Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[[μ-1,4-bis(4,5-dihydro-1,3-oxazol-2-yl)benzene-κ^2N:N']di-μ-bromido-cadmium]

Maw-Cherng Suen,[a]* Chun-Wei Yeh,[b] Shui-Chuan Lin[c] and Yi-Fen Hsu[b]

[a]Department of Material and Fiber, Nanya Institute of Technology, Chung-Li, Taiwan, [b]Department of Chemistry, Chung-Yuan Christian University, Chung-Li, Taiwan, and [c]Department of Polymer Materials, Vanung University, Jhongli, Taiwan
Correspondence e-mail: sun@nanya.edu.tw

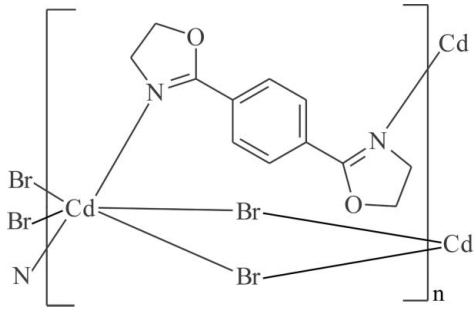
Received 6 July 2011; accepted 11 July 2011

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.026; wR factor = 0.067; data-to-parameter ratio = 48.1.

In the title coordination polymer, $[CdBr_2(C_{12}H_{12}N_2O_2)]_n$, the Cd^{II} ion, situated on an inversion centre, is coordinated by four bridging Br atoms and two N atoms from two 1,4-bis(4,5-dihydro-1,3-oxazol-2-yl)benzene (L) ligands in a distorted octahedral geometry. The L ligand, which also lies across an inversion centre, bridges two Cd^{II} ions, forming layers parallel to (010).

Related literature

For background to coordination polymers with organic ligands, see: Chiang *et al.* (2008); Hsu *et al.* (2009); Kitagawa *et al.* (2004); Yeh *et al.* (2008, 2009). For Cd(II) coordination polymers, see: Suen & Wang (2007*a*,*b*). For related structures, see: Wang *et al.* (2008, 2011).



Experimental

Crystal data

$[CdBr_2(C_{12}H_{12}N_2O_2)]$ M_r = 488.46
Triclinic, $P\overline{1}$
a = 4.0595 (2) Å
b = 8.1114 (3) Å
c = 10.1132 (4) Å
α = 84.503 (2)°
β = 81.963 (2)°
γ = 84.898 (2)°
V = 327.26 (2) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 7.77 mm^{-1}
T = 296 K
0.16 × 0.06 × 0.06 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.769, T_{max} = 0.971
15213 measured reflections
4234 independent reflections
3127 reflections with $I > 2\sigma(I)$
R_{int} = 0.081

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.067
S = 0.96
4234 reflections
88 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.99 e Å^{-3}
$\Delta\rho_{min}$ = −1.55 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd—N	2.5189 (12)	Cd—Br^{i}	2.7901 (2)
Cd—Br	2.7085 (2)		

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

We are grateful to the National Science Council of the Republic of China and the Nanya Institute of Technology for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2448).

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supplementary materials

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Poly[[μ-1,4-bis(4,5-dihydro-1,3-oxazol-2-yl)benzene-κ^2N:N']di-μ-bromido-cadmium]

M.-C. Suen, C.-W. Yeh, S.-C. Lin and Y.-F. Hsu

Comment

The synthesis of metal coordination polymers has been a subject of intense research due to their interesting structural chemistry and potential applications in gas storage, separation, catalysis, magnetism, luminescence, and drug delivery (Kitagawa *et al.*, 2004). Roles of anions, solvents and ligand conformations in the self-assembly of coordination complexes containing polydentate nitrogen ligands are very interesting (Chiang *et al.*, 2008; Hsu *et al.*, 2009; Yeh *et al.*, 2008, 2009). The Cd(II) complexes containing polydentate ligands showing various types of frameworks are also reported (Suen & Wang, 2007*a*,b). The Ag(I) and Cu(II) complexes containing 1,4-bis(4,5-dihydro-2-oxazolyl)benzene (*L*) ligands have been reported, which show various one- and two-dimensional networks (Wang, Lee *et al.*, 2008; Wang, Yeh *et al.*, 2011).

In the title complex, the Cd^{II} ion is six-coordinated with four Br atoms and two N atoms from two *L* ligands (Fig. 1, Table 1). The Cd···Cd distances separated by the bridging *L* ligands and Br atoms are 10.3574 (4) and 4.0595 (2) Å. The ligand adopts an *anti* conformation in the structure (Fig. 2).

Experimental

An aqueous solution (5.0 ml) of cadmium bromide (1.0 mmol) was layered carefully over a methanolic solution (5.0 ml) of 1,4-bis(4,5-dihydro-2-oxazolyl)benzene (1.0 mmol) in a tube. Colourless crystals were obtained after several weeks. These were washed with methanol and collected in 69.8% yield.

Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (phenyl) and 0.97 (methylene) Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

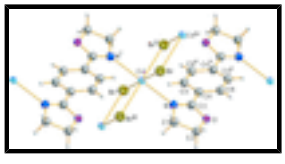

Fig. 1. A portion of the two-dimensional network in the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) -*x* + 1, -*y* + 1, -*z*; (ii) -*x*, -*y* + 1, -*z*; (iii) *x* + 1, *y*, *z*; (iv) *x* - 1, *y*, *z*; (v) -*x*, -*y* + 1, -*z* + 1.]

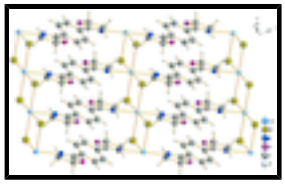

Fig. 2. A drawing of the two-dimensional network.

Poly[[μ-1,4-bis(4,5-dihydro-1,3-oxazol-2-yl)benzene- $\kappa^2N:N'$]di-μ-bromido-cadmium]

Crystal data

$[CdBr_2(C_{12}H_{12}N_2O_2)]$	$Z = 1$
$M_r = 488.46$	$F(000) = 232$
Triclinic, $P\overline{1}$	$D_x = 2.478$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 4.0595$ (2) Å	Cell parameters from 7163 reflections
$b = 8.1114$ (3) Å	$\theta = 3.1$–$41.1°$
$c = 10.1132$ (4) Å	$\mu = 7.77$ mm^{-1}
$\alpha = 84.503$ (2)°	$T = 296$ K
$\beta = 81.963$ (2)°	Columnar, colourless
$\gamma = 84.898$ (2)°	0.16 × 0.06 × 0.06 mm
$V = 327.26$ (2) Å^3	

Data collection

Bruker APEXII CCD diffractometer	4234 independent reflections
Radiation source: fine-focus sealed tube	3127 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.081$
φ and ω scans	$\theta_{max} = 41.1°$, $\theta_{min} = 3.1°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)	$h = -7 \rightarrow 6$
$T_{min} = 0.769$, $T_{max} = 0.971$	$k = -14 \rightarrow 14$
15213 measured reflections	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.026$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.067$	H-atom parameters constrained
$S = 0.96$	$w = 1/[\sigma^2(F_o^2) + (0.0224P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
4234 reflections	$(\Delta/\sigma)_{max} < 0.001$
88 parameters	$\Delta\rho_{max} = 0.99$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -1.55$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd	0.5000	0.0000	0.0000	0.02232 (4)

N	0.4635 (3)	−0.21212 (15)	0.19936 (11)	0.0222 (2)
O	0.2887 (3)	−0.39410 (14)	0.37175 (11)	0.0361 (3)
C1	0.5970 (4)	−0.37792 (18)	0.15877 (14)	0.0282 (3)
H1B	0.8389	−0.3851	0.1436	0.034*
H1A	0.5149	−0.4007	0.0773	0.034*
C2	0.4731 (5)	−0.4991 (2)	0.27480 (16)	0.0333 (3)
H2B	0.3300	−0.5751	0.2468	0.040*
H2A	0.6583	−0.5627	0.3115	0.040*
C3	0.3062 (4)	−0.23541 (17)	0.31777 (13)	0.0212 (2)
C4	0.1447 (3)	−0.11180 (17)	0.40873 (12)	0.0200 (2)
C5	0.2347 (4)	0.05114 (18)	0.39301 (13)	0.0227 (2)
H5	0.3917	0.0853	0.3219	0.027*
C6	−0.0891 (4)	−0.16227 (18)	0.51607 (13)	0.0229 (2)
H6	−0.1479	−0.2714	0.5267	0.027*
Br	0.91841 (3)	0.179762 (17)	0.103470 (13)	0.02270 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd	0.01836 (6)	0.02238 (7)	0.02671 (7)	−0.00089 (5)	−0.00254 (4)	−0.00583 (5)
N	0.0272 (5)	0.0202 (5)	0.0181 (5)	−0.0007 (4)	0.0012 (4)	−0.0038 (4)
O	0.0540 (8)	0.0203 (5)	0.0268 (5)	0.0041 (5)	0.0134 (5)	0.0000 (4)
C1	0.0369 (8)	0.0205 (6)	0.0237 (6)	0.0029 (5)	0.0056 (5)	−0.0034 (5)
C2	0.0432 (9)	0.0211 (7)	0.0304 (7)	0.0038 (6)	0.0093 (6)	−0.0029 (6)
C3	0.0253 (6)	0.0189 (6)	0.0187 (5)	−0.0003 (5)	−0.0008 (4)	−0.0026 (4)
C4	0.0234 (6)	0.0216 (6)	0.0149 (5)	0.0007 (5)	−0.0018 (4)	−0.0036 (4)
C5	0.0269 (6)	0.0241 (6)	0.0160 (5)	−0.0025 (5)	0.0020 (4)	−0.0019 (4)
C6	0.0288 (6)	0.0205 (6)	0.0188 (5)	−0.0031 (5)	0.0005 (4)	−0.0032 (4)
Br	0.02070 (7)	0.02520 (7)	0.02242 (7)	−0.00113 (5)	−0.00048 (4)	−0.00718 (5)

Geometric parameters (Å, °)

Cd—N	2.5189 (12)	C2—H2B	0.9700
Cd—Br	2.70850 (16)	C2—H2A	0.9700
Cd—Br^{i}	2.79006 (16)	C3—C4	1.4739 (17)
N—C3	1.2813 (17)	C4—C5	1.3910 (19)
N—C1	1.4781 (18)	C4—C6	1.3940 (19)
O—C3	1.3530 (18)	C5—C6^{ii}	1.3855 (18)
O—C2	1.4451 (17)	C5—H5	0.9300
C1—C2	1.516 (2)	C6—C5^{ii}	1.3855 (18)
C1—H1B	0.9700	C6—H6	0.9300
C1—H1A	0.9700		
N—Cd—N^{iii}	180.00 (6)	N—C1—H1A	110.7
N—Cd—Br^{iii}	86.94 (3)	C2—C1—H1A	110.7
N^{iii}—Cd—Br^{iii}	93.06 (3)	H1B—C1—H1A	108.8
N—Cd—Br	93.06 (3)	O—C2—C1	103.97 (11)
N^{iii}—Cd—Br	86.94 (3)	O—C2—H2B	111.0

Br^{iii}—Cd—Br	180.000 (5)	C1—C2—H2B	111.0
N—Cd—Br^{iv}	87.67 (3)	O—C2—H2A	111.0
N^{iii}—Cd—Br^{iv}	92.33 (3)	C1—C2—H2A	111.0
Br^{iii}—Cd—Br^{iv}	95.159 (5)	H2B—C2—H2A	109.0
Br—Cd—Br^{iv}	84.841 (5)	N—C3—O	117.42 (12)
N—Cd—Br^{i}	92.33 (3)	N—C3—C4	129.11 (13)
N^{iii}—Cd—Br^{i}	87.67 (3)	O—C3—C4	113.44 (11)
Br^{iii}—Cd—Br^{i}	84.841 (5)	C5—C4—C6	119.85 (12)
Br—Cd—Br^{i}	95.159 (5)	C5—C4—C3	121.06 (11)
Br^{iv}—Cd—Br^{i}	180.000 (6)	C6—C4—C3	119.00 (12)
C3—N—C1	106.43 (12)	$C6^{ii}$—C5—C4	119.60 (12)
C3—N—Cd	140.65 (10)	$C6^{ii}$—C5—H5	120.2
C1—N—Cd	110.60 (8)	C4—C5—H5	120.2
C3—O—C2	106.97 (11)	$C5^{ii}$—C6—C4	120.55 (13)
N—C1—C2	105.15 (11)	$C5^{ii}$—C6—H6	119.7
N—C1—H1B	110.7	C4—C6—H6	119.7
C2—C1—H1B	110.7	Cd—Br—Cd^{v}	95.159 (5)

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

Fig. 1

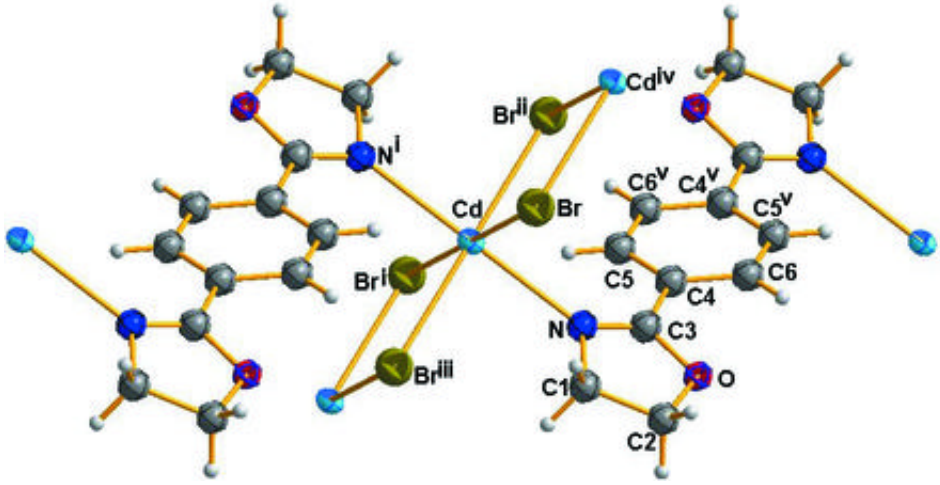

Fig. 2