metal-organic compounds

Dichlorobis[2-(*o*-tolyliminiomethyl)-phenolato-*O*]zinc(II)

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In the mononuclear title compound, [ZnCl$_2$(C$_{14}$H$_{13}$NO)$_2$], the Zn^{II} ion is located on a twofold axis of the monoclinic space group so that the whole molecule has a twofold symmetry. The Zn^{II} ion has a tetrahedral coordination consisting of two chlorine ions and the O atoms of the ligands. The coordination angles around zinc have values between 102.89 (8) (O—Zn—O) and 115.83 (5)° (Cl—Zn—O). The Zn—O and Zn—Cl bond lengths are 1.977 (2) and 2.2401 (7) Å, respectively. There are intra- and intermolecular hydrogen bonds in the structure.

Comment

The structures of zinc complexes having different ligands have been a subject of interest in our laboratory. The coordination properties and geometric parameters are available from the crystal structure studies of tetraaquabis(*p*-nitrosalicyl-ato)zinc(II) (Tahir *et al.*, 1997), bis[1-(3-chloro-4-methyl-phenyl)iminomethylbenzen-2-oxy-*O*,*N*]zinc(II) (Tatar, Canel *et al.*, 1999), [*μ*-*N*,*N*'-bis(salicylidene)-1,3-propanediaminato]-methanolatozinc(II) dichlorozinc(II) (Atakol *et al.*, 1999) and zinc(II) complexes of bidentate Schiff base ligands containing methoxyphenyl and nitrophenyl groups (Tatar, Ülkü & Atakol, 1999). Zinc is known to activate several enzymes, which makes it an essential element in living organisms.
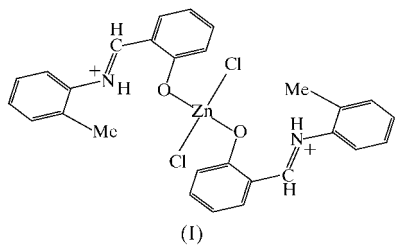
Therefore, its chemical and structural properties are constantly under investigation. Among the zinc compounds, there are monomeric complexes in which the Zn atom is tetrahedrally coordinated, as well as dimeric complexes with phenolate bridges and a trigonal bipyramidal coordination, as reported in the literature cited above and the references therein. We report here the structure of a new zinc complex, (I), obtained from the reaction of a Schiff base with ZnCl$_2$.

The [ZnCl$_2$(C$_{14}$H$_{13}$NO)$_2$] molecule has a twofold symmetry with respect to the twofold rotation axis, on which the Zn^{II} ion is located. The tetrahedral coordination around the Zn^{II} ion, involving two Cl and two ligand O atoms, is slightly distorted; the Zn—Cl and Zn—O bond lengths are 2.2401 (7) and 1.977 (2) Å, respectively. The degree of distortion from ideal tetrahedral geometry is also given by the minimum [102.89 (5)° for O1—Zn—O1^i] and maximum [115.83 (5)° for Cl—Zn—O1] coordination angles around zinc. The six-membered rings of the ligand have usual values. The dihedral angle between the two rings defined by the C1–C6 and C8–C13 atoms is 20.29 (13)°. An inspection of the possible hydrogen bonds indicate an intramolecular N1—H1···O1 hydrogen bond, with a *D*—H distance of 2.600 (2) Å, and two intermolecular hydrogen bonds, C7—H7···Cl^i and C9—H9···Cl^i, with *D*—*A* distances of 3.6058 (17) and 3.766 (3) Å, respectively [symmetry code: (i) $x, -y, \frac{1}{2} + z$]. These hydrogen bonds are rather weak interactions, as can be seen from the details given in Table 2.
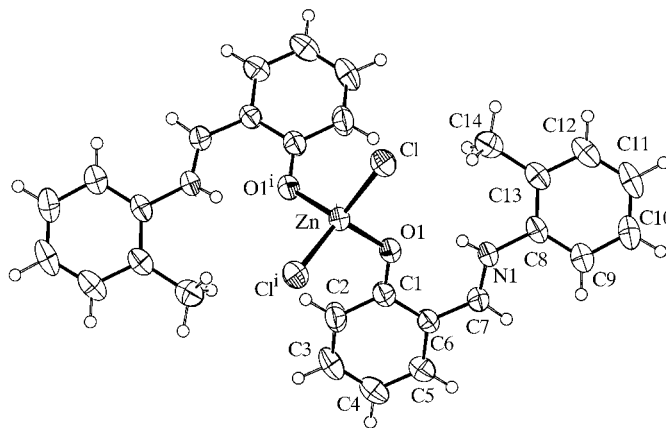

Figure 1
PLATON (Spek, 1999) drawing of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level [symmetry code: (i) $1 - x, y, \frac{1}{2} - z$].

Experimental

To obtain the title compound, 2-(2-methylphenyliminomethyl)phenol (0.211 g, 0.001 mmol) was dissolved in hot methanol (40 ml). ZnCl$_2$ (0.069 g, 0.0005 mol) in hot methanol (20 ml) was then added and the resulting solution set aside for 48 h. Crystals suitable for X-ray measurements were filtered off and dried in air.

Crystal data

[ZnCl$_2$(C$_{14}$H$_{13}$NO)$_2$]	$D_x = 1.450$ Mg m^{-3}
$M_r = 558.808$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 25
$a = 16.0495\ (11)$ Å	reflections
$b = 10.5240\ (13)$ Å	$\theta = 11.80$–$20.98°$
$c = 15.6324\ (12)$ Å	$\mu = 1.197$ mm^{-1}
$\beta = 104.232\ (2)°$	$T = 295$ K
$V = 2559.4\ (4)$ Å^3	Prism, yellow
$Z = 4$	$0.35 \times 0.25 \times 0.15$ mm

Data collection

Enraf–Nonius CAD-4 diffract-ometer	$R_{int} = 0.010$
$\omega/2\theta$ scans	$\theta_{max} = 25.26°$
Absorption correction: empirical *via* ψ scans (Fair, 1990)	$h = -18 \rightarrow 19$
	$k = -12 \rightarrow 0$
$T_{min} = 0.694$, $T_{max} = 0.836$	$l = -18 \rightarrow 0$
2565 measured reflections	3 standard reflections
2467 independent reflections	frequency: 120 min
1929 reflections with $I > 3\sigma(I)$	intensity decay: 1.792%

Refinement

Refinement on F	$w = 1/[\sigma F^2 + (0.02F)^2 + 0.4]$, except $w = 0$ if $F^2 <$ cutoff $\times \sigma F^2$ (cutoff is 3.0)
$R = 0.028$	
$wR = 0.037$	
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
1929 reflections	$\Delta\rho_{max} = 0.27$ e Å^{-3}
159 parameters	$\Delta\rho_{min} = -0.19$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Zn—Cl	2.2401 (7)	N1—C7	1.299 (3)
Zn—O1	1.977 (2)	N1—C8	1.423 (3)
O1—C1	1.311 (3)		
Cl—Zn—O1	106.14 (5)	O1—Zn—O1^i	102.89 (8)
Cl—Zn—Cl^i	110.16 (3)	Zn—O1—C1	125.7 (1)
Cl—Zn—O1^i	115.83 (5)	C7—N1—C8	126.8 (2)

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

H atoms were placed geometrically at distances of 0.95 Å from their parent atoms and were refined as riding with $U_{iso} = 1.3U_{eq}(C)$. The hydrogen-bond calculations were carried out with *PARST*95 (Nardelli, 1995). The difference map clearly shows a peak 0.91 Å from the N atom and no residual density around oxygen.

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$\cdots$O1	0.95	1.8442	2.600 (2)	134
C7—H7$\cdots$Cl^i	0.95	2.7056	3.606 (2)	158
C9—H9$\cdots$Cl^i	0.95	2.8185	3.766 (3)	170

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

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1993); data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SIR* in *MolEN*; program(s) used to refine structure: *LSFM* in *MolEN*; molecular graphics: *PLATON*99 (Spek, 1999); software used to prepare material for publication: *MolEN*.

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