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Crystal structure of dichloro-2-[(3-cyclohexylaminopropylimino)-methyl]-5-methoxyphenolatozinc(II), $Zn(C_{17}H_{26}N_2O_2)Cl_2$

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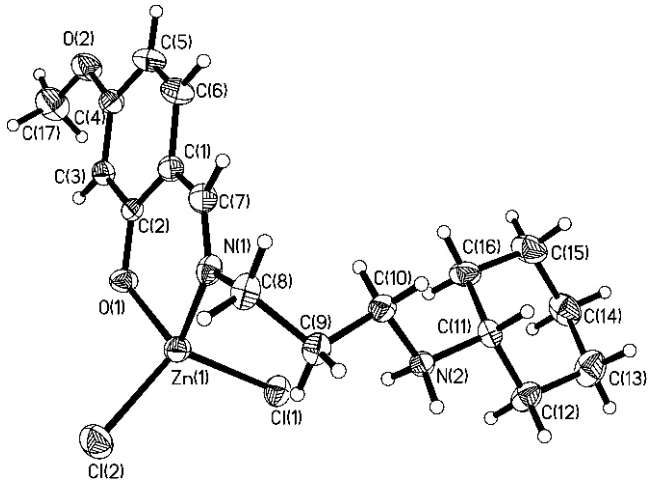
Received February 17, 2011, accepted and available on-line June 17, 2011; CCDC no. 1267/3406



Abstract

$C_{17}H_{26}Cl_2N_2O_2Zn$, monoclinic, *C*12/*c*1 (no. 15), a = 25.102(4) Å, b = 10.540(2) Å, c = 14.994(2) Å, β = 91.445(2)°, V = 3965.9 Å^3, Z = 8, $R_{gt}(F)$ = 0.034, $wR_{ref}(F^2)$ = 0.092, T = 298 K.

Source of material

A methanol solution of $ZnCl_2$ (0.14 g, 1 mmol) was added to a methanol solution (30 ml) of the Schiff base ligand (0.29 g, 1 mmol) with stirring. The resulting solution was allowed to stand at room temperature for a few days, yielding colorless block-shaped single crystals.

Experimental details

H atoms were constrained to ideal bonding parameters, with d(C—H) = 0.93 - 0.97 Å, d(N—H) = 0.90 Å, and with U_{iso}(H) = 1.2 U_{eq}(C, N) and 1.5 U_{eq}(C17).

Discussion

Schiff bases and their complexes have been attracted much attention for the interesting structures and applications [1-4]. The zinc(II) complexes with Schiff bases have been widely investigated for their biological properties [5-7].

The Zn atom in the title complex is coordinated by the phenolic O atom and the imino N atom of the Schiff base ligand, and by two chloride atoms in a tetrahedral environment. The distortion of the tetrahedral coordination can be observed from the coordinate bond angles, ranging from 95.69(6)° to 116.37(5)°. The bond lengths are comparable to those observed in similar zinc(II) complexes with Schiff bases [8-11]. The crystal structure is stabilized by intermolecular hydrogen bonds: d(N2–H2A···Cl1) = 3.210(2) Å, ∠N2–H2A···Cl1 = 159.7° and d(N2–H2B···O1) = 2.777(2) Å, ∠N2–H2B···O1 = 173.2°.

Table 1. Data collection and handling.

Crystal:	colorless block, size 0.30 × 0.30 × 0.32 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	15.19 cm^{-1}
Diffractometer, scan mode:	Bruker SMART 1000 CCD, ω
$2\theta_{max}$:	54°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	11323, 4327
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3324
$N(param)_{refined}$:	218
Programs:	SHELXS-97, SHELXL-97 [12]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(2A)	8*f*	0.0999	0.4225	0.3297	0.040
H(2B)	8*f*	0.1262	0.4406	0.4161	0.040
H(3)	8*f*	0.1158	0.3056	–0.1475	0.044
H(5)	8*f*	0.1693	–0.0415	–0.0821	0.066
H(6)	8*f*	0.2059	0.0371	0.0457	0.064
H(7)	8*f*	0.2303	0.1963	0.1419	0.051
H(8A)	8*f*	0.2673	0.4461	0.2261	0.054
H(8B)	8*f*	0.2576	0.3040	0.2525	0.054
H(9A)	8*f*	0.2283	0.4477	0.3639	0.049
H(9B)	8*f*	0.1861	0.5018	0.2950	0.049
H(10A)	8*f*	0.1574	0.2721	0.2892	0.049
H(10B)	8*f*	0.1827	0.2719	0.3860	0.049
H(11)	8*f*	0.0977	0.2403	0.4614	0.044
H(12A)	8*f*	0.0170	0.4184	0.4165	0.060
H(12B)	8*f*	0.0507	0.4192	0.5062	0.060
H(13A)	8*f*	0.0125	0.2277	0.5495	0.079
H(13B)	8*f*	–0.0333	0.3250	0.5279	0.079
H(14A)	8*f*	–0.0521	0.1254	0.4620	0.074
H(14B)	8*f*	–0.0496	0.2321	0.3892	0.074
H(15A)	8*f*	–0.0012	0.0601	0.3404	0.077
H(15B)	8*f*	0.0327	0.0576	0.4297	0.077
H(16A)	8*f*	0.0841	0.1520	0.3203	0.058
H(16B)	8*f*	0.0387	0.2504	0.2979	0.058
H(17A)	8*f*	0.0610	0.1808	–0.2410	0.111
H(17B)	8*f*	0.0817	0.0959	–0.3187	0.111
H(17C)	8*f*	0.1144	0.2153	–0.2874	0.111

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Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zn(1)	8*f*	0.15905(1)	0.50171(2)	0.10734(2)	0.0468(2)	0.0383(2)	0.0326(2)	0.0034(1)	–0.0020(1)	–0.00047(9)
Cl(1)	8*f*	0.08295(2)	0.50684(5)	0.18661(4)	0.0431(3)	0.0577(3)	0.0409(3)	0.0054(2)	0.0003(2)	0.0050(2)
Cl(2)	8*f*	0.19581(3)	0.68995(6)	0.08635(4)	0.0743(4)	0.0539(3)	0.0616(4)	–0.0206(3)	0.0001(3)	–0.0009(3)
N(1)	8*f*	0.20743(6)	0.3650(2)	0.1547(1)	0.0319(8)	0.050(1)	0.0334(8)	0.0054(7)	0.0020(7)	0.0029(7)
N(2)	8*f*	0.11695(6)	0.3820(1)	0.3749(1)	0.0359(8)	0.0333(8)	0.0297(8)	–0.0035(6)	–0.0021(7)	–0.0021(6)
O(1)	8*f*	0.14587(6)	0.4231(1)	–0.00911(8)	0.0602(9)	0.0335(7)	0.0341(7)	0.0104(6)	–0.0050(7)	–0.0001(6)
O(2)	8*f*	0.12106(6)	0.0706(1)	–0.2049(1)	0.073(1)	0.0403(8)	0.057(1)	–0.0146(8)	–0.0044(8)	–0.0083(7)
C(1)	8*f*	0.18227(7)	0.2203(2)	0.0330(1)	0.034(1)	0.039(1)	0.041(1)	0.0068(8)	0.0029(9)	0.0044(8)
C(2)	8*f*	0.15371(7)	0.3019(2)	–0.0263(1)	0.0307(9)	0.0325(9)	0.035(1)	0.0035(7)	0.0077(8)	0.0011(7)
C(3)	8*f*	0.13352(7)	0.2522(2)	–0.1072(1)	0.036(1)	0.037(1)	0.039(1)	–0.0029(8)	0.0040(9)	0.0018(8)
C(4)	8*f*	0.13941(8)	0.1257(2)	–0.1282(1)	0.041(1)	0.036(1)	0.048(1)	–0.0066(9)	0.008(1)	–0.0040(9)
C(5)	8*f*	0.1661(1)	0.0443(2)	–0.0690(2)	0.065(2)	0.031(1)	0.068(2)	0.005(1)	0.001(1)	–0.005(1)
C(6)	8*f*	0.18717(9)	0.0918(2)	0.0076(2)	0.055(1)	0.041(1)	0.064(2)	0.014(1)	–0.005(1)	0.006(1)
C(7)	8*f*	0.20897(8)	0.2579(2)	0.1145(1)	0.034(1)	0.047(1)	0.045(1)	0.0110(9)	0.0014(9)	0.008(1)
C(8)	8*f*	0.23999(8)	0.3830(2)	0.2366(1)	0.032(1)	0.065(1)	0.039(1)	–0.0004(9)	–0.0023(9)	0.002(1)
C(9)	8*f*	0.20555(8)	0.4260(2)	0.3130(1)	0.036(1)	0.051(1)	0.035(1)	–0.0075(9)	–0.0022(8)	–0.0026(9)
C(10)	8*f*	0.16629(8)	0.3252(2)	0.3403(1)	0.041(1)	0.040(1)	0.042(1)	–0.0008(9)	0.0080(9)	–0.0022(9)
C(11)	8*f*	0.07851(7)	0.2906(2)	0.4160(1)	0.035(1)	0.038(1)	0.037(1)	–0.0023(8)	–0.0005(9)	0.0076(8)
C(12)	8*f*	0.03508(8)	0.3649(2)	0.4604(2)	0.041(1)	0.057(1)	0.052(1)	–0.008(1)	0.010(1)	–0.014(1)
C(13)	8*f*	–0.00497(9)	0.2757(3)	0.5020(2)	0.050(1)	0.084(2)	0.064(2)	–0.010(1)	0.017(1)	–0.004(1)
C(14)	8*f*	–0.02862(9)	0.1848(2)	0.4330(2)	0.046(1)	0.055(1)	0.085(2)	–0.012(1)	0.011(1)	0.011(1)
C(15)	8*f*	0.0147(1)	0.1129(2)	0.3869(2)	0.059(2)	0.040(1)	0.095(2)	–0.012(1)	0.010(1)	–0.000(1)
C(16)	8*f*	0.05563(9)	0.2016(2)	0.3456(2)	0.047(1)	0.036(1)	0.062(1)	–0.0067(9)	0.006(1)	–0.010(1)
C(17)	8*f*	0.0922(1)	0.1469(2)	–0.2682(2)	0.100(2)	0.062(2)	0.059(2)	–0.021(2)	–0.018(2)	–0.005(1)

Acknowledgment. The financial support from Zhoukou Normal University is greatly acknowledged.

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