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{*N*,*N*′-Bis[1-(2-hydroxy-4-methoxyphenyl)ethylidene]ethylenediamine-κ^2O,O'}dichlorozinc(II)

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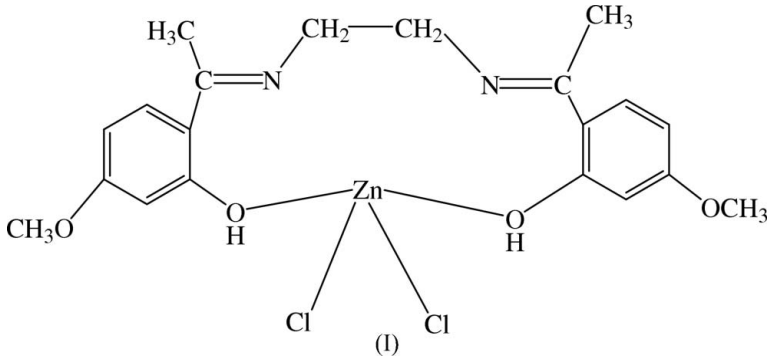
In the title Schiff base complex, $[ZnCl_2(C_{10}H_{12}NO_2)_2]$, the Zn^{II} ion is in a distorted tetrahedral ZnO_2Cl_2 coordination environment.

Comment

The Schiff base 2-hydroxy-4-methoxyacetophenone has potential biological properties. We report here the preparation and crystal structure of the title Zn^{II} complex, (I), with 2-hydroxy-4-methoxyacetophenone.



(I)

The molecular structure of (I) is shown in Fig. 1. The Zn^{II} ion is in a distorted tetrahedral coordination geometry (Table 1), formed by two hydroxyl O atoms and two Cl^- anions. Atoms O1, O2 and N1 are almost coplanar with the C3–C8 benzene ring, while atoms O3, O4 and N2 are almost coplanar with the C12–C17 benzene ring. The dihedral angle between the two nine-atom mean planes is 14.6 (2)°. Intramolecular hydrogen bonding occurs between the hydroxyl O atoms and imine N atoms (Table 2).

Experimental

To a stirred solution of 2-hydroxy-4-methoxyacetophenone (1.0 mmol) and $ZnCl_2{\cdot}2H_2O$ (1.0 mmol) in 30 ml absolute methanol was added dropwise a solution of ethylenediamine (1.0 mmol) in 10 ml absolute methanol at room temperature. After stirring for 2 h at 320 K, the precipitate was filtered off. Single crystals of (I) were obtained from the filtrate after 10 d.

Crystal data

$[ZnCl_2(C_{10}H_{12}NO_2)_2]$
M_r = 492.68
Monoclinic, $P2_1/c$
a = 11.547 (3) Å
b = 10.503 (3) Å
c = 17.469 (3) Å
β = 91.000 (3)°
V = 2118.3 (9) Å^3
Z = 4
D_x = 1.545 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.44 mm^{-1}
T = 298 (2) K
Block, yellow
0.22 × 0.14 × 0.10 mm

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.011 Å
R factor = 0.074
wR factor = 0.217
Data-to-parameter ratio = 14.2

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

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.742, T_{max} = 0.869
10504 measured reflections
3729 independent reflections
2165 reflections with $I > 2\sigma(I)$
R_{int} = 0.079
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.217
S = 1.03
3729 reflections
262 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.091P)^2 + 9.1479P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.88 e Å^{-3}
$\Delta\rho_{min}$ = −0.87 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.975 (5)	Zn1—Cl1	2.233 (2)
Zn1—O3	1.957 (5)	Zn1—Cl2	2.219 (2)
O3—Zn1—O1	88.4 (2)	O3—Zn1—Cl1	108.8 (2)
O3—Zn1—Cl2	115.46 (18)	O1—Zn1—Cl1	108.74 (19)
O1—Zn1—Cl2	116.08 (19)	Cl2—Zn1—Cl1	116.02 (10)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.85	2.582 (8)	149
O3—H3···N2	0.82	1.78	2.529 (8)	150

All H atoms were positioned geometrically and refined as riding on their parent atoms, with aromatic C—H distances of 0.93 Å, methyl C—H distances of 0.96 Å, methylene C—H distances of 0.97 Å and hydroxyl O—H distances of 0.82 Å, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C,O).

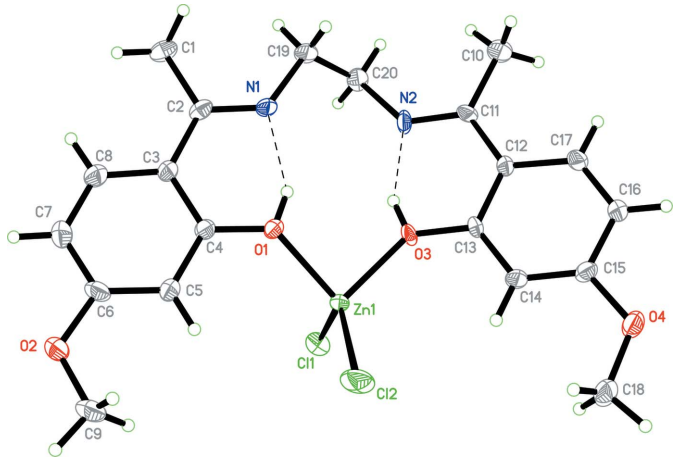


Figure 1
The molecular structure of (I) with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). Dashed lines indicate hydrogen bonds.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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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