Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[cadmium(II)-μ-benzene-1,2-diamine-κ^2N:N'-di-μ-chlorido]

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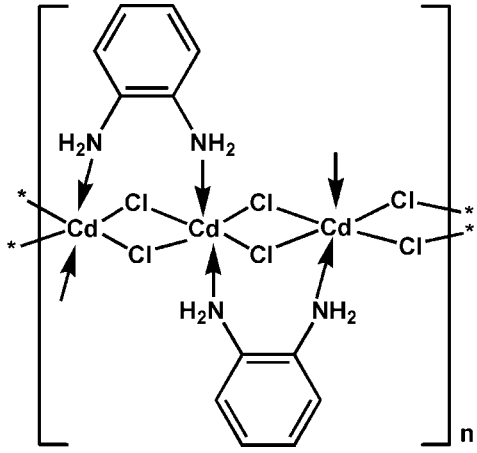
Received 27 August 2008; accepted 2 September 2008

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.018; wR factor = 0.040; data-to-parameter ratio = 19.8.

The title compound, $[CdCl_2(C_6H_8N_2)]_n$, is a coordination polymer prepared by the hydrothermal reaction of cadmium chloride and *o*-diaminobenzene. The cadmium cation, located on an inversion center, is octahedrally coordinated by four Cl atoms at equatorial sites and two N atoms from two ligands at the axial sites. Cd atoms are bridged by Cl atoms, forming extended chains parallel to [010]. Neighboring chains are connected by N—H···Cl hydrogen bonds.

Related literature

For related literature, see: Choi *et al.* (1999); Spingler *et al.* (2001); Fu & Zhao (2007).



Experimental

Crystal data

$[CdCl_2(C_6H_8N_2)]$
M_r = 291.44
Monoclinic, $P2_1/m$
a = 6.1235 (6) Å
b = 7.5473 (5) Å
c = 10.1081 (6) Å
β = 105.23 (10)°
V = 450.75 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.95 mm^{-1}
T = 293 (2) K
0.18 × 0.15 × 0.14 mm

Data collection

Rigaku SCXmini diffractometer
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_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.040
S = 1.22
1109 reflections
56 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1B···Cl1^{i}	0.89	2.51	3.3960 (18)	171

Symmetry code: (i) $x+1, y, z$.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL/PC* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

This work was supported by a Start-up Grant from Southeast University to ZRQ.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2174).

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supplementary materials

Acta Cryst. (2008). E**64**, m1254 [**doi:10.1107/S1600536808027980**]

catena-Poly[cadmium(II)-μ-benzene-1,2-diamine-κ^2N:N'-di-μ-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*-diamminedichloroplatium(II) received Food and Drug Administration's approval in 1979 for use as an anticancer drug (Spingler *et al.*, 2001). The title compound, $[CdCl_2(C_6H_8N_2)]_n$, 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···Cl hydrogen bonds.(Table 1) to form a two-dimensional network (Fig. 2).

Experimental

A mixture of $CdCl_2$ (0.0366 g, 0.2 mmol) and benzene-1,2-diamine (0.0216 g, 0.2 mmol) in H_2O (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_{iso}(H) = 1.2 U_{eq}(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) *1-x, -y, 1-z*; (B) 1-*x*, -12+*y*, 1-*z*; (C) *+x, 1/2-y, +z*.]

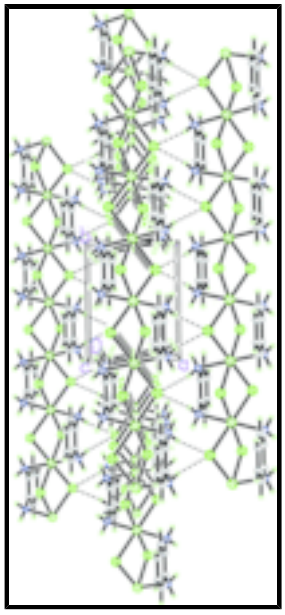

Fig. 2. Part of the structure of (I), showing two-dimensional extended polymeric network. Dotted lines show intermolecular hydrogen bonding.

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Crystal data

$[CdCl_2(C_6H_8N_2)]$	F_{000} = 280
M_r = 291.44	D_x = 2.147 Mg m^{-3}
Monoclinic, $P2_1/m$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yb	Cell parameters from 4460 reflections
a = 6.1235 (6) Å	θ = 3.1–27.5º
b = 7.5473 (5) Å	μ = 2.95 mm^{-1}
c = 10.1081 (6) Å	T = 293 (2) K
β = 105.2300 (10)º	Prism, colourless
V = 450.75 (6) Å^3	0.18 × 0.15 × 0.14 mm
Z = 2	

Data collection

Rigaku SCXmini diffractometer	1109 independent reflections
Radiation source: fine-focus sealed tube	1020 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.029
Detector resolution: 13.6612 pixels mm^{-1}	θ_{max} = 27.5º
T = 293(2) K	θ_{min} = 3.4º
CCD profile fitting scans	h = −7→7
Absorption correction: multi-scan (CrystalClear; Rigaku, 2005)	k = −9→9
T_{min} = 0.595, T_{max} = 0.660	l = −13→13
4700 measured reflections	

Refinement

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

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{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 (Å^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)

Cl1	0.0293 (4)	0.0263 (4)	0.0466 (4)	0.000	0.0218 (3)	0.000
Cl2	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 (Å, °)

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

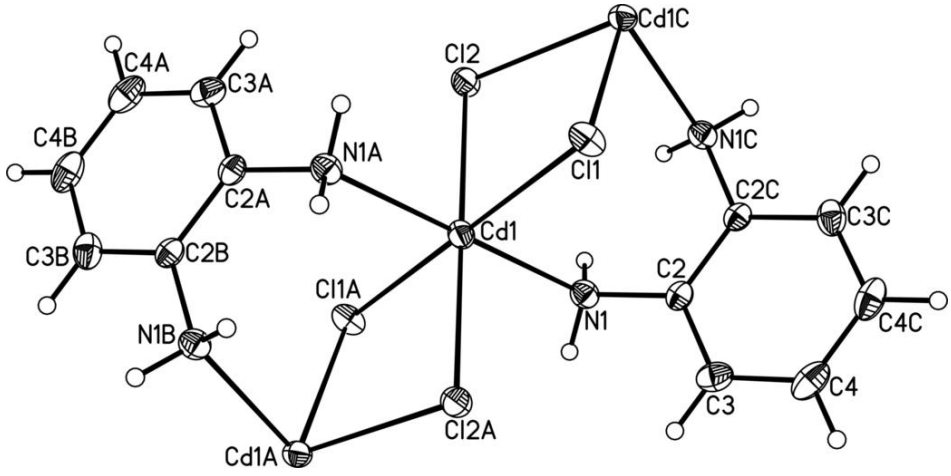
Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) −*x*+1, *y*+1/2, −*z*+1; (iii) *x*, −*y*+1/2, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1B···Cl1^{iv}	0.89	2.51	3.3960 (18)	171

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

Fig. 1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C4A
C3A
C4B
N1A
Cl1
N1C
C2A
C2C
C3C
Cd1
C3B
C2B
C2
Cl1A
N1
C4C
N1B
C3
C4
Cl2A
Cd1A

Fig. 2