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catena-Poly[[(4,4′-dimethyl-2,2′-bipyridine-κ^2N,N')cadmium]-di-μ-bromido]

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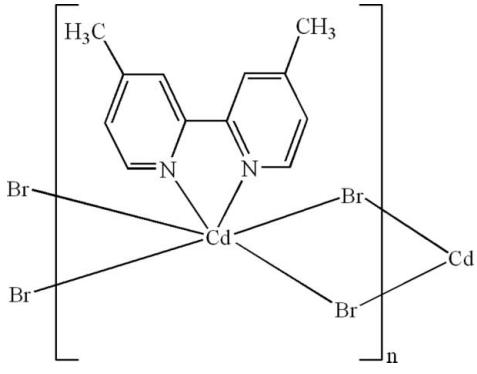
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.019 Å; R factor = 0.079; wR factor = 0.155; data-to-parameter ratio = 16.8.

In the crystal of the title polymeric compound, $[CdBr_2(C_{12}H_{12}N_2)]_n$, the Cd^{II} cation is located on a twofold rotation axis and is six-coordinated in a distorted octahedral geometry formed by two N atoms from the 4,4′-dimethyl-2,2′-bipyridine ligand and by four bridging Br^- anions. The bridging function of the Br^- anions leads to a polymeric chain running along the c axis. Weak C—H$\cdots\pi$ interactions observed between adjacent chains are effective in the stabilization of the three-dimensional packing.

Related literature

For related structures, see: Ahmadi *et al.* (2008); Alizadeh *et al.* (2010); Amani *et al.* (2009); Bellusci *et al.* (2008); Han *et al.* (2006); Hojjat Kashani *et al.* (2008); Kalateh *et al.* (2008, 2010); Shirvan & Haydari Dezfuli (2012); Sofetis *et al.* (2006); Willett *et al.* (2001); Yousefi *et al.* (2008); Zhang (2007).



Experimental

Crystal data

$[CdBr_2(C_{12}H_{12}N_2)]$
M_r = 456.45
Monoclinic, $C2/c$
a = 17.979 (4) Å
b = 10.5319 (18) Å
c = 7.4496 (16) Å
β = 108.403 (17)°
V = 1338.5 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 7.58 mm^{-1}
T = 298 K
0.25 × 0.21 × 0.20 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.188, T_{max} = 0.246
3392 measured reflections
1313 independent reflections
909 reflections with $I > 2\sigma(I)$
R_{int} = 0.095

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.155
S = 1.24
1313 reflections
78 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.88 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—N1	2.357 (10)	Cd1—Br1^{i}	2.8789 (16)
Cd1—Br1	2.6852 (17)		

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

Table 2
Hydrogen-bond geometry (Å, °).

Cg is the centroid of the N1-pyridine ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C4—H4$B\cdots Cg^{ii}$	0.96	2.84	3.575 (16)	135

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: XU5649).

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supporting information

Acta Cryst. (2012). E**68**, m1493–m1494 [doi:10.1107/S1600536812046636]

catena-Poly[[(4,4′-dimethyl-2,2′-bipyridine-κ^2N,N')cadmium]-di-μ-bromido]

Sadif A. Shirvan, Sara Haydari Dezfuli, Fereydoon Khazali and Ali Borsalani

S1. Comment

Recently, we reported the synthes and crystal structure of [$CdBr_2$(4,4′-dmbpy)(DMSO)], (Shirvan & Haydari Dezfuli, 2012) [where 4,4′-dmbpy is 4,4′-dimethyl-2,2′-bipyridine and DMSO is dimethyl sulfoxide]. 4,4′-Dimethyl-2,2′-bipyridine is a good bidentate ligand, and numerous complexes with 4,4′-dmbipy have been prepared, such as that of mercury (Kalateh *et al.*, 2008; Yousefi *et al.*, 2008), indium (Ahmadi *et al.*, 2008), iron (Amani *et al.*, 2009), platin (Hojjat Kashani *et al.*, 2008), silver (Bellusci *et al.*, 2008), gallium (Sofetis *et al.*, 2006), copper (Willett *et al.*, 2001), cadmium (Kalateh *et al.*, 2010) and zinc (Alizadeh *et al.*, 2010). Here, we report the synthesis and structure of the title compound.

The asymmetric unit of the title compound, (Fig. 1), contains half-molecule; a twofold rotation axis passes through the Cd atom. The Cd^{II} cation is six-coordinated in a distorted octahedral geometry formed by two N atoms from the 4,4′-dimethyl-2,2′-bipyridine ligand and four bridging Br^- anions. The bridging function of the Br^- anions leads to a polymeric chain running along the *b* axis. The Cd—N and Cd—Br bond lengths and angles (Table 1) are within normal range [Cd(phen)(μ-Br)$_2$]$_n$, (Zhang, 2007) and [Cd(bipy)(μ-Br)$_2$]$_n$, (Han *et al.*, 2006) [where phen is 1,10-phenanthroline and bipy is 2,2′-bipyridine].

S2. Experimental

For the preparation of the title compound, a solution of 4,4′-dimethyl-2,2′-bipyridine (0.25 g, 1.33 mmol) in methanol (10 ml) was added to a solution of $CdBr_2.4H_2O$, (0.46 g, 1.33 mmol) in methanol (5 ml) at room temperature. The suitable crystals for X-ray diffraction experiment were obtained by methanol diffusion to a colorless solution in dimethylformamide. Suitable crystals were isolated after one week (yield; 0.45 g, 74.1%).

S3. Refinement

H atoms were positioned geometrically with C—H = 0.93–0.96 Å and constrained to ride on their parent atoms, U_{iso}(H) = 1.2U_{eq}(C).

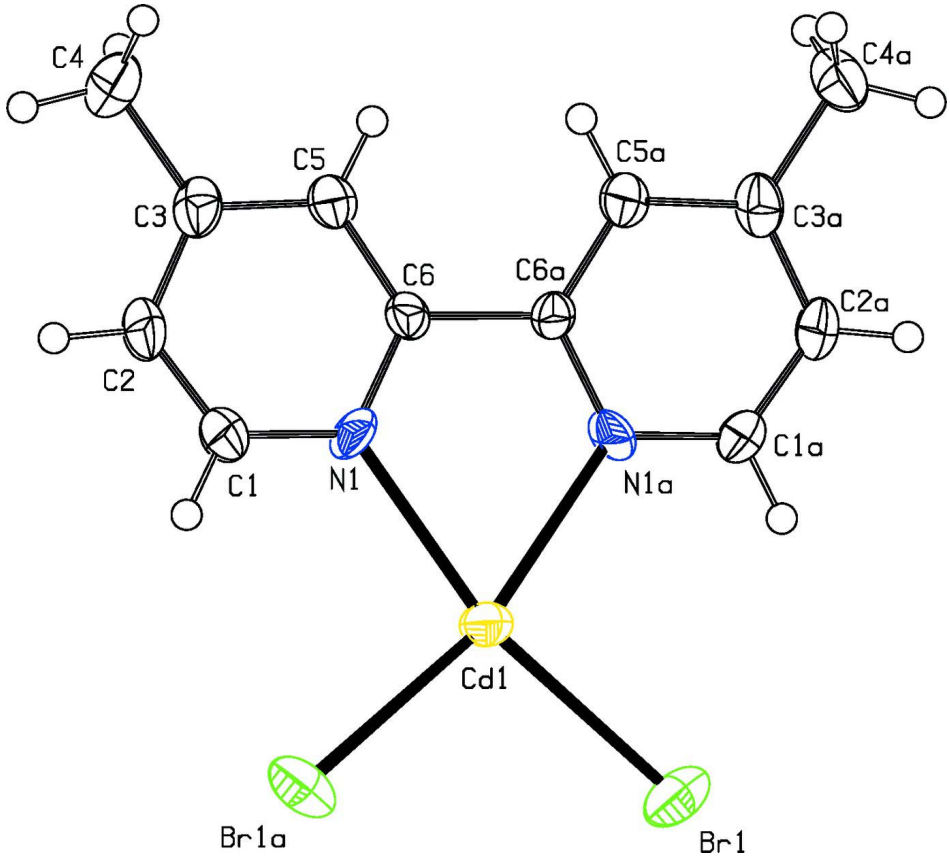

Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

***catena*-Poly[[(4,4′-dimethyl-2,2′-bipyridine- κ^2N,N')cadmium]-di-μ-bromido]**

Crystal data

$[CdBr_2(C_{12}H_{12}N_2)]$
$M_r = 456.45$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 17.979\ (4)$ Å
$b = 10.5319\ (18)$ Å
$c = 7.4496\ (16)$ Å
$\beta = 108.403\ (17)°$
$V = 1338.5\ (5)$ Å^3
$Z = 4$
$F(000) = 864$
$D_x = 2.265$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3392 reflections
$\theta = 2.3–26.0°$
$\mu = 7.58$ mm^{-1}
$T = 298$ K
Prism, colorless
0.25 × 0.21 × 0.20 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.188$, $T_{max} = 0.246$
3392 measured reflections
1313 independent reflections
909 reflections with $I > 2\sigma(I)$

R_{int} = 0.095
θ_{max} = 26.0°, θ_{min} = 2.3°
h = −22→22
k = −12→12
l = −7→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.155
S = 1.24
1313 reflections
78 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0098P)^2 + 54.7076P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.022
$\Delta\rho_{max}$ = 1.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.88 e Å^{-3}

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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Cd1	0.0000	0.92501 (14)	0.2500	0.0312 (4)
Br1	0.09337 (9)	1.08683 (16)	0.4997 (2)	0.0439 (5)
N1	−0.0688 (6)	0.7414 (11)	0.1090 (15)	0.030 (3)
C6	−0.0397 (7)	0.6266 (12)	0.1779 (18)	0.023 (3)
C5	−0.0804 (7)	0.5157 (13)	0.111 (2)	0.030 (3)
H5	−0.0585	0.4376	0.1574	0.036*
C1	−0.1384 (8)	0.7427 (15)	−0.025 (2)	0.042 (4)
H1	−0.1579	0.8209	−0.0767	0.050*
C3	−0.1535 (8)	0.5209 (14)	−0.025 (2)	0.031 (3)
C4	−0.2002 (8)	0.4012 (14)	−0.094 (2)	0.040 (4)
H4A	−0.2098	0.3586	0.0101	0.048*
H4B	−0.1712	0.3462	−0.1505	0.048*
H4C	−0.2493	0.4229	−0.1869	0.048*
C2	−0.1825 (8)	0.6396 (14)	−0.091 (2)	0.036 (3)
H2	−0.2318	0.6478	−0.1806	0.043*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0363 (8)	0.0203 (7)	0.0304 (9)	0.000	0.0011 (6)	0.000
Br1	0.0434 (10)	0.0394 (9)	0.0520 (12)	−0.0169 (7)	0.0195 (8)	−0.0153 (8)
N1	0.032 (6)	0.027 (5)	0.022 (6)	−0.009 (5)	−0.005 (4)	−0.006 (5)

C6	0.018 (6)	0.024 (6)	0.030 (7)	0.002 (5)	0.009 (5)	0.002 (6)
C5	0.019 (6)	0.031 (7)	0.045 (9)	0.002 (5)	0.015 (6)	−0.002 (6)
C1	0.034 (8)	0.030 (7)	0.046 (9)	0.003 (6)	−0.008 (7)	0.010 (7)
C3	0.027 (7)	0.042 (8)	0.023 (7)	0.001 (6)	0.005 (5)	−0.010 (6)
C4	0.037 (8)	0.044 (9)	0.035 (8)	−0.012 (7)	0.006 (6)	−0.003 (7)
C2	0.026 (7)	0.042 (8)	0.031 (8)	0.002 (6)	−0.005 (6)	0.004 (7)

Geometric parameters (Å, º)

Cd1—N1^{i}	2.357 (10)	C5—C3	1.383 (18)
Cd1—N1	2.357 (10)	C5—H5	0.9300
Cd1—Br1^{i}	2.6852 (17)	C1—C2	1.34 (2)
Cd1—Br1	2.6852 (17)	C1—H1	0.9300
Cd1—Br1^{ii}	2.8789 (16)	C3—C2	1.39 (2)
Cd1—Br1^{iii}	2.8790 (16)	C3—C4	1.513 (19)
Br1—Cd1^{iii}	2.8789 (16)	C4—H4A	0.9600
N1—C1	1.331 (16)	C4—H4B	0.9600
N1—C6	1.353 (17)	C4—H4C	0.9600
C6—C5	1.384 (18)	C2—H2	0.9300
C6—C6^{i}	1.49 (2)		
N1^{i}—Cd1—N1	69.7 (5)	N1—C6—C6^{i}	116.2 (7)
N1^{i}—Cd1—Br1^{i}	162.8 (3)	C5—C6—C6^{i}	122.4 (7)
N1—Cd1—Br1^{i}	95.0 (3)	C3—C5—C6	120.1 (13)
N1^{i}—Cd1—Br1	95.0 (3)	C3—C5—H5	119.9
N1—Cd1—Br1	162.8 (3)	C6—C5—H5	119.9
Br1^{i}—Cd1—Br1	101.21 (9)	N1—C1—C2	125.0 (14)
N1^{i}—Cd1—Br1^{ii}	85.5 (3)	N1—C1—H1	117.5
N1—Cd1—Br1^{ii}	90.4 (3)	C2—C1—H1	117.5
Br1^{i}—Cd1—Br1^{ii}	86.77 (5)	C5—C3—C2	117.4 (13)
Br1—Cd1—Br1^{ii}	96.39 (5)	C5—C3—C4	121.0 (13)
N1^{i}—Cd1—Br1^{iii}	90.4 (3)	C2—C3—C4	121.6 (12)
N1—Cd1—Br1^{iii}	85.5 (3)	C3—C4—H4A	109.5
Br1^{i}—Cd1—Br1^{iii}	96.39 (5)	C3—C4—H4B	109.5
Br1—Cd1—Br1^{iii}	86.77 (5)	H4A—C4—H4B	109.5
Br1^{ii}—Cd1—Br1^{iii}	175.03 (9)	C3—C4—H4C	109.5
Cd1—Br1—Cd1^{iii}	93.23 (5)	H4A—C4—H4C	109.5
C1—N1—C6	116.9 (12)	H4B—C4—H4C	109.5
C1—N1—Cd1	124.3 (10)	C1—C2—C3	119.1 (12)
C6—N1—Cd1	118.6 (8)	C1—C2—H2	120.4
N1—C6—C5	121.3 (11)	C3—C2—H2	120.4
N1^{i}—Cd1—Br1—Cd1^{iii}	−90.1 (3)	Br1^{iii}—Cd1—N1—C6	−89.3 (10)
N1—Cd1—Br1—Cd1^{iii}	−63.5 (10)	C1—N1—C6—C5	0 (2)
Br1^{i}—Cd1—Br1—Cd1^{iii}	95.88 (5)	Cd1—N1—C6—C5	175.0 (10)
Br1^{ii}—Cd1—Br1—Cd1^{iii}	−176.16 (7)	C1—N1—C6—C6^{i}	177.6 (15)
Br1^{iii}—Cd1—Br1—Cd1^{iii}	0.0	Cd1—N1—C6—C6^{i}	−7.7 (19)
N1^{i}—Cd1—N1—C1	177.1 (15)	N1—C6—C5—C3	−2 (2)

Br1^{i}—Cd1—N1—C1	−11.0 (12)	C6^{i}—C6—C5—C3	−179.3 (14)
Br1—Cd1—N1—C1	148.7 (10)	C6—N1—C1—C2	2 (2)
Br1^{ii}—Cd1—N1—C1	−97.8 (12)	Cd1—N1—C1—C2	−171.9 (13)
Br1^{iii}—Cd1—N1—C1	85.0 (12)	C6—C5—C3—C2	1 (2)
N1^{i}—Cd1—N1—C6	2.9 (7)	C6—C5—C3—C4	−177.8 (13)
Br1^{i}—Cd1—N1—C6	174.7 (9)	N1—C1—C2—C3	−3 (3)
Br1—Cd1—N1—C6	−25.6 (17)	C5—C3—C2—C1	1 (2)
Br1^{ii}—Cd1—N1—C6	87.9 (10)	C4—C3—C2—C1	−179.7 (15)

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

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the N1-pyridine ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4*B*···*Cg*^{iv}	0.96	2.84	3.575 (16)	135

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