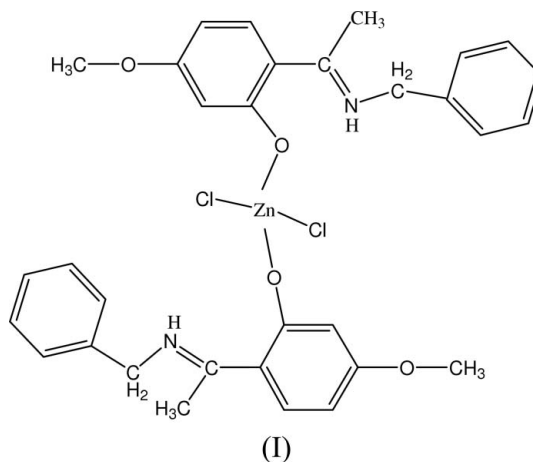


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xutongtao_1968@163.com**Key indicators**Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.007$ Å
 R factor = 0.042
 wR factor = 0.119
Data-to-parameter ratio = 15.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**Bis{2-[1-(benzylimino)ethyl]-5-methoxyphenol}dichlorozinc(II)**

The title complex, $[\text{ZnCl}_2(\text{C}_{16}\text{H}_{17}\text{NO}_2)_2]$, displays a distorted tetrahedral coordination geometry around the Zn^{II} ion. The Schiff base inner salt, (benzylimino)ethyl-5-methoxyphenol, coordinates in a monodentate manner to the Zn^{II} ion *via* the deprotonated hydroxy groups. The protonated imino groups form intramolecular hydrogen bonds with the deprotonated hydroxyl groups of the same Schiff base ligand.

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Paenol, 2-hydroxyl-4-methoxyacetophenone, is an effective component of traditional Chinese medicines, and its derivatives have attracted considerable attention because of their potential biological properties. As part of our ongoing investigation on Schiff base compounds of paenol, we present here the structure of the title Zn^{II} complex, (I).

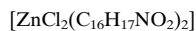


The molecular structure of (I) is shown in Fig. 1. Two Schiff base inner salts, (benzylimino)ethyl-5-methoxyphenol, coordinate to the Zn^{II} ion *via* their deprotonated hydroxyl groups; two Cl^- ions coordinate to the Zn^{II} ion to complete the distorted tetrahedral coordination geometry (Table 1). The protonated imino groups form intramolecular hydrogen bonds with the deprotonated hydroxyl groups of the same Schiff base (Table 2).

Experimental

To a stirred absolute methanol solution (30 ml) of paenol (1 mmol) and $\text{ZnCl}_2 \cdot 2\text{H}_2\text{O}$ (1 mmol) was added dropwise an absolute methanol solution (10 ml) of benzylamine (1 mmol) at room temperature. After stirring for 2 h at 320 K, the precipitate was filtered off, washed with methanol and dried *in vacuo*. Single crystals of (I) were obtained by slow evaporation of the resulting filtrate after 16 d.

Crystal data

 $M_r = 646.88$ Monoclinic, $P2_1/c$ $a = 11.1785$ (18) Å $b = 16.082$ (3) Å $c = 17.555$ (3) Å $\beta = 97.928$ (3)° $V = 3125.7$ (9) Å³ $Z = 4$ $D_x = 1.375$ Mg m⁻³Mo $K\alpha$ radiation $\mu = 1.00$ mm⁻¹ $T = 298$ (2) K

Prism, colorless

 $0.49 \times 0.45 \times 0.40$ mm

Data collection

Bruker APEX area-detector diffractometer

 φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 2002)

 $T_{\min} = 0.618$, $T_{\max} = 0.670$

16847 measured reflections

5827 independent reflections

3546 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.053$ $\theta_{\text{max}} = 25.5^\circ$

Refinement

Refinement on F^2 $R[F^2 > 2\sigma(F^2)] = 0.042$ $wR(F^2) = 0.119$ $S = 1.04$

5827 reflections

374 parameters

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0436P)^2 + 1.2861P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} = 0.001$ $\Delta\rho_{\text{max}} = 0.46$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.30$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Zn1—O1	1.964 (2)	N1—C2	1.308 (5)
Zn1—O3	1.987 (2)	N1—C10	1.453 (5)
Zn1—Cl1	2.2303 (12)	N2—C18	1.292 (5)
Zn1—Cl2	2.2178 (11)	N2—C26	1.470 (5)
O1—Zn1—O3	108.13 (10)	O1—Zn1—Cl1	102.80 (8)
O1—Zn1—Cl2	113.27 (8)	O3—Zn1—Cl1	110.58 (8)
O3—Zn1—Cl2	102.41 (7)	Cl1—Zn1—Cl2	119.42 (5)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 \cdots O1	0.97	1.63	2.543 (4)	156
N2—H2 \cdots O3	0.97	1.77	2.545 (4)	134

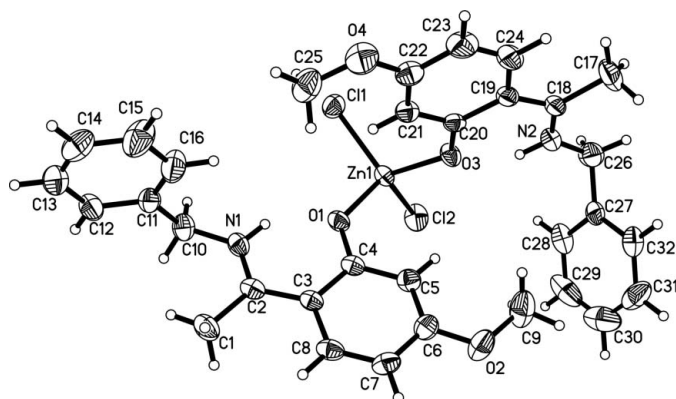


Figure 1

The molecular structure of (I), with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

The H atoms on imino N atoms were located in a difference Fourier map and refined as riding in their as-found relative positions with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{N})$. Methyl H atoms were placed in calculated positions with $C-H = 0.96$ Å and torsion angles were refined to fit the electron density, $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$. Other H atoms were placed geometrically with $C-H = 0.93$ (aromatic) or 0.97 Å (methylene), and refined in riding mode with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: SMART (Bruker, 2003); cell refinement: SAINT (Bruker, 2003); 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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