

{4-Bromo-2-[3-(dimethylamino)propylimino-methyl]phenolato}dichlorozinc(II)**Xiao-Yang Qiu**

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Key indicators

Single-crystal X-ray study
 $T = 298\text{ K}$
 Mean $\sigma(\text{C}-\text{C}) = 0.010\text{ \AA}$
 R factor = 0.050
 wR factor = 0.139
 Data-to-parameter ratio = 13.8

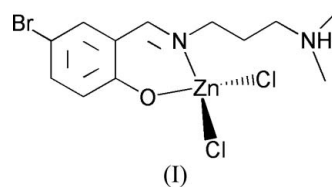
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound, $[\text{ZnCl}_2(\text{C}_{12}\text{H}_{17}\text{BrN}_2\text{O})]$, is a mononuclear Schiff base zinc(II) complex. The Zn atom is tetrahedrally coordinated by one phenolate O atom and one imine N atom of the Schiff base, and by two chloride anions. In the crystal structure, molecules are linked through intermolecular N—H \cdots O and C—H \cdots Cl interactions, forming layers parallel to the bc plane.

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Comment

Zinc(II) complexes are very important in biological chemistry (Weston, 2005; Henkel & Krebs, 2004). They function as the active site of hydrolytic enzymes, such as carboxypeptidase and carbonic anhydrase (Bertini *et al.*, 1994; Lipscomb & Sträter, 1996). The structure of a new zinc(II) complex, (I), derived from the Schiff base 4-bromo-2-[3-(dimethylamino)propyliminomethyl]phenol is reported here.



Compound (I) is a mononuclear zinc(II) complex, in which the Schiff base ligand is in a zwitterionic form, with the dimethylamino N atom protonated (Fig. 1). The Zn atom is

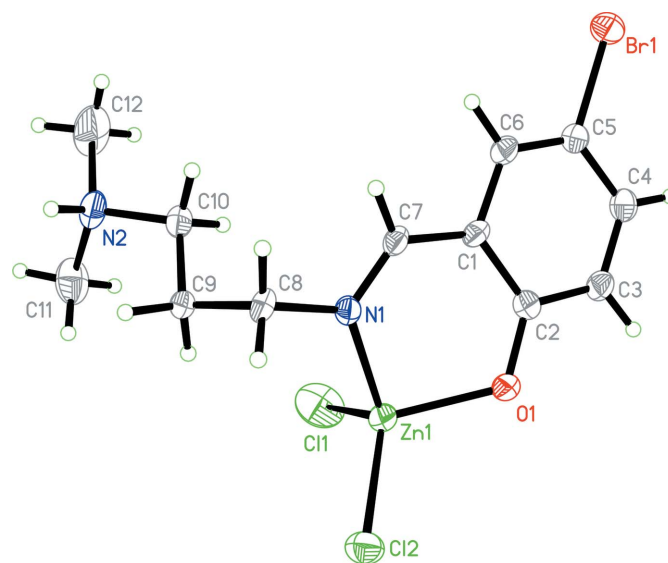


Figure 1
 The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

tetrahedrally coordinated by the phenolate O atom and the imine N atom of the Schiff base, and by two chloride anions. The Zn—O and Zn—N bond lengths (Table 1) are comparable to the corresponding values observed in other Schiff base zinc(II) complexes (Tatar *et al.*, 1999; Qiu, 2006). Atoms in the N1/C8—C10/N2/C11 (or C12) chain adopts a *trans* configuration to minimize steric effects.

In the crystal structure, molecules are linked through intermolecular N—H···O and C—H···Cl interactions (Table 2), forming layers parallel to the *bc* plane (Fig. 2).

Experimental

A mixture of 5-bromosalicylaldehyde (1.0 mmol, 202.1 mg), *N,N*-dimethyl-1,3-diaminopropane (1.0 mmol, 102.3 mg) and ZnCl₂ (1.0 mmol, 136.3 mg) was dissolved in ethanol (100 ml). The mixture was stirred for about 1 h at room temperature to give a clear colourless solution. After allowing the solution to stand still in air for 9 d, colourless block-shaped crystals were formed.

Crystal data

[ZnCl ₂ (C ₁₂ H ₁₇ BrN ₂ O)]	Z = 4
<i>M_r</i> = 421.46	<i>D_x</i> = 1.673 Mg m ⁻³
Monoclinic, <i>P</i> 2 ₁ / <i>n</i>	Mo <i>K</i> α radiation
<i>a</i> = 6.938 (1) Å	<i>μ</i> = 4.17 mm ⁻¹
<i>b</i> = 15.202 (1) Å	<i>T</i> = 298 (2) K
<i>c</i> = 15.906 (1) Å	Block, colourless
<i>β</i> = 94.058 (1)°	0.18 × 0.17 × 0.12 mm
<i>V</i> = 1673.4 (3) Å ³	

Data collection

Bruker SMART APEX 1000 CCD area-detector diffractometer	7159 measured reflections
<i>ω</i> scans	2457 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1682 reflections with <i>I</i> > 2σ(<i>I</i>)
<i>T_{min}</i> = 0.521, <i>T_{max}</i> = 0.635	<i>R_{int}</i> = 0.048
	<i>θ_{max}</i> = 23.5°

Refinement

Refinement on <i>F</i> ²	$w = 1/[\sigma^2(F_o^2) + (0.0627P)^2 + 2.2538P]$
$R[F^2 > 2\sigma(F^2)] = 0.050$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.139$	(Δ/σ) _{max} < 0.001
<i>S</i> = 1.05	$\Delta\rho_{max} = 0.96 \text{ e } \text{Å}^{-3}$
2457 reflections	$\Delta\rho_{min} = -0.80 \text{ e } \text{Å}^{-3}$
178 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1

Selected geometric parameters (Å, °).

Zn1—O1	1.967 (5)	Zn1—Cl2	2.205 (2)
Zn1—N1	2.006 (5)	Zn1—Cl1	2.233 (3)
O1—Zn1—N1	94.8 (2)	O1—Zn1—Cl1	113.23 (18)
O1—Zn1—Cl2	110.32 (16)	N1—Zn1—Cl1	107.09 (18)
N1—Zn1—Cl2	113.49 (18)	Cl2—Zn1—Cl1	115.99 (10)

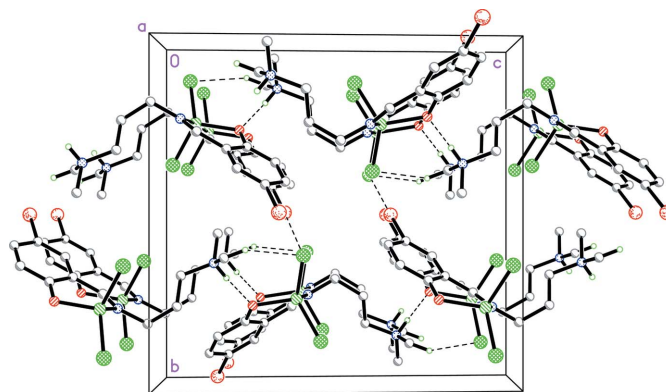


Figure 2

The crystal packing of (I). Intermolecular N—H···O and C—H···Cl hydrogen bonds are shown as dashed lines.

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N2—H2···O1 ¹	0.91 (5)	1.98 (5)	2.867 (8)	168 (6)
C11—H11A···Cl2 ²	0.96	2.80	3.609 (8)	142 (6)

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

The crystal was very weakly diffracting and data of significant intensity could not be obtained beyond $\theta = 23.5^\circ$. Atom H2 was located in a difference Fourier map and refined isotropically, with the N—H distance restrained to 0.90 (1) Å. The other H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H = 0.93–0.97 Å and *U_{iso}*(H) = 1.2 or 1.5*U_{eq}*(C).

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

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