Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[(2,2′-bipyridine-κ^2N,N')cadmium(II)]-μ-5-carboxyimidazole-4-carboxylato-$\kappa^4N^3,O^4:N^1,O^5$]

Shan Gao,* Ji-Wei Liu, Li-Hua Huo and Hui Zhao

School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China

Correspondence e-mail: shangao67@yahoo.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.019
wR factor = 0.054
Data-to-parameter ratio = 15.5

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

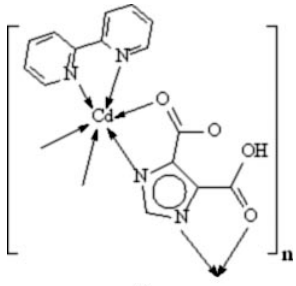
© 2004 International Union of Crystallography
Printed in Great Britain – all rights reserved

Received 15 October 2004
Accepted 22 October 2004
Online 30 October 2004

In the title one-dimensional coordination polymer, $[Cd(HIDC)(2,2'\text{-bipy})]_n$ ($HIDC^{2-}$ is the imidazole-4,5-dicarboxylate dianion, $C_5H_2N_2O_4$, and 2,2′-bipy is 2,2′-bipyridine, $C_{10}H_8N_2$), each Cd^{II} atom exists in a distorted trigonal prismatic coordination geometry, involving two N and two O atoms from two bidentate $HIDC^{2-}$ groups, and two N atoms from the 2,2′-bipy co-ligand. Adjacent Cd^{II} ions are bridged by $HIDC^{2-}$ groups, giving rise to a one-dimensional chain structure. The Cd···Cd separation within the polymer is 6.707 (2) Å.

Comment

1*H*-Imidazole-4,5-dicarboxylic acid (H_3IDC) has great potential for the construction of supramolecular architectures, owing to its versatile binding modes. To date, a few mononuclear (Zhang *et al.*, 2004; Xiao *et al.*, 2004; Ma *et al.*, 2003) and dinuclear (Rajendiran *et al.*, 2003; Bayón & Net, 1987) complexes have already been reported. However, coordination polymers based on the H_3IDC ligand remain largely unexplored (Wang *et al.*, 2004). In the present work, we report the crystal structure of the title one-dimensional chain Cd^{II} coordination polymer, (I), $[Cd(HIDC)(2,2'\text{-bipy})]_n$ (2,2′-bipy = 2,2′-bipyridine), which was obtained by the hydrothermal reaction of cadmium dinitrate tetrahydrate, 1*H*-imidazole-4,5-dicarboxylic acid and 2,2′-bipyridine.



(I)

As shown in Fig. 1, the carboxylic acid (H_3IDC) ligand of (I) bears a formal charge of −2, representing the removal of two H atoms, from the imidazole atom N4 and the carboxyl atom O1. The Cd^{II} ion is six-coordinated by two N atoms [Cd—N 2.2706 (14) and 2.2209 (15) Å] and two O atoms [Cd—O 2.3895 (14) and 2.4306 (13) Å] from two bidentate $HIDC^{2-}$ ligands, and two N atoms from one 2,2′-bipy co-ligand [mean Cd—N 2.352 (2) Å]. The O—Cd—O angles around the Cd^{II} centre are in the range 69.81 (5)–165.65 (5)° (Table 1). The coordination geometry of the Cd^{II} atom can be described as a distorted trigonal prismatic; this can be attributed to the chelating effects of the $HIDC^{2-}$ and 2,2′-bipy ligands, which

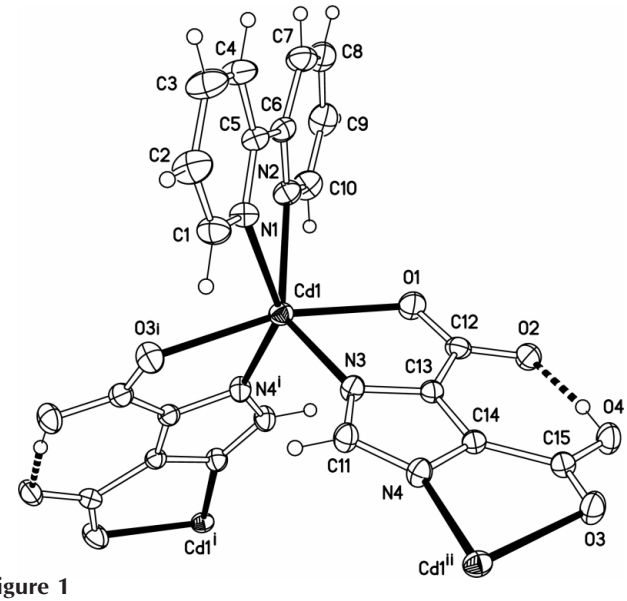


Figure 1
A view of the title complex, with 30% probability displacement ellipsoids. Intramolecular hydrogen bonds are shown as dashed lines. [Symmetry codes: (i) $x+\frac{1}{2}, \frac{1}{2}-y, \frac{1}{2}-z$; (ii) $x-\frac{1}{2}, \frac{1}{2}-y, \frac{1}{2}-z$].

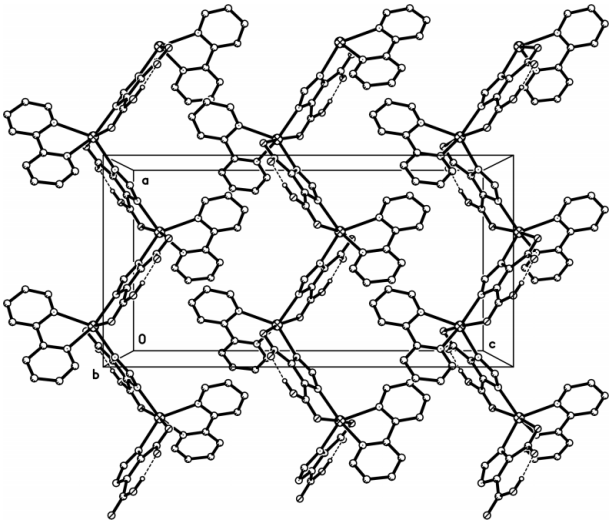


Figure 2
A packing diagram for the title complex. Hydrogen bonds are shown as dashed lines. H atoms bound to C atoms have been omitted.

form three five-membered chelate rings. The $HIDC^{2-}$ ligand is planar, with an overall r.m.s. deviation of 0.06 (3) Å. The dihedral angle between the 2,2′-bipy and $HIDC^{2-}$ ligands is 77.0 (5)°.

The C12—O2 [1.278 (2) Å] and C15—O4 [1.290 (2) Å] bonds are longer than the C12—O1 [1.244 (2) Å] and C17—O3 [1.238 (2) Å] bonds, in accord with the monodentate coordination mode of carboxyl groups. The free carboxy atom O4 and the uncoordinated atom O2 form an intramolecular hydrogen bond (Table 2).

Each $HIDC^{2-}$ group of (I) acts as a bis-bidentate bridging ligand to link two Cd^{II} ions, generating a one-dimensional chain running along the *a* axis direction. Within this chain, the adjacent Cd···Cd separation is 6.707 (2) Å. The antiparallel 2,2′-bipy ligands lie on alternate sides of the chain. The crystal packing (Fig. 2) shows a short distance of 3.680 (3) Å between the centroids of the 2,2′-bipy rings, which suggests the existence of π–π stacking interactions.

Experimental

Cadmium dinitrate tetrahydrate (6.16 g, 20 mmol), 2,2′-bipyridine (3.12 g, 20 mmol) and 1*H*-imidazole-4,5-dicarboxylic acid (4.60 g, 20 mmol) were dissolved in an ethanol–water solution (1:5). The mixture was sealed in a 50 ml Teflon-lined stainless steel bomb and held at 403 K for 3 d. The bomb was cooled naturally to room temperature, and colourless prismatic crystals of (I) were obtained after several days. CHN analysis, calculated for $C_{15}H_{10}N_4O_4Cd$: C 42.62, H 2.38, N 13.26%; found: C 42.81, H 2.45, N 13.31%.

Crystal data

$[Cd(C_5H_2N_2O_4)(C_{10}H_8N_2)]$
$M_r = 422.68$
Orthorhombic, *Pbca*
$a = 10.776$ (2) Å
$b = 13.283$ (3) Å
$c = 20.890$ (4) Å
$V = 2990.1$ (10) Å^3
$Z = 8$
$D_x = 1.878$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 776 reflections
$\theta = 3.1$–$27.3°$
$\mu = 1.49$ mm^{-1}
$T = 293$ (2) K
Prism, colourless
0.37 × 0.26 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID area-detector diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.635$, $T_{max} = 0.765$
27 506 measured reflections
3410 independent reflections
3123 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 27.5°$
$h = -13 \rightarrow 13$
$k = -17 \rightarrow 17$
$l = -27 \rightarrow 27$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.019$
$wR(F^2) = 0.054$
$S = 1.03$
3410 reflections
220 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0328P)^2 + 1.2915P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.3239 (15)	Cd1—O3^{i}	2.4306 (13)
Cd1—N2	2.3793 (16)	O1—C12	1.244 (2)
Cd1—N3	2.2706 (14)	O2—C12	1.278 (2)
Cd1—N4^{i}	2.2209 (15)	O3—C15	1.238 (2)
Cd1—O1	2.3895 (14)	O4—C15	1.290 (2)
N1—Cd1—N2	69.81 (5)	N3—Cd1—O3^{i}	97.58 (5)
N1—Cd1—O1	112.74 (5)	N4^{i}—Cd1—N1	144.81 (5)
N1—Cd1—O3^{i}	78.36 (5)	N4^{i}—Cd1—N2	105.16 (6)
N2—Cd1—O1	77.81 (5)	N4^{i}—Cd1—N3	108.15 (6)
N2—Cd1—O3^{i}	115.53 (5)	N4^{i}—Cd1—O1	99.39 (5)
N3—Cd1—N1	95.04 (5)	N4^{i}—Cd1—O3^{i}	72.76 (5)
N3—Cd1—N2	138.54 (5)	O1—Cd1—O3^{i}	165.65 (5)
N3—Cd1—O1	73.07 (5)		

Symmetry code: (i) $\frac{1}{2}+x, \frac{1}{2}-y, 1-z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H16···O2	0.85 (3)	1.60 (3)	2.454 (3)	174 (3)

The H atom of the carboxy group was located in a difference map, and refined with an O—H distance restraint of 0.85 (1) Å and with U_{iso}(H) = 1.5U_{eq}(O). H atoms bound to C atoms were placed in calculated positions, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) and refined using a riding model.

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

The authors thank the National Natural Science Foundation of China (grant No. 20101003), Heilongjiang Province Natural Science Foundation (grant No. B0007), the Scientific Fund of Remarkable Teachers of Heilongjiang Province (grant No. 1054 G036) and Heilongjiang University for supporting this study.

References

Bayón, T. C & Net, G. (1987). *J. Chem. Soc. Dalton Trans.* pp. 3003–3007.
Higashi, T. (1995). *ABSCOR.* Rigaku Corporation, Tokyo, Japan.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA.
Ma, C. B., Chen, F., Chen, C. N. & Liu, Q. T. (2003). *Acta Cryst.* C**59**, m516–m518.
Rajendiran, T. M., Kirk, M. L., Setyawati, I. A., Caudle, M. T., Kampf, J. W. & Pecoraro, V. L. (2003). *Chem. Commun.* pp. 824–825.
Rigaku Corporation (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure.* Rigaku/MSC, 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Wang, C. F., Gao, E. Q., He, Z. & Yan, C. H. (2004). *Chem. Commun.* pp. 720–721.
Xiao, H. P., Li, X. H. & Shi, Q. (2004). *Acta Cryst.* E**60**, m1519–m1521.
Zhang, X. M., Fang, R. Q., Wu, H. S. & Ng, S. W. (2004). *Acta Cryst.* E**60**, m12–m13.