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catena-Poly[[(1,10-phenanthroline-κ^2N,N')cadmate(II)]-di-μ-bromido]

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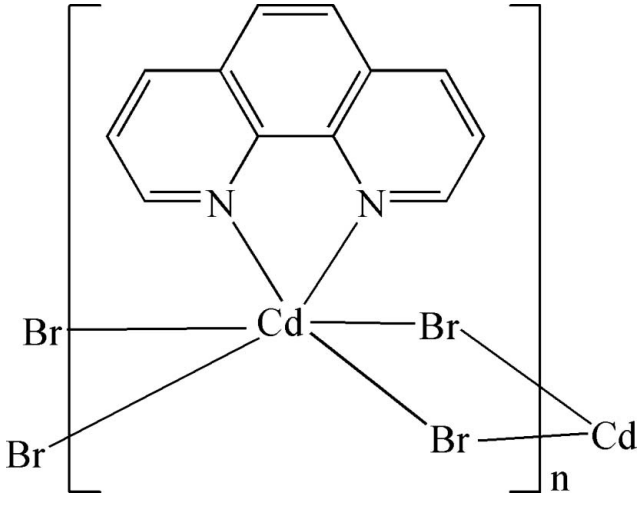
Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.011 Å; R factor = 0.029; wR factor = 0.067; data-to-parameter ratio = 15.8.

The title compound, $[CdBr_2(C_{12}H_8N_2)]_n$, is a 1:1 adduct of cadmium bromide with 1,10-phenanthroline (phen), which contains an infinite chain consisting of Cd_2Br_2 parallelograms sharing the Cd coners. The chain propagates along the c axis. Both the Cd^{II} atom and the phen molecule lie on a twofold rotation axis. The Cd^{II} atom is coordinated by two N atoms from a chelating phen ligand and four Br atoms to complete a distorted octahedral geometry. The closest atom-to-atom distance of 3.35 (1) Å between the phen ligands of two adjacent chains indicates the existence of π–π interactions, which result in a two-dimensional layer parallel to the bc plane. The layers are associated through weak C—H···Br hydrogen bonds.

Related literature

For related literature, see: Bell *et al.* (1982); Bigoli *et al.* (1983); Bonomo *et al.* (1989); Huang *et al.* (1998); Kimachi *et al.* (1995); Chen *et al.* (2003); Zhou *et al.* (2003).



Experimental

Crystal data

$[CdBr_2(C_{12}H_8N_2)]$
M_r = 452.42
Monoclinic, $C2/c$
a = 16.7781 (7) Å
b = 10.7594 (7) Å
c = 7.4213 (3) Å
β = 108.664 (4)°
V = 1269.26 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 7.99 mm^{-1}
T = 290 (2) K
0.23 × 0.12 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.340, T_{max} = 0.511
(expected range = 0.304–0.457)
7231 measured reflections
1247 independent reflections
998 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.067
S = 1.06
1247 reflections
79 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···Br1^{i}	0.96	2.88	3.816 (12)	166
C5—H5···Br1^{ii}	0.96	2.87	3.815 (5)	167

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2057).

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supplementary materials

Acta Cryst. (2007). E**63**, m1562 [**doi:10.1107/S1600536807020831**]

catena-Poly[[(1,10-phenanthroline-κ^2N,N')cadmate(II)]-di-μ-bromido]

B.-S. Zhang

Comment

Polynuclear d^{10} metal complexes have been found to exhibit intriguing structural and photoluminescent properties. Cl-bridged Cd^{II} polymeric complexes are of considerable interest because they may act as photoactive materials. Structures of Cl-bridged Cd^{II} polymeric complexes have been studied (Bell *et al.*, 1982; Bigoli *et al.*, 1983; Bonomo *et al.*, 1989; Huang *et al.*, 1998). However, Cd^{II} polymeric complexes with a $CdBr_2N_2$ coordination polydedron have been rarely reported. The phosphorescence and zero-field optically detected magnetic resonance studies with powder of CdX_2(phen), (phen = 1,10-phenanthroline; *X* = Cl, Br, and I) (Kimachi *et al.*, 1995) and the crystal structures of $CdCl_2$(phen) and $CdCl_2$ (2,2'-bipyridine) have been reported (Chen *et al.*, 2003; Zhou *et al.*, 2003). We have introduced Br^- ion as a bridging ligand, and synthesized the Br-bridged Cd complex, $[CdBr_2(phen)]_n$, (I), by a hydrothermal reaction.

The structure of compound (I) (Fig. 1), contains one-dimensional chains extending in the c direction (Fig 2). Both Cd^{II} atom and phen molecule lie on the twofold rotation axis. The Cd^{II} atom is coordinated by two N atoms from a chelating phen ligand and four Br atoms to complete a distorted CdN_2Br_4 octahedral geometry. The average Cd—N bond length is 2.350 (3) Å and the bond lengths of Cd—Br are 2.6813 (5)Å and 2.9003 (5) Å. The Cd···Cd distance in the chain is 4.047 (1) Å, which is longer than that of the Cl-bridged Cd complex [3.931 (9) Å]. The closest atom-to-atom distance of 3.35 (1)Å between the phen ligands of two adjacent chains indicates the existence of π–π interactions, which result in a two-dimensional layer parallel to the *bc* plane (Fig. 3). The layers are associated through weak C—H···Br hydrogen bonds (Table 1).

Experimental

Freshly prepared $CdCO_3$ (0.14 g, 0.812 mmol), phen·H_2O (0.10 g, 0.505 mmol), 2-bromobenzoic acid (0.10 g, 0.498 mmol), CH_3OH/H_2O (12 ml; *v*/*v*=1:2) were mixed and stirred for 2 h. The resulting suspension was heated in a 23 ml Teflon-lined stainless steel autoclave at 393 K for 7 d. After the autoclave was cooled to room temperature, colorless block crystals suitable for X-ray analysis were obtained.

Refinement

All H atoms were positioned geometrically and treated as riding atoms, with C—H = 0.96 Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

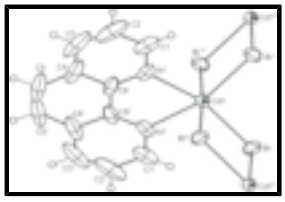

Fig. 1. The structure of (I), showing the coordination geometry of Cd ^{II} atom. Displacement ellipsoids are drawn at the 40% probability level. H atoms have been omitted for clarity. [symmetry codes: (i) 1 − *x*, *y*, 1/2 − *z*; (ii) 1 − *x*, 1 − *y*, 1 − *z*; (iii) 1 − *x*, 1 − *y*, −*z*; (iv) *x*, 1 − *y*, *z* − 1/2.]

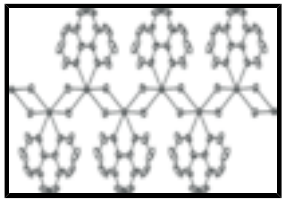

Fig. 2. A view of the one-dimensional chain along the *c* axis in (I). H atoms have been omitted for clarity.

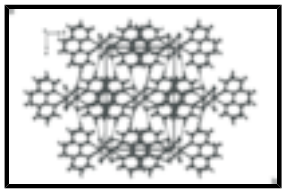

Fig. 3. A packing diagram for (I), viewed down the *c* axis. Dashed lines indicate hydrogen bonds.

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Crystal data

$[CdBr_2(C_{12}H_8N_2)]$	F_{000} = 848
M_r = 452.42	D_x = 2.368 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 961 reflections
a = 16.7781 (7) Å	θ = 2.3–26.0º
b = 10.7594 (7) Å	μ = 7.99 mm^{-1}
c = 7.4213 (3) Å	*T* = 290 (2) K
β = 108.664 (4)º	Block, colourless
V = 1269.26 (11) Å^3	0.23 × 0.12 × 0.10 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	1247 independent reflections
Radiation source: fine-focus sealed tube	998 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.039
T = 290(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −20→18
T_{min} = 0.340, T_{max} = 0.511	*k* = −13→10

7231 measured reflections

$l = -9 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.029$

$wR(F^2) = 0.067$

$S = 1.06$

1247 reflections

79 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + 3.3613P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.59$ e Å^{-3}

$\Delta\rho_{min} = -0.46$ e Å^{-3}

Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.00093 (19)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.5000	0.42497 (3)	0.2500	0.04136 (18)
Br1	0.60185 (3)	0.58225 (4)	0.49961 (6)	0.04905 (19)
N1	0.4258 (2)	0.2472 (3)	0.1038 (5)	0.0462 (9)
C1	0.3527 (3)	0.2477 (6)	−0.0359 (8)	0.0699 (15)
H1	0.3291	0.3253	−0.0919	0.084*
C2	0.3095 (5)	0.1378 (9)	−0.1055 (11)	0.105 (3)
H2	0.2563	0.1406	−0.2050	0.125*
C3	0.3414 (7)	0.0289 (8)	−0.0353 (13)	0.112 (4)
H3	0.3095	−0.0452	−0.0812	0.135*
C4	0.4194 (6)	0.0225 (5)	0.1050 (10)	0.085 (2)
C5	0.4646 (8)	−0.0905 (4)	0.1855 (12)	0.131 (7)
H5	0.4391	−0.1695	0.1417	0.157*
C6	0.4603 (3)	0.1372 (4)	0.1760 (6)	0.0534 (13)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0494 (3)	0.0298 (2)	0.0357 (3)	0.000	0.00083 (19)	0.000
Br1	0.0535 (4)	0.0480 (3)	0.0414 (3)	−0.0127 (2)	0.0092 (2)	−0.00875 (17)
N1	0.049 (2)	0.044 (2)	0.051 (2)	−0.0127 (17)	0.0228 (18)	−0.0174 (16)
C1	0.053 (3)	0.093 (4)	0.065 (3)	−0.018 (3)	0.021 (3)	−0.037 (3)
C2	0.074 (5)	0.157 (7)	0.096 (5)	−0.061 (5)	0.044 (4)	−0.083 (5)
C3	0.150 (8)	0.110 (6)	0.120 (6)	−0.090 (6)	0.103 (6)	−0.083 (6)
C4	0.149 (7)	0.049 (3)	0.099 (5)	−0.049 (4)	0.098 (5)	−0.039 (3)
C5	0.29 (2)	0.032 (3)	0.151 (11)	−0.038 (5)	0.178 (12)	−0.027 (3)
C6	0.082 (4)	0.035 (2)	0.064 (3)	−0.018 (2)	0.052 (2)	−0.0149 (19)

Geometric parameters (Å, °)

Cd1—N1	2.349 (3)	C1—H1	0.9600
Cd1—N1^{i}	2.349 (3)	C2—C3	1.323 (12)
Cd1—Br1	2.6813 (5)	C2—H2	0.9600
Cd1—Br1^{i}	2.6813 (5)	C3—C4	1.389 (11)
Cd1—Br1^{ii}	2.9003 (5)	C3—H3	0.9600
Cd1—Br1^{iii}	2.9003 (5)	C4—C6	1.429 (7)
Br1—Cd1^{ii}	2.9003 (5)	C4—C5	1.456 (11)
N1—C1	1.328 (6)	C5—C5^{i}	1.27 (2)
N1—C6	1.351 (6)	C5—H5	0.9600
C1—C2	1.396 (8)	C6—C6^{i}	1.429 (10)
N1—Cd1—N1^{i}	71.03 (19)	N1—C1—C2	121.7 (6)
N1—Cd1—Br1	163.57 (9)	N1—C1—H1	119.4
N1^{i}—Cd1—Br1	93.92 (10)	C2—C1—H1	118.9
N1—Cd1—Br1^{i}	93.92 (10)	C3—C2—C1	120.5 (7)
N1^{i}—Cd1—Br1^{i}	163.57 (9)	C3—C2—H2	119.3
Br1—Cd1—Br1^{i}	101.73 (2)	C1—C2—H2	120.2
N1—Cd1—Br1^{ii}	86.58 (9)	C2—C3—C4	120.3 (6)
N1^{i}—Cd1—Br1^{ii}	90.92 (9)	C2—C3—H3	119.1
Br1—Cd1—Br1^{ii}	87.145 (15)	C4—C3—H3	120.6
Br1^{i}—Cd1—Br1^{ii}	94.797 (16)	C3—C4—C6	117.4 (7)
N1—Cd1—Br1^{iii}	90.92 (9)	C3—C4—C5	126.3 (7)
N1^{i}—Cd1—Br1^{iii}	86.58 (9)	C6—C4—C5	116.4 (8)
Br1—Cd1—Br1^{iii}	94.797 (16)	C5^{i}—C5—C4	123.4 (5)
Br1^{i}—Cd1—Br1^{iii}	87.145 (15)	C5^{i}—C5—H5	117.7
Br1^{ii}—Cd1—Br1^{iii}	176.93 (2)	C4—C5—H5	118.9
Cd1—Br1—Cd1^{ii}	92.855 (15)	N1—C6—C6^{i}	118.7 (3)
C1—N1—C6	119.0 (4)	N1—C6—C4	121.1 (6)
C1—N1—Cd1	125.3 (3)	C6^{i}—C6—C4	120.2 (4)
C6—N1—Cd1	115.7 (3)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···Br1^{iv}	0.96	2.88	3.816 (12)	166
C5—H5···Br1^{v}	0.96	2.87	3.815 (5)	167

Symmetry codes: (iv) *x*−1/2, *y*−1/2, *z*−1; (v) −*x*+1, *y*−1, −*z*+1/2.

Fig. 1

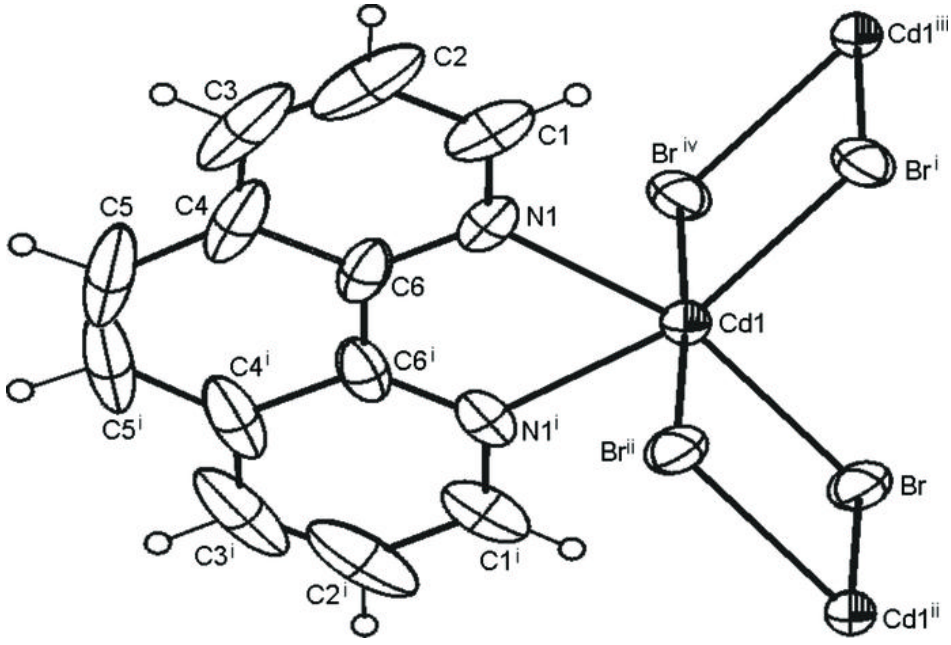
C2
C3
C1
C5
C4
N1
C6
Cd1
C4i
C6i
C5i
N1i
Brii
Br
C3i
C1i
C2i
Cd1ii
Br iv
Cd1iii
Bri

Fig. 2

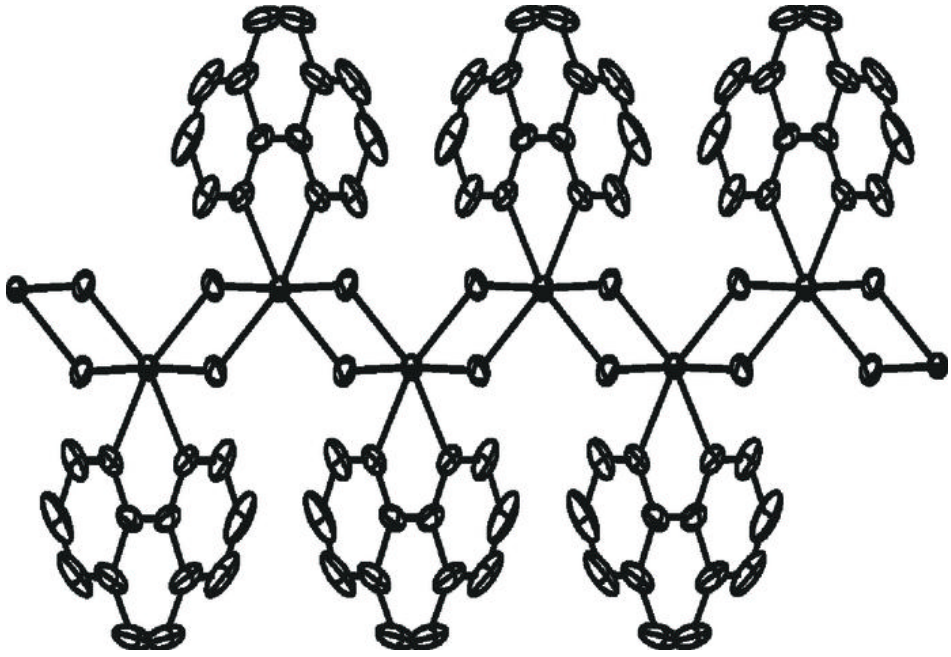

Fig. 3