cd1—N5 <sup>ii</sup>	94.83 (8)	N5 <sup>ii</sup> —Cd1—O1	98.57 (7)
N2 <sup>i</sup> —Cd1—O1	84.09 (7)	N5 <sup>iii</sup> —Cd1—O1	81.43 (7)

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

H atoms were positioned geometrically at distances of 0.93 (CH), 0.97 (CH<sub>2</sub>) and 0.96  $\text{\AA}$  (CH<sub>3</sub>) from the parent C atoms; a riding model was used during the refinement process. The  $U_{\text{iso}}(\text{H})$  values were constrained to be  $1.2U_{\text{eq}}$  of the carrier atom, except for methyl H atoms, which were constrained to be  $1.5U_{\text{eq}}$  of the parent C atom.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2001); 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: SF3054). Services for accessing these data are described at the back of the journal.

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