Crystal Structure of Bis[1-(3-chloro-4-methylphenyl)-iminomethylbenzen-2-oxy-*O*,*N*]zinc(II)

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The Zn^{2+} ion as well as the zinc complexes are important for biochemical reactions. Some complexes formed by the reaction of ON type Schiff bases and Zn^{2+} ion have been reported previously.[1-4] The coordination around zinc in these compounds is tetrahedral. We describe here a new zinc complex with 3-chloro-4-methylphenylsalicylaldimine as an ON type ligand.

To synthesize the title compound 0.497 g (0.002 mol) of the ligand was dissolved in 70 ml of hot methanol. To this solution a hot methanol solution of 0.219 g (0.001 mol) of $Zn(AcO)_2 \cdot H_2O$ was added with mixing. After a few days light yelow crystals were filtered and dried at room temperature in air. Chemical reaction scheme and the chemical structure are shown in Fig. 1.

The triclinic unit cell of the title compound consists of two centro-symmertically related molecules of $[C_{28}H_{22}Cl_2ZnN_2O_2]$. The coordination around zinc (Fig. 2) is a distorted terahedron involving two O and N atoms of the ligand. In the coordination sphere, the Zn–O and Zn–N bond lengths are [1.839(3) – 1.922(4)]Å and [2.014(4) – 2.019(3)]Å, respectively. The bond angles in the distorted tetrahedron are in the range 95.7(1)˚ – 123.1(2)˚, the smallest value belonging to the O2–Zn–N2 angle and the largest value to the N1–Zn–N2 angle. These bond lengths and angle values are comparable with the values reported in the cited literature.[2,4]

The authors acknowledge the purchase of the CAD-4 diffractometer under Grant DPT/TABAG1 of the Scientific and Technical Research Council of Turkey.

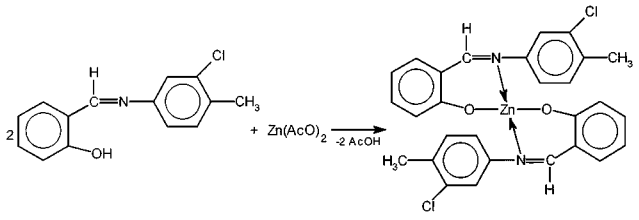

Fig. 1 Synthesis and chemical structure.

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Table 1 Crystal and experimental data

Formula: $C_{28}H_{22}Cl_2ZnN_2O_2$
Formula weight: 554.78
Crystal system: triclinic
Space group: $P\bar{1}$ Z=2
a=8.6922(9)Å
b=12.5875(16)Å
c=12.8425(20)Å
α=62.315(12)˚
β=77.709(11)˚
γ=83.950(9)˚
V=1215.7(3)Å^3
D_x=1.5140 g/cm^3
μ(Mo K$_\alpha$)=1.282 mm^{-1}
T=295 K
Yellow
F(0 0 0)=568
Crystal size: 0.35×0.25×0.15 mm
Radiation=Mo K$_\alpha$
R=0.0515
Rw=0.0580
No. of reflections used=3562
No. of parameters=320
$2\theta_{max}$=54.7˚
$(\Delta/\sigma)_{max}$=0.00076
$(\Delta\rho)_{max}$=0.70 eÅ^{-3}
$(\Delta\rho)_{min}$=–0.15 eÅ^{-3}
Goodness-of-fit=0.99
Measurement: Enraf Nonius CAD-4 diffractometer
Program system: CAD-4 EXPRESS Software
Structure determination: MolEN
Treatment of hydrogen atoms: hydrogen atoms of phenyl ring carbon were located at the positions calculated geometrically, while the positions of hydrogen atoms bonded to C7, C21 and methyl carbons were taken from a difference map and a riding model was used.
Refinement: full matrix least-squares (MolEN)

References

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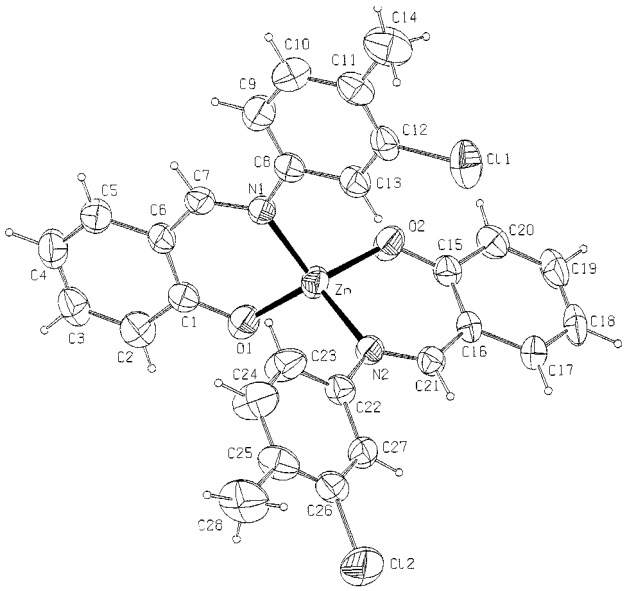

Fig. 2 The ORTEP drawing of the title compound with atom labeling.

Table 2 Final atomic coordinates and equivalent isotropic thermal parameters for non-hydrogen atoms

Atom	*x*	*y*	*z*	B_{eq}/Å^2
Zn	0.34446(7)	0.44635(5)	0.75032(4)	3.29(1)
Cl1	0.6735(2)	0.0403(1)	0.8226(1)	5.79(4)
Cl2	-0.1372(2)	0.0894(2)	1.2811(1)	6.58(5)
O1	0.1914(4)	0.5706(3)	0.7123(3)	4.08(8)
O2	0.5553(4)	0.4795(3)	0.7506(3)	4.28(8)
N1	0.3451(4)	0.4071(3)	0.6152(3)	2.77(8)
N2	0.2984(4)	0.3238(3)	0.9241(3)	2.82(8)
C1	0.1348(5)	0.6205(4)	0.6127(4)	3.1(1)
C2	0.0320(6)	0.7184(4)	0.5929(4)	4.2(1)
C3	-0.0316(6)	0.7758(4)	0.4912(4)	4.2(1)
C4	0.0061(6)	0.7379(4)	0.4029(4)	4.4(1)
C5	0.1054(6)	0.6432(4)	0.4191(4)	3.9(1)
C6	0.1726(5)	0.5802(4)	0.5231(3)	3.0(1)
C7	0.2684(5)	0.4800(4)	0.5299(4)	3.1(1)
C8	0.4302(5)	0.3094(4)	0.6053(4)	3.0(1)
C9	0.4500(6)	0.2838(4)	0.5101(4)	4.1(1)
C10	0.5365(7)	0.1845(4)	0.5105(4)	4.5(1)
C11	0.6070(6)	0.1055(4)	0.6061(4)	4.1(1)
C12	0.5870(5)	0.1346(4)	0.6994(4)	3.4(1)
C13	0.5038(5)	0.2310(4)	0.7017(4)	3.3(1)
C14	0.6979(8)	-0.0005(5)	0.6028(5)	6.0(2)
C15	0.6125(5)	0.4515(4)	0.8463(4)	3.1(1)
C16	0.5383(5)	0.3741(4)	0.9636(3)	2.8(1)
C17	0.6115(6)	0.3527(4)	1.0610(4)	3.5(1)
C18	0.7505(6)	0.4040(4)	1.0439(4)	4.2(1)
C19	0.8236(6)	0.4765(4)	0.9288(4)	4.3(1)
C20	0.7586(6)	0.5001(4)	0.8324(4)	4.0(1)
C21	0.3929(5)	0.3136(4)	0.9948(3)	2.9(1)
C22	0.1574(5)	0.2555(4)	0.9725(4)	3.0(1)
C23	0.0877(6)	0.2364(5)	0.8966(4)	5.0(1)
C24	-0.0480(7)	0.1692(5)	0.9387(5)	5.9(1)
C25	-0.1191(6)	0.1202(4)	1.0577(4)	4.4(1)
C26	-0.0496(6)	0.1421(4)	1.1311(4)	3.6(1)
C27	0.0850(6)	0.2093(4)	1.0916(4)	3.3(1)
C28	-0.2685(7)	0.0494(5)	1.1003(5)	6.6(2)

a. $B_{eq}=(8\pi^2/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*(\boldsymbol{a}_i\cdot\boldsymbol{a}_j)$.

Table 3 Bond distances (Å) and angles (°)

Zn - O1	1.893(3)	N1 - C7	1.317(5)
Zn - O2	1.922(4)	N1 - C8	1.411(6)
Zn - N1	2.014(4)	N2 - C21	1.305(6)
Zn - N2	2.019(3)	N2 - C22	1.424(6)
Cl1 - C12	1.747(5)	C6 - C7	1.415(6)
Cl2 - C26	1.742(5)	C11 - C14	1.492(8)
O1 - C1	1.314(6)	C16 - C21	1.427(6)
O2 - C15	1.305(6)	C25 - C28	1.505(8)
Zn - O2 - O1	120.2(2)	C7 - C6 - N1	128.8(5)
Zn - N1 - O1	97.9(2)	C8 - C9 - N1	126.4(4)
Zn - N2 - O1	112.0(1)	C8 - C13 - N1	116.9(4)
Zn - N1 - O2	109.7(1)	C11 - C14 - C10	120.4(6)
Zn - N2 - O2	95.7(1)	C11 - C14 - C12	124.7(5)
Zn - N2 - N1	123.1(2)	C12 - C13 - Cl1	118.0(4)
O1 - C1 - Zn	125.1(3)	C15 - C16 - O2	124.2(4)
O2 - C15 - Zn	125.0(2)	C15 - C20 - O2	118.3(3)
N1 - C7 - Zn	117.7(3)	C16 - C21 - C15	125.4(4)
N1 - C8 - Zn	122.9(3)	C16 - C21 - C17	115.8(3)
N1 - C8 - C7	119.3(4)	C21 - C16 - N2	127.8(3)
N2 - C21 - Zn	119.5(3)	C22 - C23 - N2	118.1(4)
N2 - C22 - Zn	120.7(3)	C22 - C27 - N2	123.7(5)
N2 - C22 - C21	119.5(3)	C25 - C28 - C24	120.4(6)
C1 - C2 - O1	118.6(5)	C25 - C28 - C26	123.0(5)
C1 - C6 - O1	123.5(4)	C26 - C25 - Cl2	119.5(4)
C6 - C7 - C1	125.8(4)	C26 - C27 - Cl2	117.4(4)

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(Received May 21, 1998)
(Accepted August 31, 1998)