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## Key indicators

Single-crystal X-ray study  
 $T = 298\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$   
 $R$  factor = 0.044  
 $wR$  factor = 0.100  
Data-to-parameter ratio = 21.3

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

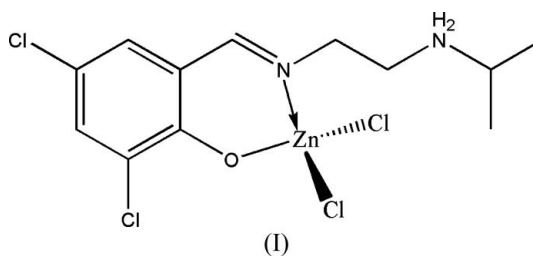
## Dichloro{2,4-dichloro-6-[2-(isopropylammonio)-ethyliminomethyl]phenolato}zinc(II)

The title complex,  $[\text{ZnCl}_2(\text{C}_{12}\text{H}_{16}\text{Cl}_2\text{N}_2\text{O})]$ , is a mononuclear Schiff base zinc(II) compound. The tetrahedral Zn atom is coordinated by one imine N and one phenolate O atoms of the Schiff base ligand and by two chloride anions. The crystal structure is stabilized by intermolecular  $\text{N}-\text{H}\cdots\text{Cl}$  and  $\text{C}-\text{H}\cdots\text{Cl}$  hydrogen bonds.

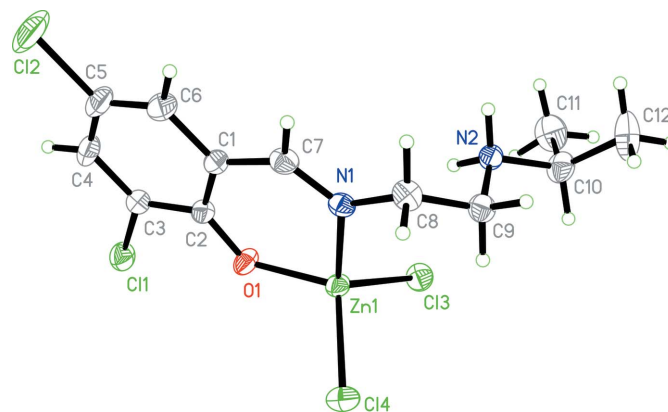
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## Comment

Zinc(II) complexes derived from Schiff bases have been studied extensively due to their interesting structures and applications (Lacroix *et al.*, 1996; Chisholm *et al.*, 2001; Jian *et al.*, 2004; Tatar *et al.*, 2002; Bhosekar *et al.*, 2006). The condensation reaction of aromatic carbaldehydes with primary amines has been shown to offer an easy and inexpensive way of forming a variety of polydentate Schiff base ligands and, as part of a further investigation of the structures of Schiff base zinc(II) complexes, the title mononuclear zinc(II) complex, (I), is reported here.



The tetrahedral  $\text{Zn}^{\text{II}}$  in (I) is coordinated by one imine N and one phenolate O atoms of the Schiff base ligand and by



**Figure 1**  
The molecular structure of the title complex, shown with 30% probability displacement ellipsoids.

two Cl anions (Fig. 1). The coordination bond distances are typical (Table 1). The O1–Zn1–N1 and N1–Zn1–Cl3 angles deviate most from ideal tetrahedral geometry, with values of 97.15 (10) and 114.97 (8)°, respectively. The other angles in the coordination environment are in the range 108.66 (7)–113.82 (7)° (Table 1). The crystal structure is stabilized by intermolecular N–H···Cl and C–H···Cl hydrogen bonds (Table 2).

### Experimental

Compound (I) was obtained by refluxing 3,5-dichloro-2-hydroxybenzaldehyde (0.2 mmol, 38.3 mg), *N*-isopropyl-1,2-diaminoethane (0.2 mmol, 20.6 mg) and zinc(II) chloride (0.2 mmol, 27.2 mg) in methanol (30 ml) for 1 h. After cooling, the reaction mixture was filtered. Colourless single crystals suitable for X-ray diffraction were formed from the filtrate after 3 d.

#### Crystal data

[ZnCl <sub>2</sub> (C <sub>12</sub> H <sub>16</sub> Cl <sub>2</sub> N <sub>2</sub> O)]	Z = 4
<i>M<sub>r</sub></i> = 411.44	<i>D<sub>x</sub></i> = 1.595 Mg m <sup>-3</sup>
Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>c</i>	Mo <i>K</i> α radiation
<i>a</i> = 12.345 (2) Å	<i>μ</i> = 2.05 mm <sup>-1</sup>
<i>b</i> = 10.390 (1) Å	<i>T</i> = 298 (2) K
<i>c</i> = 13.569 (2) Å	Block, colourless
<i>β</i> = 100.143 (2)°	0.22 × 0.18 × 0.15 mm
<i>V</i> = 1713.2 (4) Å <sup>3</sup>	

#### Data collection

Bruker SMART APEX area detector diffractometer	14232 measured reflections
<i>ω</i> scans	3902 independent reflections
Absorption correction: multi-scan ( <i>SADABS</i> ; Sheldrick, 1996)	2856 reflections with <i>I</i> > 2σ( <i>I</i> )
<i>T<sub>min</sub></i> = 0.661, <i>T<sub>max</sub></i> = 0.748	<i>R<sub>int</sub></i> = 0.049
	<i>θ<sub>max</sub></i> = 27.5°

#### Refinement

Refinement on <i>F</i> <sup>2</sup>	H-atom parameters constrained
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )] = 0.044	<i>w</i> = 1/[σ <sup>2</sup> ( <i>F<sub>o</sub></i> <sup>2</sup> ) + (0.039 <i>P</i> ) <sup>2</sup> + 0.3267 <i>P</i> ]
<i>wR</i> ( <i>F</i> <sup>2</sup> ) = 0.100	where <i>P</i> = ( <i>F<sub>o</sub></i> <sup>2</sup> + 2 <i>F<sub>c</sub></i> <sup>2</sup> )/3
<i>S</i> = 1.04	(Δ/σ) <sub>max</sub> < 0.001
3902 reflections	Δρ <sub>max</sub> = 0.37 e Å <sup>-3</sup>
183 parameters	Δρ <sub>min</sub> = -0.39 e Å <sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Zn1–O1	1.922 (2)	Zn1–Cl3	2.2314 (9)
Zn1–N1	2.013 (3)	Zn1–Cl4	2.2473 (9)
O1–Zn1–N1	97.15 (10)	O1–Zn1–Cl4	113.82 (7)
O1–Zn1–Cl3	111.98 (7)	N1–Zn1–Cl4	108.66 (7)
N1–Zn1–Cl3	114.97 (8)	Cl3–Zn1–Cl4	109.82 (4)

**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 <i>A</i> ···Cl4 <sup>i</sup>	0.90	2.34	3.241 (3)	177
N2–H2 <i>B</i> ···Cl3	0.90	2.65	3.302 (3)	130
N2–H2 <i>B</i> ···Cl4 <sup>ii</sup>	0.90	2.72	3.369 (3)	130
C9–H9 <i>A</i> ···Cl1 <sup>iii</sup>	0.97	2.74	3.553 (3)	141
C10–H10···Cl2 <sup>iv</sup>	0.98	2.81	3.660 (3)	146

Symmetry codes: (i) *x*, -*y* + ½, *z* + ½; (ii) -*x*, *y* + ½, -*z* + ½; (iii) -*x*, *y* - ½, -*z* + ½; (iv) *x* + 1, *y*, *z*.

All H atom positions were positioned geometrically (C–H = 0.93–0.97 Å and N–H = 0.90 Å) and refined as riding, with *U<sub>iso</sub>*(H) values set at 1.2 or 1.5*U<sub>eq</sub>*(C,N).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINTE* (Siemens, 1996); data reduction: *SAINTE*; 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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