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Bis{2-bromo-4-chloro-6-[(2-dimethylaminoethylimino)methyl]phenolato}-cadmium(II) monohydrate

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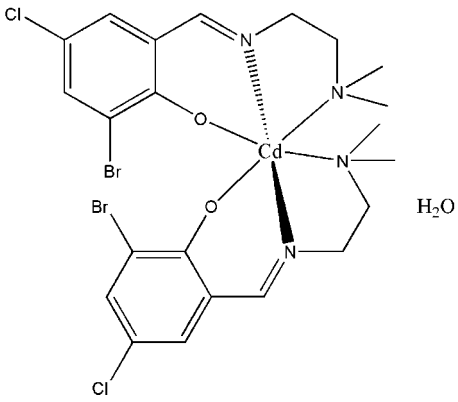
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.039; wR factor = 0.087; data-to-parameter ratio = 19.2.

In the title compound, $[Cd(C_{11}H_{13}BrClN_2O)_2]\cdot H_2O$, both the mononuclear cadmium(II) complex and the solvent water molecule lie on a crystallographic twofold rotation axis, which passes through the metal centre and the O atom of the water molecule. The Cd^{II} atom is six-coordinated in a severely distorted octahedral geometry by two phenolate O, two imine N and two amine N atoms from two Schiff base ligands. The water molecule is linked to the Cd^{II} complex molecule through O—H···O hydrogen bonds.

Related literature

For related literature, see: Cai *et al.* (2006); Cao (2007); Chakraborty *et al.* (2007); Das *et al.* (2007); Ghosh *et al.* (2007); Keypour *et al.* (2007); Li & Wang (2007*a*,*b*); Li & You (2007); Rahaman *et al.* (2006); Shashidhar *et al.* (2007); Wang & Li (2007); You *et al.* (2006).



Experimental

Crystal data

$[Cd(C_{11}H_{13}BrClN_2O)_2]\cdot H_2O$
M_r = 739.60
Orthorhombic, *Pbcn*
a = 12.4517 (18) Å
b = 9.2937 (14) Å
c = 23.254 (4) Å
V = 2691.1 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.01 mm^{-1}
T = 298 (2) K
0.32 × 0.30 × 0.27 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.293, T_{max} = 0.331
21549 measured reflections
3076 independent reflections
2184 reflections with $I > 2\sigma(I)$
R_{int} = 0.067

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.087
S = 1.02
3076 reflections
160 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O1	2.236 (3)	Cd1—N2	2.477 (3)
Cd1—N1	2.319 (3)		
O1^{i}—Cd1—O1	86.12 (14)	N1—Cd1—N2^{i}	95.34 (12)
O1—Cd1—N1	79.68 (10)	O1—Cd1—N2	147.12 (11)
O1—Cd1—N1^{i}	115.90 (11)	N1—Cd1—N2	72.83 (11)
N1—Cd1—N1^{i}	159.69 (16)	N2^{i}—Cd1—N2	110.01 (16)
O1—Cd1—N2^{i}	89.90 (11)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{ii}	0.85 (4)	2.14 (3)	2.911 (5)	152 (5)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: CI2399).

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supplementary materials

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Bis{2-bromo-4-chloro-6-[(2-dimethylaminoethylimino)methyl]phenolato}cadmium(II) monohydrate

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Comment

Cadmium complexes derived from Schiff bases have been widely studied for their structures and applications (Shashidhar *et al.*, 2007; Keypour *et al.*, 2007; Cao, 2007; Das *et al.*, 2007; Chakraborty *et al.*, 2007). Recently, we have reported a few transition metal complexes derived from Schiff bases (Li & Wang, 2007*a*,b; Li & You, 2007; Wang & Li, 2007). As a further investigation of the work on the structural characterization of such complexes, the title cadmium(II) complex, (I), is reported here.

The asymmetric unit of (I) contains one-half of the mononuclear cadmium(II) complex, with the other half related by a crystallographic twofold axis passing through the metal atom; the lattice water molecule also lies on the twofold axis (Fig. 1). The Cd^{II} atom is six-coordinated in an anti-trigonal bipyramidal geometry by two phenolate O, two imine N and two amine N atoms from two Schiff base ligands. The Cd—O and Cd—N bond lengths (Table 1) are comparable to the corresponding values observed in other Schiff base cadmium(II) complexes (Ghosh *et al.*, 2007; Rahaman *et al.*, 2006; You *et al.*, 2006; Cai *et al.*, 2006).

The water molecule is linked to the Cd^{II} complex molecule through O—H···O hydrogen bonds (Table 2).

Experimental

3-Bromo-5-chlorosalicylaldehyde (0.2 mmol, 47.0 mg) and *N*,*N*-dimethyl-1,2-diaminoethane (0.2 mmol, 17.6 mg) were dissolved in a methanol solution (20 ml). The mixture was stirred at room temperature for 30 min, giving a clear yellow solution. To this solution was added an aqueous solution (2 ml) of $Cd(NO_3)_2{\cdot}4H_2O$ (0.1 mmol, 30.8 mg) with stirring. The resulting mixture was stirred for a further 30 min at room temperature, giving a clear colourless solution. After allowing the solution to stand in air for a week, colourless block-shaped crystals were formed.

Refinement

Atom H2 was located from a difference Fourier map and its positional parameters were refined, with thw O—H distance restrained to 0.85 (1) Å. Other H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

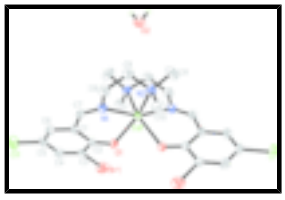

Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids. unlabelled atoms are related to labelled atoms by the symmetry operation (−*x*, *y*, 1/2 − *z*).

Bis{2-bromo-4-chloro-6-[(2-dimethylaminoethylimino)methyl]phenolato}cadmium(II) monohydrate

Crystal data

$[Cd(C_{11}H_{13}BrClN_2O)_2]\cdot H_2O$	F_{000} = 1456
M_r = 739.60	D_x = 1.826 Mg m^{-3}
Orthorhombic, *Pbcn*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2n 2ab	Cell parameters from 2827 reflections
a = 12.4517 (18) Å	θ = 2.5–24.3º
b = 9.2937 (14) Å	μ = 4.01 mm^{-1}
c = 23.254 (4) Å	*T* = 298 (2) K
V = 2691.1 (7) Å^3	Block, colourless
Z = 4	0.32 × 0.30 × 0.27 mm

Data collection

Bruker SMART CCD area-detector diffractometer	3076 independent reflections
Radiation source: fine-focus sealed tube	2184 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.067
T = 298(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −16→16
T_{min} = 0.293, T_{max} = 0.331	*k* = −11→11
21549 measured reflections	*l* = −30→29

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.039	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.087	$w = 1/[\sigma^2(F_o^2) + (0.0149P)^2 + 3.7768P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.001
3076 reflections	$\Delta\rho_{max}$ = 0.62 e Å^{-3}

160 parameters	$\Delta\rho_{min} = -0.58$ e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.0000	0.16643 (4)	0.2500	0.03424 (12)
Br1	−0.05873 (5)	−0.18375 (6)	0.41005 (2)	0.07325 (19)
Cl1	0.31949 (15)	−0.02044 (18)	0.51342 (6)	0.1009 (6)
O1	0.0340 (2)	−0.0093 (3)	0.31307 (11)	0.0424 (7)
O2	0.0000	0.7240 (5)	0.2500	0.0646 (12)
N1	0.1798 (3)	0.2104 (4)	0.26903 (15)	0.0417 (8)
N2	0.0692 (3)	0.3193 (4)	0.17098 (15)	0.0447 (8)
C1	0.1937 (3)	0.0785 (4)	0.35954 (17)	0.0406 (9)
C2	0.0964 (3)	−0.0023 (4)	0.35705 (17)	0.0394 (9)
C3	0.0726 (4)	−0.0801 (4)	0.40812 (18)	0.0477 (11)
C4	0.1371 (5)	−0.0844 (5)	0.45538 (18)	0.0585 (13)
H4	0.1171	−0.1367	0.4878	0.070*
C5	0.2326 (4)	−0.0096 (6)	0.45414 (19)	0.0593 (13)
C6	0.2605 (4)	0.0715 (5)	0.40785 (19)	0.0545 (12)
H6	0.3246	0.1228	0.4083	0.065*
C7	0.2305 (3)	0.1734 (4)	0.31383 (18)	0.0455 (10)
H7	0.2992	0.2112	0.3180	0.055*
C8	0.2352 (4)	0.3090 (5)	0.2292 (2)	0.0542 (12)
H8A	0.2760	0.2535	0.2014	0.065*
H8B	0.2852	0.3687	0.2505	0.065*
C9	0.1559 (4)	0.4034 (5)	0.1981 (2)	0.0549 (12)
H9A	0.1249	0.4711	0.2251	0.066*
H9B	0.1933	0.4581	0.1688	0.066*
C10	0.1122 (4)	0.2283 (6)	0.1254 (2)	0.0680 (15)
H10A	0.0541	0.1872	0.1038	0.102*
H10B	0.1546	0.1526	0.1420	0.102*
H10C	0.1564	0.2851	0.1003	0.102*
C11	−0.0104 (4)	0.4182 (6)	0.1473 (2)	0.0741 (16)
H11A	0.0225	0.4771	0.1183	0.111*

H11B	−0.0379	0.4784	0.1775	0.111*
H11C	−0.0683	0.3643	0.1306	0.111*
H2	0.002 (5)	0.783 (4)	0.2779 (15)	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0320 (2)	0.0349 (2)	0.0359 (2)	0.000	−0.00174 (18)	0.000
Br1	0.0855 (4)	0.0647 (3)	0.0695 (4)	−0.0195 (3)	0.0068 (3)	0.0153 (3)
Cl1	0.1271 (14)	0.1097 (13)	0.0658 (9)	0.0133 (11)	−0.0591 (9)	0.0031 (8)
O1	0.0469 (16)	0.0394 (15)	0.0407 (16)	−0.0071 (13)	−0.0115 (13)	0.0045 (12)
O2	0.065 (3)	0.052 (3)	0.077 (4)	0.000	−0.003 (3)	0.000
N1	0.0326 (18)	0.045 (2)	0.048 (2)	−0.0032 (15)	0.0034 (15)	0.0044 (15)
N2	0.046 (2)	0.043 (2)	0.046 (2)	−0.0001 (17)	0.0015 (16)	0.0080 (16)
C1	0.043 (2)	0.037 (2)	0.042 (2)	0.0086 (19)	−0.0100 (19)	−0.0043 (18)
C2	0.043 (2)	0.032 (2)	0.043 (2)	0.0052 (18)	−0.0038 (18)	−0.0039 (18)
C3	0.063 (3)	0.035 (2)	0.045 (2)	0.002 (2)	−0.001 (2)	0.0033 (19)
C4	0.091 (4)	0.052 (3)	0.032 (2)	0.011 (3)	−0.006 (2)	0.005 (2)
C5	0.079 (4)	0.056 (3)	0.042 (3)	0.018 (3)	−0.024 (2)	−0.007 (2)
C6	0.055 (3)	0.049 (3)	0.059 (3)	0.011 (2)	−0.019 (2)	−0.009 (2)
C7	0.033 (2)	0.044 (2)	0.059 (3)	−0.0027 (19)	−0.005 (2)	−0.010 (2)
C8	0.042 (3)	0.061 (3)	0.059 (3)	−0.010 (2)	0.003 (2)	0.009 (2)
C9	0.057 (3)	0.047 (3)	0.061 (3)	−0.009 (2)	0.007 (2)	0.007 (2)
C10	0.089 (4)	0.066 (3)	0.049 (3)	−0.017 (3)	0.014 (3)	0.001 (2)
C11	0.059 (3)	0.078 (4)	0.085 (4)	0.007 (3)	0.002 (3)	0.043 (3)

Geometric parameters (Å, °)

Cd1—O1^{i}	2.236 (3)	C2—C3	1.421 (6)
Cd1—O1	2.236 (3)	C3—C4	1.361 (6)
Cd1—N1	2.319 (3)	C4—C5	1.378 (7)
Cd1—N1^{i}	2.319 (3)	C4—H4	0.93
Cd1—N2^{i}	2.477 (3)	C5—C6	1.359 (7)
Cd1—N2	2.477 (3)	C6—H6	0.93
Br1—C3	1.899 (5)	C7—H7	0.93
Cl1—C5	1.756 (4)	C8—C9	1.505 (6)
O1—C2	1.286 (4)	C8—H8A	0.97
O2—H2	0.85 (4)	C8—H8B	0.97
N1—C7	1.266 (5)	C9—H9A	0.97
N1—C8	1.475 (5)	C9—H9B	0.97
N2—C10	1.459 (6)	C10—H10A	0.96
N2—C11	1.459 (6)	C10—H10B	0.96
N2—C9	1.475 (5)	C10—H10C	0.96
C1—C6	1.400 (5)	C11—H11A	0.96
C1—C2	1.426 (6)	C11—H11B	0.96
C1—C7	1.455 (6)	C11—H11C	0.96
O1^{i}—Cd1—O1	86.12 (14)	C3—C4—H4	120.8
O1^{i}—Cd1—N1	115.90 (11)	C5—C4—H4	120.8

O1—Cd1—N1	79.68 (10)	C6—C5—C4	121.2 (4)
O1^{i}—Cd1—N1^{i}	79.68 (10)	C6—C5—Cl1	119.7 (4)
O1—Cd1—N1^{i}	115.90 (11)	C4—C5—Cl1	119.1 (4)
N1—Cd1—N1^{i}	159.69 (16)	C5—C6—C1	120.6 (5)
O1^{i}—Cd1—N2^{i}	147.12 (11)	C5—C6—H6	119.7
O1—Cd1—N2^{i}	89.90 (11)	C1—C6—H6	119.7
N1—Cd1—N2^{i}	95.34 (12)	N1—C7—C1	127.5 (4)
N1^{i}—Cd1—N2^{i}	72.83 (11)	N1—C7—H7	116.3
O1^{i}—Cd1—N2	89.90 (11)	C1—C7—H7	116.3
O1—Cd1—N2	147.12 (11)	N1—C8—C9	110.9 (4)
N1—Cd1—N2	72.83 (11)	N1—C8—H8A	109.5
N1^{i}—Cd1—N2	95.34 (12)	C9—C8—H8A	109.5
N2^{i}—Cd1—N2	110.01 (16)	N1—C8—H8B	109.5
C2—O1—Cd1	126.8 (2)	C9—C8—H8B	109.5
C7—N1—C8	116.9 (4)	H8A—C8—H8B	108.0
C7—N1—Cd1	126.2 (3)	N2—C9—C8	112.1 (4)
C8—N1—Cd1	116.2 (3)	N2—C9—H9A	109.2
C10—N2—C11	109.9 (4)	C8—C9—H9A	109.2
C10—N2—C9	110.4 (4)	N2—C9—H9B	109.2
C11—N2—C9	108.9 (4)	C8—C9—H9B	109.2
C10—N2—Cd1	109.6 (3)	H9A—C9—H9B	107.9
C11—N2—Cd1	113.9 (3)	N2—C10—H10A	109.5
C9—N2—Cd1	104.0 (2)	N2—C10—H10B	109.5
C6—C1—C2	120.9 (4)	H10A—C10—H10B	109.5
C6—C1—C7	115.3 (4)	N2—C10—H10C	109.5
C2—C1—C7	123.9 (4)	H10A—C10—H10C	109.5
O1—C2—C3	120.8 (4)	H10B—C10—H10C	109.5
O1—C2—C1	124.9 (4)	N2—C11—H11A	109.5
C3—C2—C1	114.3 (4)	N2—C11—H11B	109.5
C4—C3—C2	124.5 (4)	H11A—C11—H11B	109.5
C4—C3—Br1	118.3 (4)	N2—C11—H11C	109.5
C2—C3—Br1	117.2 (3)	H11A—C11—H11C	109.5
C3—C4—C5	118.5 (4)	H11B—C11—H11C	109.5

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{ii}	0.85 (4)	2.14 (3)	2.911 (5)	152 (5)

Symmetry codes: (ii) *x*, *y*+1, *z*.

Fig. 1