



**supplementary materials**

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***catena*-Poly[*cadmium*(II)- $\mu$ -benzene-1,2-diamine- $\kappa^2$ N:N'-di- $\mu$ -chlorido]**

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**Comment**

Coordination frameworks have received much attention over the past decade due to their potential applications. Scientists have dedicated much attention to coordination compounds which constructed by ligands with diamino coordination sites (Choi *et al.*, 1999; Fu *et al.*, 2007), since *cis*-diamminedichloroplatinum(II) received Food and Drug Administration's approval in 1979 for use as an anticancer drug (Spingler *et al.*, 2001). The title compound,  $[\text{CdCl}_2(\text{C}_6\text{H}_8\text{N}_2)]_n$ , is a coordination polymer prepared by the hydrothermal reaction of cadmium chloride and *o*-diaminobenzene. The Cd cation is located on the inversion center and octahedrally coordinated by four Cl atoms at equatorial sites and two N atoms from two ligands at the axial sites. Cd cations are bridged by Cl atoms to form a one-dimensional extended chain. The neighboring chains are binded by N—H $\cdots$ Cl hydrogen bonds.(Table 1) to form a two-dimensional network (Fig. 2).

**Experimental**

A mixture of  $\text{CdCl}_2$  (0.0366 g, 0.2 mmol) and benzene-1,2-diamine (0.0216 g, 0.2 mmol) in  $\text{H}_2\text{O}$  (4 ml) was heated in Pyrex tube at 100°C for two days. After slowly cooling down to room temperature over a period of 10 h, colorless crystals of the title compound suitable for diffraction were isolated.

**Refinement**

Positional parameters of all the H atoms were calculated geometrically and were allowed to ride on the C, N atoms to which they are bonded, with C—H = 0.93 Å, N—H = 0.90 Å and with  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ .

**Figures**



Fig. 1. A partial packing diagram of the title compound, with the displacement ellipsoids were drawn at the 30% probability level. [Symmetry codes: (A)  $I-x, -y, I-z$ ; (B)  $1-x, -1/2+y, 1-z$ ; (C)  $+x, 1/2-y, +z$ .]

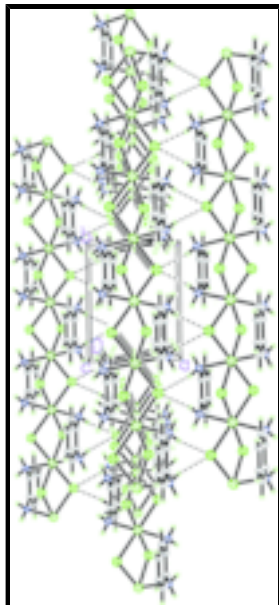


Fig. 2. Part of the structure of (I), showing two-dimensional extended polymeric network. Dotted lines show intermolecular hydrogen bonding.

**catena-Poly[cadmium(II)- $\mu$ -benzene-1,2-diamine- $\kappa^2$ N:N'-di- $\mu$ -chlorido]**

*Crystal data*

[CdCl<sub>2</sub>(C<sub>6</sub>H<sub>8</sub>N<sub>2</sub>)]

$M_r = 291.44$

Monoclinic,  $P2_1/m$

Hall symbol: -P 2yb

$a = 6.1235$  (6) Å

$b = 7.5473$  (5) Å

$c = 10.1081$  (6) Å

$\beta = 105.2300$  (10)°

$V = 450.75$  (6) Å<sup>3</sup>

$Z = 2$

$F_{000} = 280$

$D_x = 2.147$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 4460 reflections

$\theta = 3.1$ – $27.5$ °

$\mu = 2.95$  mm<sup>-1</sup>

$T = 293$  (2) K

Prism, colourless

$0.18 \times 0.15 \times 0.14$  mm

*Data collection*

Rigaku SCXmini  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 13.6612 pixels mm<sup>-1</sup>

$T = 293$ (2) K

CCD profile fitting scans

Absorption correction: multi-scan  
(CrystalClear; Rigaku, 2005)

$T_{\min} = 0.595$ ,  $T_{\max} = 0.660$

4700 measured reflections

1109 independent reflections

1020 reflections with  $I > 2\sigma(I)$

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

$\theta_{\text{max}} = 27.5$ °

$\theta_{\text{min}} = 3.4$ °

$h = -7 \rightarrow 7$

$k = -9 \rightarrow 9$

$l = -13 \rightarrow 13$

Refinement

Refinement on $F^2$	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.018$	$w = 1/[\sigma^2(F_o^2) + (0.0114P)^2 + 0.0467P]$
$wR(F^2) = 0.040$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.22$	$(\Delta/\sigma)_{\max} < 0.001$
1109 reflections	$\Delta\rho_{\max} = 0.25 \text{ e } \text{\AA}^{-3}$
56 parameters	$\Delta\rho_{\min} = -0.35 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL97 (Sheldrick, 1997), $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.115 (2)

Special details

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

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.5000	0.0000	0.5000	0.02699 (11)
Cl1	0.26524 (11)	0.2500	0.58281 (8)	0.03186 (18)
Cl2	0.62145 (13)	0.2500	0.35295 (7)	0.03336 (19)
N1	0.8292 (3)	0.0596 (2)	0.67983 (17)	0.0290 (4)
H1A	0.8687	-0.0546	0.7042	0.043*
H1B	0.9341	0.1080	0.6439	0.043*
C2	0.7996 (3)	0.1574 (2)	0.79569 (18)	0.0249 (4)
C3	0.7561 (3)	0.0677 (3)	0.9058 (2)	0.0348 (5)
H3	0.7530	-0.0555	0.9056	0.042*
C4	0.7174 (3)	0.1588 (3)	1.0153 (2)	0.0411 (5)
H4	0.6913	0.0971	1.0893	0.049*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cd1	0.03100 (15)	0.02342 (14)	0.02722 (15)	-0.00010 (7)	0.00882 (10)	-0.00260 (7)

## supplementary materials

Cd1	0.0293 (4)	0.0263 (4)	0.0466 (4)	0.000	0.0218 (3)	0.000
Cd2	0.0499 (4)	0.0270 (4)	0.0289 (4)	0.000	0.0205 (3)	0.000
N1	0.0290 (9)	0.0270 (8)	0.0324 (9)	-0.0003 (7)	0.0108 (8)	-0.0011 (7)
C2	0.0180 (8)	0.0319 (10)	0.0234 (9)	-0.0015 (7)	0.0031 (7)	-0.0008 (8)
C3	0.0284 (10)	0.0391 (12)	0.0348 (11)	-0.0017 (9)	0.0045 (9)	0.0089 (10)
C4	0.0308 (11)	0.0662 (15)	0.0271 (10)	-0.0034 (10)	0.0093 (9)	0.0071 (10)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

Cd1—N1 <sup>i</sup>	2.3758 (17)	N1—H1A	0.9113
Cd1—N1	2.3758 (17)	N1—H1B	0.8946
Cd1—Cl2	2.6274 (5)	C2—C3	1.387 (3)
Cd1—Cl2 <sup>i</sup>	2.6274 (5)	C2—C2 <sup>iii</sup>	1.398 (4)
Cd1—Cl1 <sup>i</sup>	2.6381 (5)	C3—C4	1.375 (3)
Cd1—Cl1	2.6381 (5)	C3—H3	0.9300
Cl1—Cd1 <sup>ii</sup>	2.6381 (5)	C4—C4 <sup>iii</sup>	1.377 (5)
Cl2—Cd1 <sup>iii</sup>	2.6274 (5)	C4—H4	0.9300
N1—C2	1.436 (2)		
N1 <sup>i</sup> —Cd1—N1	180.00 (7)	Cd1—Cl2—Cd1 <sup>ii</sup>	91.80 (2)
N1 <sup>i</sup> —Cd1—Cl2	90.71 (4)	C2—N1—Cd1	117.26 (11)
N1—Cd1—Cl2	89.29 (4)	C2—N1—H1A	110.3
N1 <sup>i</sup> —Cd1—Cl2 <sup>i</sup>	89.29 (4)	Cd1—N1—H1A	98.0
N1—Cd1—Cl2 <sup>i</sup>	90.71 (4)	C2—N1—H1B	112.2
Cl2—Cd1—Cl2 <sup>i</sup>	180.0	Cd1—N1—H1B	108.8
N1 <sup>i</sup> —Cd1—Cl1 <sup>i</sup>	92.61 (4)	H1A—N1—H1B	109.2
N1—Cd1—Cl1 <sup>i</sup>	87.39 (4)	C3—C2—C2 <sup>iii</sup>	119.20 (13)
Cl2—Cd1—Cl1 <sup>i</sup>	94.319 (17)	C3—C2—N1	119.72 (18)
Cl2 <sup>i</sup> —Cd1—Cl1 <sup>i</sup>	85.682 (17)	C2 <sup>iii</sup> —C2—N1	120.96 (10)
N1 <sup>i</sup> —Cd1—Cl1	87.39 (4)	C4—C3—C2	120.8 (2)
N1—Cd1—Cl1	92.61 (4)	C4—C3—H3	119.6
Cl2—Cd1—Cl1	85.682 (17)	C2—C3—H3	119.6
Cl2 <sup>i</sup> —Cd1—Cl1	94.318 (17)	C3—C4—C4 <sup>iii</sup>	119.98 (13)
Cl1 <sup>i</sup> —Cd1—Cl1	180.00 (3)	C3—C4—H4	120.0
Cd1 <sup>ii</sup> —Cl1—Cd1	91.32 (2)	C4 <sup>iii</sup> —C4—H4	120.0

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

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1B $\cdots$ Cl1 <sup>iv</sup>	0.89	2.51	3.3960 (18)	171

Symmetry codes: (iv)  $x+1, y, z$ .

Fig. 1

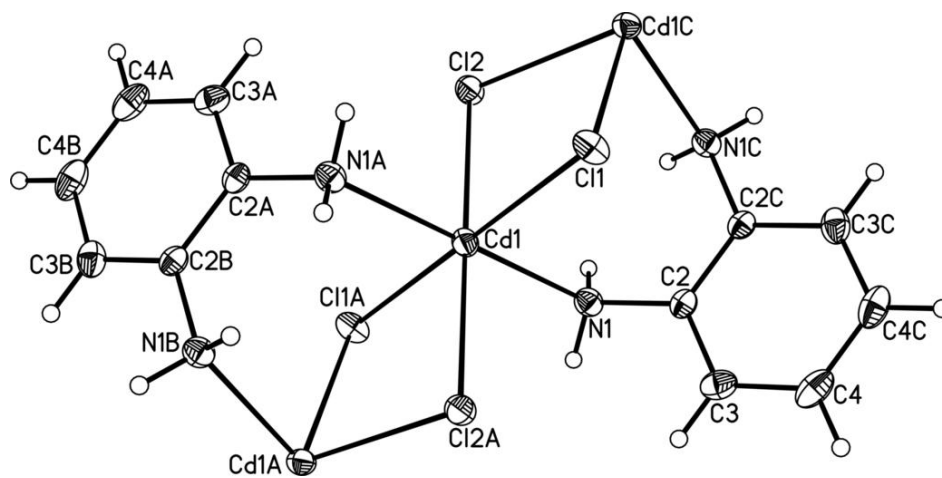


Fig. 2

