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catena-Poly[[(2,2′-bipyridine)cadmium(II)]-di-μ-bromo]

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.006 Å
R factor = 0.025
wR factor = 0.063
Data-to-parameter ratio = 17.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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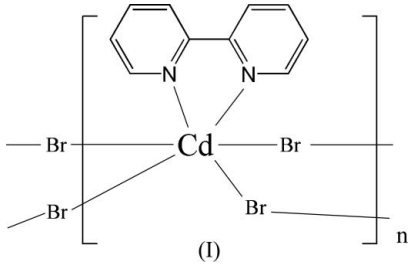
The title compound, $[CdBr_2(C_{10}H_8N_2)]_n$, has been hydrothermally synthesized and structurally characterized by single-crystal X-ray diffraction. The cadmium(II) ion lies on a twofold rotation axis and has a distorted octahedral geometry. The compound exhibits a one-dimensional chain structure extending parallel to the c axis.

Comment

The construction of metal-organic frameworks (MOF) is currently receiving considerable attention owing to their potential properties as functional solid materials, as well as their facinating framework structures (Evans & Lin, 2002; Lu *et al.*, 2001; Li *et al.*, 1999). These compounds are interesting for their potential applications as gas-storage devices, size- and shape-selective catalysts, molecular sieves and optoelectronic devices (Eddaoudi *et al.*, 2002; Kitaura *et al.*, 2003; Moulton & Zaworotko, 2001; Millange *et al.*, 2002). These MOF structures can be rapidly, reliably and efficiently synthesized from relatively simple subunits, where the metal ions, multidentate organic ligands, and coordinate bonding are the parameters for directing the self-assembly processes. In the course of our studies on the synthesis of new cadmium complexes with 2,2′-bipyridine (bpy), we obtained the metal-organic framework (MOF) $[Cd(bpy)Br_2]_n$, (I), which is isostructural with $[Cu(bpy)Br_2]_n$ (Garland *et al.*, 1988).



(I)

The monomeric unit of (I) consists of one Cd atom, one bpy ligand and two Br atoms. The cadmium(II) centre lies on a twofold rotation axis and is six-coordinated by two N atoms of a bpy bidentate ligand and four Br atoms in a distorted octahedral geometry (Fig. 1). The Br atoms of the monomeric unit play a bridging role, linking adjacent units in a chain running parallel to the c axis (Fig. 2). The shortest contact between chains is H4$\cdots$Br1^{i} = 2.96 Å [symmetry code: (i) $\frac{1}{2}-x$, $-\frac{1}{2}+y$, $\frac{5}{2}-z$].

Experimental

The title compound was obtained by a hydrothermal reaction. The starting materials $Cd(OAC)_2{\cdot}4H_2O$ (0.533 g, 2 mmol), bpy (0.1562 g,

1 mmol), KBr (0.238 g, 2 mmol), and deionized water (15 ml) were mixed, and the pH of the solution was adjusted to 6.5 by the addition of a sodium hydroxide solution. The resulting suspension was stirred for 1 h, and sealed in a 40 ml stainless steel bomb with a Teflon liner at 453 K for 4 days. The autoclave was cooled at 6 K h^{-1} to 373 K and the temperature was kept constant for 12 h. After cooling to room temperature at the same cooling rate, colourless crystals suitable for X-ray analysis were obtained.

Crystal data

$[CdBr_2(C_{10}H_8N_2)]$	D_x = 2.463 Mg m^{-3}
M_r = 428.40	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 1329 reflections
a = 17.227 (5) Å	θ = 2.5–26.4°
b = 9.618 (3) Å	μ = 8.77 mm^{-1}
c = 7.362 (2) Å	T = 294 (2) K
β = 108.728 (4)°	Prism, colourless
V = 1155.2 (6) $Å^3$	0.34 × 0.32 × 0.28 mm
Z = 4	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	1191 independent reflections
	896 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.029
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)	θ_{max} = 26.4°
	$h = -14 \rightarrow 21$
T_{min} = 0.068, T_{max} = 0.085	$k = -11 \rightarrow 12$
3190 measured reflections	$l = -9 \rightarrow 8$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0311P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.026	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.063	$\Delta\rho_{max}$ = 0.47 e $Å^{-3}$
S = 1.01	$\Delta\rho_{min}$ = −0.48 e $Å^{-3}$
1191 reflections	Extinction correction: *SHELXL97*
70 parameters	Extinction coefficient: 0.0029 (2)
H-atom parameters constrained	

Table 1
Selected bond lengths (Å).

Cd1—N1	2.337 (3)	Cd1—Br1^{i}	2.8994 (8)
Cd1—Br1	2.6761 (6)		

Symmetry code: (i) $-x, y, -z+\frac{3}{2}$.

All H atoms were placed in calculated positions and constrained to ride on their parent atoms with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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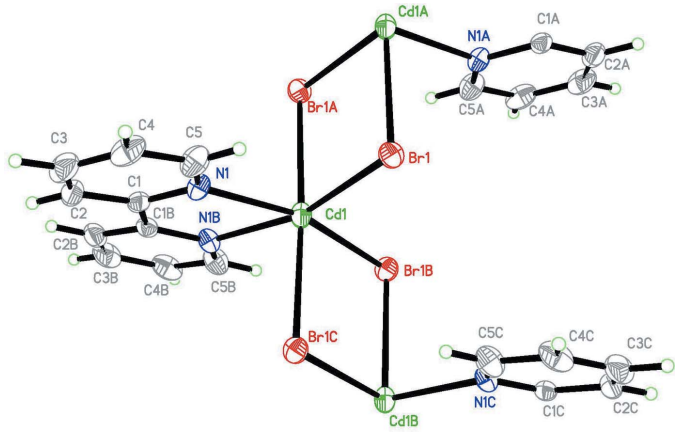

Figure 1
A segment of the polymeric chain structure of (I). Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size. Symmetry codes: A = $-x$, $1-y$, $2-z$; B = $-x$, y, $\frac{3}{2}-z$; C = x, $1-y$, $-\frac{1}{2}+z$.

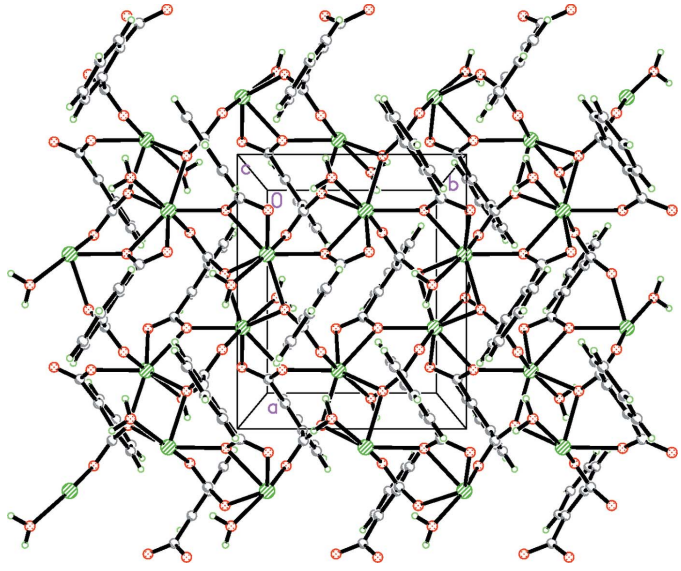

Figure 2
The packing of (I), viewed along the c axis.

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