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Bis{4-bromo-2-[(2-hydroxyethyl)iminomethyl]phenolato-κ^3O,N,O'}cadmium

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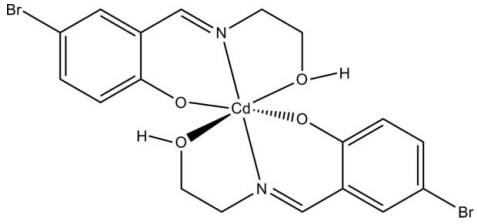
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.011 Å; R factor = 0.055; wR factor = 0.126; data-to-parameter ratio = 17.2.

The centrosymmetric title compound, $[Cd(C_9H_9BrNO_2)_2]$, was obtained by the reaction of 5-bromosalicylaldehyde, 2-aminoethanol and cadmium nitrate in ethanol. The Cd atom, located on an inversion centre, is hexacoordinated by two Schiff base ligands in an octahedral coordination through the phenolate O atom, the imine N atom and the hydroxy O atoms. In the crystal, molecules are linked through intermolecular O—H···O hydrogen bonds, forming chains along the b axis.

Related literature

For the structures and properties of Schiff base Cd complexes, see: Sarkar *et al.* (2011); Das *et al.* (2010); Fang & Nie (2010); Niu *et al.* (2010); Keypour *et al.* (2009).



Experimental

Crystal data

$[Cd(C_9H_9BrNO_2)_2]$
M_r = 598.56
Monoclinic, $P2/n$
a = 10.207 (4) Å
b = 5.3275 (19) Å
c = 18.656 (7) Å
β = 99.156 (4)°
V = 1001.5 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 5.11 mm^{-1}
T = 298 K
0.23 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.386, T_{max} = 0.428
7794 measured reflections
2172 independent reflections
1524 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.126
S = 1.02
2172 reflections
126 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.41 e Å^{-3}
$\Delta\rho_{min}$ = −1.55 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{i}	0.85 (1)	1.75 (2)	2.599 (7)	173 (9)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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* and local programs.

The School of Biological and Chemical Engineering at Jiaxing University is acknowledged for the provision of facilities to prepare and crystallize the compound. Dr Yu-Xi Sun of Qufu Normal University is acknowledged for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5060).

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supporting information

Acta Cryst. (2011). E**67**, m1035 [doi:10.1107/S1600536811025852]

Bis{4-bromo-2-[(2-hydroxyethyl)iminomethyl]phenolato-κ^3O,N,O'}cadmium

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S1. Comment

Schiff base cadmium(II) complexes have been received much attention due to their interesting structures and luminescent properties (Sarkar *et al.*, 2011; Das *et al.*, 2010; Fang & Nie, 2010; Niu *et al.*, 2010; Keypour *et al.*, 2009).

The molecule of the title complex, (I) (Fig. 1), is centrosymmetric, with the inversion center located at the Cd atom. The Cd atom is hexa-coordinated by two Schiff base ligands, forming an octahedral coordination. The Schiff base coordinates to the Co atom through the phenolate O atom, the imine N atom, and the hydroxy O atom. The bond lengths are within normal values. In the crystal, molecules are linked through intermolecular O—H···O hydrogen bonds (Table 1), to form chains along the *b* axis, Fig. 2.

S2. Experimental

To a solution of 5-bromosalicylaldehyde (0.181 g, 1.0 mmol), 2-aminoethanol (0.061 g, 1.0 mmol) in 20 ml absolute ethanol was added slowly a solution of cadmium nitrate (0.154 g, 0.5 mmol) in ethanol. The mixture was stirred for 2 h at room temperature to give a colorless solution, which was filtered and the filtrate was left to stand at room temperature. Colorless block crystals suitable for X-ray diffraction were obtained by slow evaporation.

S3. Refinement

H2 atom bonded to O2 atom was located in a difference map and refined with distance restraint of O—H = 0.85 (1) Å. Other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.97 Å.

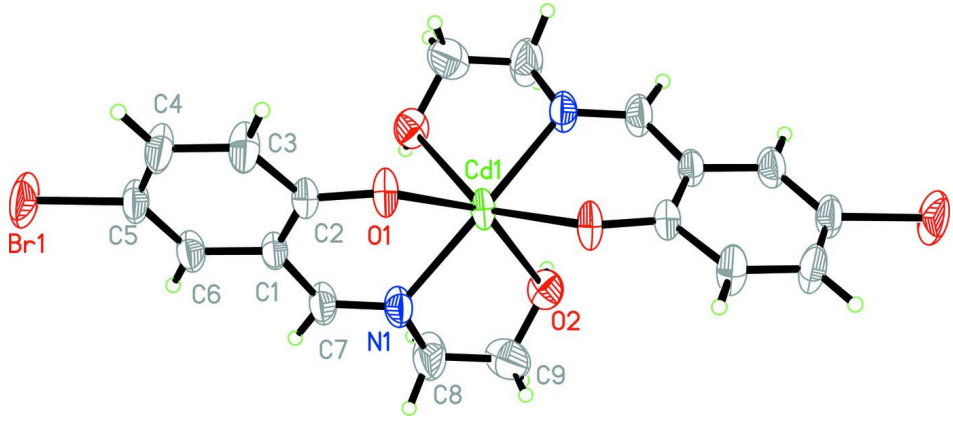

Figure 1

The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms. Unlabelled atoms are at the symmetry position 1/2 - *x*, *y*, 1/2 - *z*.

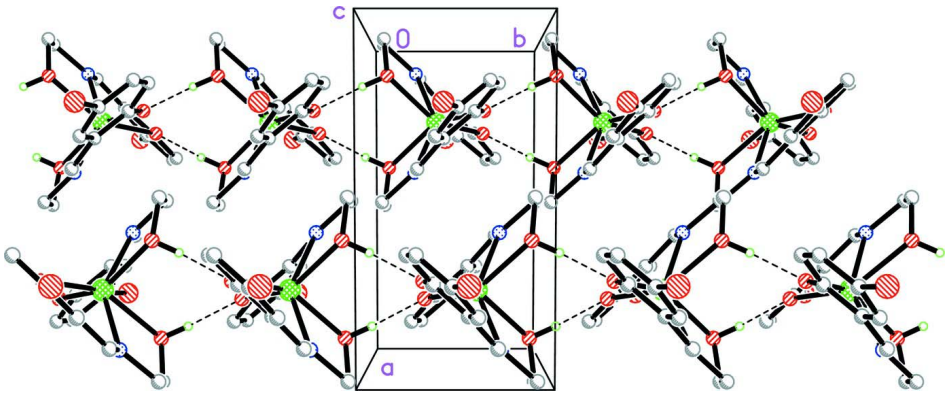

Figure 2

The packing of (I), viewed down the *c* axis. Hydrogen bonds are drawn as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

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Monoclinic, $P2/n$
Hall symbol: -P 2yac
$a = 10.207\ (4)$ Å
$b = 5.3275\ (19)$ Å
$c = 18.656\ (7)$ Å
$\beta = 99.156\ (4)°$
$V = 1001.5\ (6)$ Å^3
$Z = 2$
$F(000) = 580$
$D_x = 1.985$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1609 reflections
$\theta = 2.5–24.4°$
$\mu = 5.11$ mm^{-1}
$T = 298$ K
Block, colorless
0.23 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min} = 0.386$, $T_{max} = 0.428$
7794 measured reflections
2172 independent reflections
1524 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.1°$
$h = -13\rightarrow12$
$k = -6\rightarrow6$
$l = -23\rightarrow23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.126$
$S = 1.02$
2172 reflections
126 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.034P)^2 + 5.8476P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.41$ e Å^{-3}
$\Delta\rho_{min} = -1.55$ 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	0.2500	0.38621 (12)	0.2500	0.0491 (2)
Br1	0.21431 (12)	0.4350 (3)	0.64964 (5)	0.1157 (5)
N1	0.4104 (7)	0.2594 (14)	0.3415 (3)	0.0705 (19)
O1	0.2194 (5)	0.6681 (8)	0.3344 (2)	0.0577 (13)
O2	0.3921 (6)	0.0979 (9)	0.2021 (3)	0.0676 (14)
C1	0.3083 (7)	0.4314 (13)	0.4410 (3)	0.0529 (17)
C2	0.2245 (7)	0.6144 (12)	0.4037 (3)	0.0476 (15)
C3	0.1433 (9)	0.7475 (15)	0.4453 (4)	0.073 (2)
H3	0.0893	0.8751	0.4231	0.087*
C4	0.1407 (9)	0.6964 (18)	0.5174 (4)	0.081 (3)
H4	0.0842	0.7849	0.5428	0.097*
C5	0.2219 (9)	0.5144 (17)	0.5511 (4)	0.069 (2)
C6	0.3057 (8)	0.3868 (16)	0.5151 (4)	0.067 (2)
H6	0.3625	0.2677	0.5397	0.080*
C7	0.4004 (8)	0.2792 (17)	0.4087 (4)	0.073 (2)
H7	0.4597	0.1840	0.4407	0.088*
C8	0.5021 (11)	0.066 (2)	0.3211 (5)	0.112 (4)
H8A	0.5895	0.0913	0.3493	0.134*
H8B	0.4712	−0.0987	0.3329	0.134*
C9	0.5113 (10)	0.075 (2)	0.2490 (6)	0.113 (4)
H9A	0.5551	−0.0772	0.2366	0.136*
H9B	0.5676	0.2151	0.2409	0.136*
H2	0.358 (8)	−0.047 (7)	0.194 (5)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0826 (6)	0.0363 (3)	0.0287 (3)	0.000	0.0101 (3)	0.000
Br1	0.1431 (11)	0.1725 (13)	0.0387 (5)	0.0486 (9)	0.0363 (6)	0.0257 (6)
N1	0.082 (5)	0.092 (5)	0.038 (3)	0.029 (4)	0.011 (3)	−0.004 (3)
O1	0.107 (4)	0.038 (2)	0.030 (2)	0.007 (2)	0.018 (2)	0.0017 (18)
O2	0.084 (4)	0.056 (3)	0.064 (3)	−0.005 (3)	0.016 (3)	−0.026 (3)
C1	0.067 (5)	0.060 (4)	0.032 (3)	0.008 (3)	0.008 (3)	0.000 (3)
C2	0.074 (5)	0.037 (3)	0.033 (3)	−0.004 (3)	0.013 (3)	−0.002 (3)
C3	0.114 (7)	0.062 (5)	0.044 (4)	0.024 (5)	0.021 (4)	0.003 (4)
C4	0.111 (7)	0.095 (6)	0.042 (4)	0.033 (6)	0.030 (4)	0.000 (4)

C5	0.089 (6)	0.086 (5)	0.032 (4)	0.017 (5)	0.014 (4)	0.004 (4)
C6	0.083 (6)	0.081 (5)	0.036 (4)	0.021 (5)	0.006 (4)	0.004 (4)
C7	0.088 (6)	0.095 (6)	0.037 (4)	0.035 (5)	0.011 (4)	0.007 (4)
C8	0.112 (8)	0.166 (11)	0.059 (5)	0.078 (8)	0.020 (5)	0.005 (6)
C9	0.084 (7)	0.157 (11)	0.094 (7)	0.031 (7)	0.002 (6)	−0.069 (7)

Geometric parameters (Å, º)

Cd1—O1	2.233 (4)	C1—C7	1.443 (10)
Cd1—O1^{i}	2.233 (4)	C2—C3	1.413 (10)
Cd1—N1	2.272 (6)	C3—C4	1.376 (10)
Cd1—N1^{i}	2.272 (6)	C3—H3	0.9300
Cd1—O2^{i}	2.382 (5)	C4—C5	1.363 (11)
Cd1—O2	2.382 (5)	C4—H4	0.9300
Br1—C5	1.900 (7)	C5—C6	1.352 (11)
N1—C7	1.278 (8)	C6—H6	0.9300
N1—C8	1.482 (10)	C7—H7	0.9300
O1—C2	1.318 (7)	C8—C9	1.364 (13)
O2—C9	1.387 (11)	C8—H8A	0.9700
O2—H2	0.850 (10)	C8—H8B	0.9700
C1—C2	1.405 (9)	C9—H9A	0.9700
C1—C6	1.407 (9)	C9—H9B	0.9700
O1—Cd1—O1^{i}	95.5 (2)	C4—C3—C2	122.8 (7)
O1—Cd1—N1	80.5 (2)	C4—C3—H3	118.6
O1^{i}—Cd1—N1	124.4 (2)	C2—C3—H3	118.6
O1—Cd1—N1^{i}	124.4 (2)	C5—C4—C3	119.1 (7)
O1^{i}—Cd1—N1^{i}	80.5 (2)	C5—C4—H4	120.4
N1—Cd1—N1^{i}	145.4 (4)	C3—C4—H4	120.4
O1—Cd1—O2^{i}	90.41 (19)	C6—C5—C4	121.0 (7)
O1^{i}—Cd1—O2^{i}	149.32 (19)	C6—C5—Br1	119.7 (6)
N1—Cd1—O2^{i}	86.3 (2)	C4—C5—Br1	119.3 (6)
N1^{i}—Cd1—O2^{i}	71.4 (2)	C5—C6—C1	121.1 (7)
O1—Cd1—O2	149.32 (19)	C5—C6—H6	119.5
O1^{i}—Cd1—O2	90.41 (19)	C1—C6—H6	119.5
N1—Cd1—O2	71.4 (2)	N1—C7—C1	127.9 (7)
N1^{i}—Cd1—O2	86.3 (2)	N1—C7—H7	116.1
O2^{i}—Cd1—O2	99.7 (3)	C1—C7—H7	116.1
C7—N1—C8	117.5 (7)	C9—C8—N1	112.1 (8)
C7—N1—Cd1	123.5 (5)	C9—C8—H8A	109.2
C8—N1—Cd1	115.0 (5)	N1—C8—H8A	109.2
C2—O1—Cd1	123.9 (4)	C9—C8—H8B	109.2
C9—O2—Cd1	110.2 (5)	N1—C8—H8B	109.2
C9—O2—H2	109 (6)	H8A—C8—H8B	107.9
Cd1—O2—H2	113 (6)	C8—C9—O2	115.7 (9)
C2—C1—C6	119.8 (6)	C8—C9—H9A	108.3
C2—C1—C7	124.7 (6)	O2—C9—H9A	108.3
C6—C1—C7	115.5 (6)	C8—C9—H9B	108.3

O1—C2—C1	124.2 (6)	O2—C9—H9B	108.3
O1—C2—C3	119.7 (6)	H9A—C9—H9B	107.4
C1—C2—C3	116.2 (6)		

Symmetry code: (i) $-x+1/2, y, -z+1/2$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{ii}	0.85 (1)	1.75 (2)	2.599 (7)	173 (9)

Symmetry code: (ii) $-x+1/2, y-1, -z+1/2$.