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catena-Poly[[aquacadmium(II)]bis(μ-4,5-diphenyl-1*H*-imidazole-1-acetate)-$\kappa^3N:O,O';\kappa^3O,O':N$]

Shan Gao,[a]* Ji-Wei Liu[a,b] and Li-Hua Huo[a]

[a]Laboratory of Functional Materials, School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China, and [b]College of Chemistry and Chemical Technology, Da Qing Petroleum Institute, Da Qing 163318, People's Republic of China

Correspondence e-mail:
shangao67@yahoo.com

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Key indicators

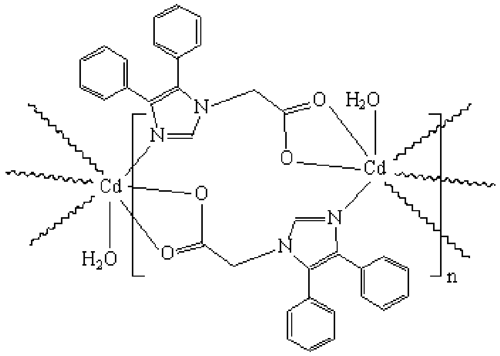
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.008 Å
R factor = 0.034
wR factor = 0.091
Data-to-parameter ratio = 15.3

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

In the title one-dimensional coordination polymer, $[Cd(\mu\text{-DPIA})_2(H_2O)]_n$ ($DPIA^-$ is the 4,5-diphenylimidazole-1-acetate monoanion, $C_{17}H_{13}N_2O_2$), each Cd^{II} atom exists in a pentagonal–bipyramidal coordination geometry, defined by four O atoms and two N atoms from two $DPIA^-$ ligands [Cd—O = 2.389 (4)–2.455 (4) Å and Cd—N = 2.362 (5)–2.372 (5) Å] and one water molecule [Cd—O(water) = 2.313 (2) Å]. Adjacent Cd^{II} ions are bridged by $DPIA^-$ groups, forming an infinite chain structure. The Cd$\cdots$Cd separation within the polymer is 7.650 (3) Å. The structure is stabilized by weak hydrogen-bonding interactions.

Comment

Recently, there has been considerable interest in the solid-state coordination chemistry and biochemistry of *N*-heterocyclic carboxylic acids, such as pyrazine 2-carboxylic acid and imidazole-4,5-dicarboxylic acid (Min *et al.*, 2001; Gao, Liu *et al.*, 2004; Gao, Gu *et al.*, 2004). 4,5-Diphenylimidazole-1-acetic acid (HDPIA), which easily binds a metal ion by its flexible carboxyl group or by the rigid *N*-heterocyclic part, is recognized as a potentially multidentate ligand (Gao, Zhao *et al.*, 2004). We report here the new one-dimensional coordination polymer, *catena*-poly[[aquacadmium(II)]bis(μ-4,5-diphenyl-1*H*-imidazole-1-acetate-$\kappa^3N:O,O'$)], (I).



(I)

As shown in Fig. 1, the carboxyl group is bonded to the Cd ion in a bidentate mode. The Cd^{II} atom is coordinated by four O atoms and two N atoms from two $DPIA^-$ ligands and one water molecule, which define a pentagonal–bipyramidal geometry. Atoms O1^i, O3^{ii}, O4^{ii}, O2^i and O1*W* (symmetry codes as in Table 1) define the equatorial plane of the coordination polyhedron, while atoms N1 and N3 occupy the axial sites of the pentagonal bipyramid. The Cd atom deviates by 0.007 (4) Å from the equatorial plane. The Cd—O distances are within the range of the corresponding bond distances [2.209 (2)–2.879 (2) Å] reported for normal Cd–carboxylate

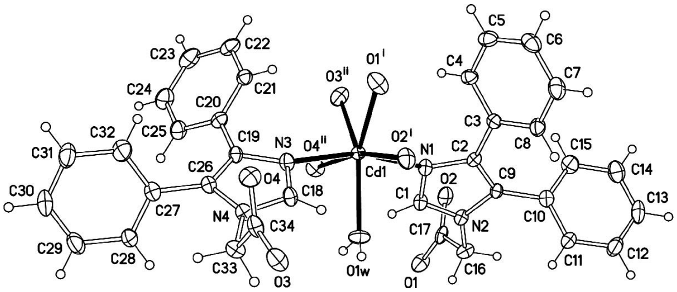


Figure 1

ORTEPII plot (Johnson, 1976) of the title complex, with displacement ellipsoids drawn at the 30% probability level. Symmetry codes are as in Table 1. H atoms are drawn as small circles of arbitrary radius.

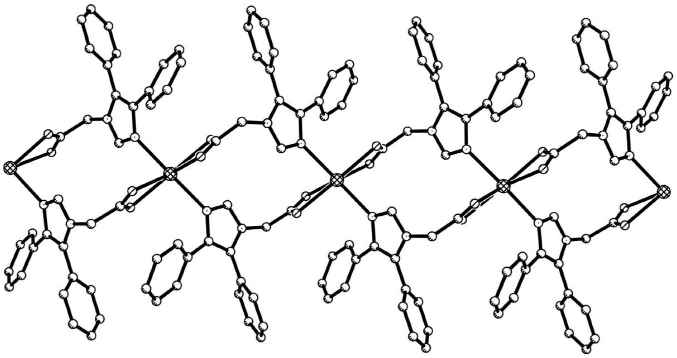


Figure 2

The chain structure of the title complex. Water molecules and H atoms on C atoms have been omitted for clarity.

complexes (Clegg *et al.*, 1995). Each DPIA$^-$ ligand bridges two adjacent Cd^{II} atoms, giving rise to a chain along the *a* axis, as shown in Fig. 2. In the chain, the Cd$\cdots$Cd distance is 7.650 (3) Å. Furthermore, the chains are connected by intermolecular hydrogen bonds involving the water molecules and carboxyl O atoms of DPIA$^-$ groups, yielding a supramolecular layer structure.

Experimental

4,5-Diphenylimidazole-1-acetic acid was prepared according to a literature procedure (Gao, Zhao *et al.*, 2004). 4,5-Diphenylimidazole-1-acetic acid (1.113 g, 4 mmol) and cadmium nitrate tetrahydrate (0.606 g, 2 mmol) were dissolved in an ethanol solution (30 ml). The mixture was sealed in a 50 ml Teflon-lined stainless steel bomb and held at 393 K for 5 d. The bomb was cooled to room temperature and colourless single crystals were obtained over several days. Analysis calculated for $C_{34}H_{28}CdN_4O_5$: C 59.61, H 4.12, N 8.18%; found: C 59.75, H 4.10, N, 8.09%.

Crystal data

$[Cd(C_{17}H_{13}N_2O_2)_2(H_2O)]$
$M_r = 685.01$
Orthorhombic, $Pca2_1$
$a = 15.096$ (3) Å
$b = 6.1108$ (12) Å
$c = 32.164$ (6) Å
$V = 2967.1$ (10) Å^3
$Z = 4$
$D_x = 1.533$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 22 239 reflections
$\theta = 3.3$–27.4°
$\mu = 0.79$ mm^{-1}
$T = 296$ (2) K
Prism, colourless
0.38 × 0.26 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.754$, $T_{max} = 0.865$
23 982 measured reflections

6181 independent reflections
5488 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 27.5°$
$h = -19 \rightarrow 19$
$k = -7 \rightarrow 7$
$l = -38 \rightarrow 41$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.091$
$S = 1.04$
6181 reflections
403 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0481P)^2 + 1.6576P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.57$ e Å^{-3}
$\Delta\rho_{min} = -0.55$ e Å^{-3}
Absolute structure: (Flack, 1983), 2734 Friedel pairs
Flack parameter = 0.02 (2)

Table 1

Selected geometric parameters (Å, °).

Cd1—N1	2.372 (5)	Cd1—O1*W*	2.313 (2)
Cd1—N3	2.362 (5)	O1—C17	1.251 (6)
Cd1—O1^i	2.455 (4)	O2—C17	1.236 (7)
Cd1—O2^i	2.409 (5)	O3—C34	1.254 (6)
Cd1—O3^{ii}	2.389 (4)	O4—C34	1.228 (7)
Cd1—O4^{ii}	2.423 (5)		
N1—Cd1—O1^i	108.48 (17)	O3^{ii}—Cd1—O1^i	88.57 (10)
N1—Cd1—O2^i	93.2 (2)	O3^{ii}—Cd1—O2^i	139.25 (16)
N1—Cd1—O3^{ii}	83.78 (16)	O3^{ii}—Cd1—O4^{ii}	53.97 (15)
N1—Cd1—O4^{ii}	83.86 (11)	O4^{ii}—Cd1—O1^i	139.79 (15)
N3—Cd1—N1	164.03 (12)	O1*W*—Cd1—N1	81.6 (2)
N3—Cd1—O1^i	83.64 (17)	O1*W*—Cd1—N3	82.4 (2)
N3—Cd1—O2^i	85.63 (11)	O1*W*—Cd1—O1^i	135.48 (14)
N3—Cd1—O3^{ii}	107.43 (17)	O1*W*—Cd1—O2^i	83.0 (2)
N3—Cd1—O4^{ii}	93.5 (2)	O1*W*—Cd1—O3^{ii}	135.95 (14)
O2^i—Cd1—O1^i	53.86 (16)	O1*W*—Cd1—O4^{ii}	83.2 (2)
O2^i—Cd1—O4^{ii}	166.19 (12)		

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

Table 2

Hydrogen-bonding geometry (Å, °).

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
O1*W*—H1*W*1$\cdots$O1^{iii}	0.85 (4)	1.86 (5)	2.673 (5)	160 (6)
O1*W*—H1*W*2$\cdots$O3^{iv}	0.85 (4)	1.96 (4)	2.665 (5)	140 (5)

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

H atoms attached to C atoms were positioned geometrically and refined as riding, with displacement parameter constraints as follows: methylene C—H = 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$, and aromatic C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. Water H atoms were located in a difference Fourier map and refined with a distance restraint of O—H = 0.85 (1) Å and $U_{iso}(H) = 1.5U_{eq}(O)$.

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*.

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