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A novel Cd^{II} coordination polymer with 1,1′-(1,4-butanediyl)diimidazole

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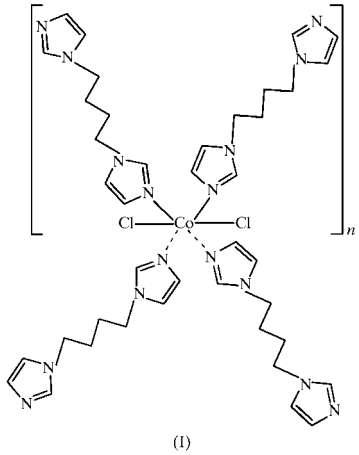
The novel title Cd^{II} coordination polymer, poly[[dichlorocadmium(II)]-di-μ-1,1′-(1,4-butanediyl)diimidazole], $[CdCl_2(C_{10}H_{14}N_4)_2]_n$, (I), was obtained by reaction of $CdCl_2\cdot 2.5H_2O$ and 1,1′-(1,4-butanediyl)diimidazole (hereafter *L*). In (I), each *L* molecule coordinates to two Cd^{II} cations through its two aromatic N atoms, thus acting as a bridging bidentate ligand. The Cd^{II} cations, which lie on the inversion centre, are bridged by four *L* molecules to form a two-dimensional (4,4)-network. The two-dimensional square-grid sheets are superimposed in an offset fashion.

Comment

In recent years, research into coordination polymers has been expanding rapidly because of their fascinating structural diversity and potential application as functional materials



(I)

(Batten & Robson, 1998; Moulton & Zaworotko, 2001). To date, a number of one-, two- and three-dimensional infinite frameworks have been generated with linear *N*,*N*′-bidentate spacers (Tong *et al.*, 2002). Much of the work has been focused on coordination polymers with rigid ligands, such as 4,4′-bipyridine, pyrazine and their analogues. However, flexible ligands such as 1,1′-(1,4-butanediyl)dibenzimidazole (*L*′) and 1,1′-(1,4-butanediyl)diimidazole (*L*) have not been well explored to date (Ma, Liu, Xing *et al.*, 2000; Ma, Liu, Liu *et al.*, 2000). In the present paper, we report the preparation and crystal structure of a novel two-dimensional coordination polymer, namely $[CdL_2Cl_2]_n$, (I).

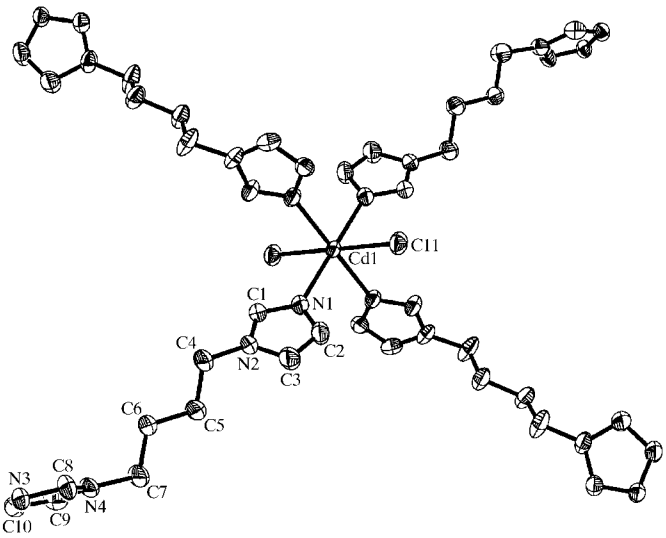


Figure 1
A view of the local coordination of the Cd^{II} cation in (I), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted for clarity.

As shown in Fig. 1, the Cd^{II} cation occupies the inversion centre and is six-coordinated by four N atoms from four *L* molecules and two Cl^- anions. Each Cd^{II} cation has a slightly distorted CdN_4Cl_2 octahedral coordination sphere. The average Cd—N distance of 2.3499 (19) Å is somewhat longer than the value of 2.275 (5) Å found in $[CdL_{1.5}(H_2O)_2(SO_4)]\cdot 4H_2O$ with a (6,3)-network (Ma, Liu, Xing *et al.*, 2000).

As illustrated in Fig. 2, each *L* molecule in (I) coordinates to two Cd^{II} cations through its two aromatic N atoms, thus acting

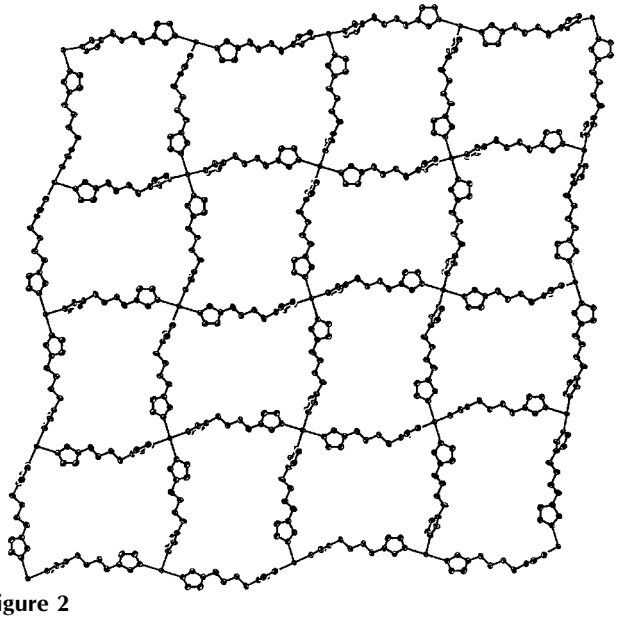


Figure 2
The two-dimensional sheet of the (4,4)-network in (I). The Cl^- anions have been omitted for clarity.

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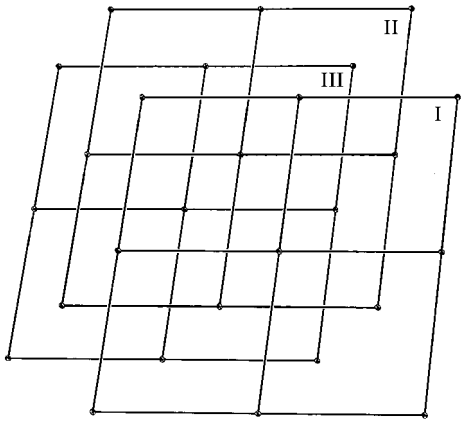

Figure 3
A top view showing the off-set superposition of the adjacent nets in (I) along the *c* axis.

as a bridging bidentate ligand. The Cd^{II} cations, which lie on the inversion centre, are bridged by four *L* molecules to form a two-dimensional neutral (4,4)-network. The networks contain square grids (44-membered ring), with a Cd^{II} cation at each corner and an *L* molecule at each edge connecting two Cd^{II} cations. Due to the symmetry of the crystal structure, the edge lengths are equal, and the edge length of 14.167 Å is similar to those of the related compound $[CdL_{1.5}(H_2O)_2(SO_4)]\cdot 4H_2O$ (Ma, Liu, Xing *et al.*, 2000).

Although large circuits exist in a single net, they are mainly overlapped by other nets. The square-grid sheets are superimposed in an interesting off-set fashion. The off-set superposition of each pair of adjacent nets by one third of the edges divides the voids into smaller rectangles (Fig. 3), which are similar to those found in A-zeolites and Pentasil zeolites (Tong *et al.*, 1998). In the superposition structure, the sheets are arranged in the sequence ···I–II–III–I–II–III···.

In conclusion, in (I), a novel two-dimensional coordination polymer, with off-set superposition, the Cd^{II} cations provide the four-connecting nodes of the net and the *L* molecules link the nodes to form a two-dimensional (4,4)-network.

Experimental

A mixture of $CdCl_2\cdot 2.5H_2O$ (0.228 g, 1 mmol) and *L* (0.380 g, 2 mmol) in water (20 ml) was refluxed for 20 min, then filtered whilst hot. Colourless crystals of (I) were obtained by evaporating the filtrate at room temperature for several days. The compound is insoluble in common organic solvents and dissolves in water only very slowly.

Crystal data

$[CdCl_2(C_{10}H_{14}N_4)_2]$
M_r = 563.80
Monoclinic, $P2_1/n$
a = 7.6488 (15) Å
b = 18.732 (4) Å
c = 8.6668 (17) Å
β = 112.11 (3)°
V = 1150.4 (5) Å^3
Z = 2
D_x = 1.628 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7161 reflections
θ = 2.2–27.5°
μ = 1.21 mm^{-1}
T = 293 (2) K
Prism, colourless
0.24 × 0.23 × 0.11 mm

Data collection

Rigaku R-AXIS RAPID CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.703, T_{max} = 0.874
9903 measured reflections
2554 independent reflections
2038 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 27.5°
$h = 0 \rightarrow 9$
$k = 0 \rightarrow 24$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.066
S = 1.02
2554 reflections
142 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0416P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—Cd1	2.3680 (19)	Cd1—Cl1	2.6569 (8)
N3—Cd1^{i}	2.3317 (19)		
N3^{ii}—Cd1—N1	90.29 (7)	N3^{iii}—Cd1—Cl1	91.39 (5)
N3^{iii}—Cd1—N1	89.71 (7)	N1—Cd1—Cl1	89.97 (5)
N3^{ii}—Cd1—Cl1	88.61 (5)	N1^{iv}—Cd1—Cl1	90.03 (5)

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

All H atoms on C atoms were generated geometrically and refined as riding atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). Analytical expressions of neutral-atom scattering factors were employed and anomalous dispersion corrections incorporated.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: AV1149). Services for accessing these data are described at the back of the journal.

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