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The crystal structure of bis((*E*)-2-((tert-butylimino)methyl)-4-chlorophenolato-κ²*N*,*O*) zinc(II), $C_{22}H_{26}Cl_2N_2O_2Zn$

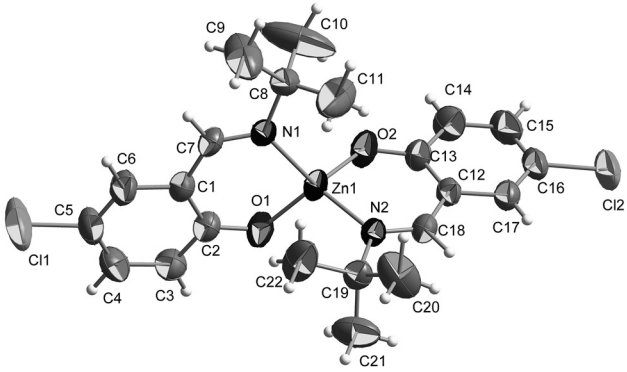

Table 1: Data collection and handling.

Crystal:	Block
Size:	039×0.37×0.32 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	1.27 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	21,975, 4208, 0.022
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 3749
$N(param)_{refined}$:	269
Programs:	Bruker [1], SHELX [2, 3]

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Abstract

$C_{22}H_{26}Cl_2N_2O_2Zn$, monoclinic, $P2_1/n$ (no. 14), a = 10.488(7) Å, b = 10.139(7) Å, c = 22.760(15) Å, β = 99.705°, V = 2386(3) Å^3, Z = 4, $R_{gt}(F)$ = 0.0395, $wR_{ref}(F^2)$ = 0.1053, T = 296(2) K.

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The molecular structure is shown in Figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

(*E*)-2-((*tert*-Butylimino)methyl)-4-chlorophenol (1.16 g, 5.5 mmol), zinc acetate monohydrate (0.50 g, 2.5 mmol) and ethanol (80 mL) were heated and stirred at 373 K for 6 h, then cooled to room temperature, resulting in a yellow solution. Crystals of the title compound were obtained by slow evaporation within three days.

Experimental details

All hydrogen atoms were identified in difference Fourier syntheses. The U_{iso} values of the hydrogen atoms of methyl groups were set to $1.5U_{eq}$(C) and the U_{iso} values of all other hydrogen atoms were set to $1.2U_{eq}$(C).

Comment

Salicylaldehyde Schiff base is a kind of ligand, which can form complexes with many metal ions [4–7]. Salicylaldehyde Schiff base metal complexes are widely used in catalysis and so on [8–10].

The crystal structure shows that the zinc complex has a distorted tetrahedral structure and the Zn is four-coordinated by two phenol oxygen atoms and imine nitrogen atoms of two Schiff bases. The Zn–O distance (O1–Zn1 = 1.917(3) Å; O2–Zn1 = 1.917(2) Å) and the Zn–N length (N1–Zn1 = 2.014(3) Å; N2–Zn1 = 2.010(3) Å) are similar to those seen in related complexes [11, 12]. The C=N bond distance is 1.285(4) Å (C7=N1) and 1.282(4) Å (C18=N2), respectively. The O–Zn–N bond angles are 97.81(9)° (O1–Zn1–N1) and 98.11(10)° (O2–Zn1–N2). Moreover, the coordination of the two NO bidentate chelate

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5995 (3)	0.2509 (3)	0.83077 (13)	0.0468 (7)
C2	0.5307 (3)	0.3638 (3)	0.84439 (13)	0.0479 (7)
C3	0.5220 (3)	0.3852 (4)	0.90477 (15)	0.0602 (8)
H3	0.477820	0.459169	0.914832	0.072*
C4	0.5759 (4)	0.3019 (4)	0.94885 (16)	0.0676 (10)
H4	0.569398	0.319941	0.988300	0.081*
C5	0.6403 (4)	0.1904 (4)	0.93484 (16)	0.0724 (10)
C6	0.6530 (4)	0.1659 (4)	0.87754 (16)	0.0656 (9)
H6	0.697992	0.091333	0.868879	0.079*
C7	0.6265 (3)	0.2160 (3)	0.77272 (14)	0.0487 (7)
H7	0.681693	0.144516	0.771691	0.058*
C8	0.6306 (3)	0.2224 (3)	0.66711 (14)	0.0540 (8)
C9	0.6852 (7)	0.0843 (5)	0.6723 (2)	0.120 (2)
H9A	0.757108	0.080710	0.704495	0.180*
H9B	0.713665	0.060668	0.635735	0.180*
H9C	0.619537	0.023707	0.679854	0.180*
C10	0.7323 (7)	0.3157 (7)	0.6552 (3)	0.173 (4)
H10A	0.699773	0.404319	0.654814	0.259*
H10B	0.756006	0.295834	0.617272	0.259*
H10C	0.806776	0.307431	0.685913	0.259*
C11	0.5185 (6)	0.2248 (8)	0.6173 (2)	0.145 (3)
H11A	0.451245	0.168738	0.626949	0.217*
H11B	0.545499	0.193922	0.581494	0.217*
H11C	0.486592	0.313433	0.611474	0.217*
C12	0.3291 (3)	0.6265 (3)	0.61896 (12)	0.0434 (6)
C13	0.4603 (3)	0.6507 (3)	0.64277 (14)	0.0491 (7)
C14	0.5204 (4)	0.7571 (3)	0.61840 (18)	0.0690 (10)
H14	0.606939	0.774886	0.633021	0.083*
C15	0.4561 (4)	0.8352 (4)	0.57401 (18)	0.0712 (10)
H15	0.498993	0.904379	0.558884	0.085*
C16	0.3279 (4)	0.8111 (3)	0.55180 (15)	0.0609 (9)
C17	0.2658 (3)	0.7094 (3)	0.57353 (14)	0.0545 (8)
H17	0.179186	0.694087	0.558065	0.065*
C18	0.2506 (3)	0.5234 (3)	0.63836 (13)	0.0441 (6)
H18	0.163975	0.523567	0.620653	0.053*
C19	0.1828 (3)	0.3364 (3)	0.69065 (15)	0.0517 (7)
C20	0.0961 (5)	0.2880 (5)	0.6346 (2)	0.1034 (17)
H20A	0.043649	0.359561	0.616584	0.155*
H20B	0.041286	0.218665	0.644755	0.155*
H20C	0.148417	0.255011	0.607097	0.155*
C21	0.1029 (5)	0.4042 (5)	0.7313 (2)	0.0962 (15)
H21A	0.158349	0.432471	0.766995	0.144*
H21B	0.039513	0.343726	0.741398	0.144*
H21C	0.060000	0.479384	0.711273	0.144*
C22	0.2519 (4)	0.2214 (5)	0.7239 (3)	0.1036 (18)
H22A	0.304695	0.178342	0.699035	0.155*
H22B	0.189494	0.160066	0.734129	0.155*
H22C	0.305548	0.252541	0.759530	0.155*
Cl1	0.7118 (2)	0.08261 (17)	0.99087 (6)	0.1442 (7)
Cl2	0.24555 (13)	0.91344 (12)	0.49620 (5)	0.0953 (4)
N1	0.5846 (2)	0.2705 (2)	0.72221 (10)	0.0431 (5)
N2	0.2841 (2)	0.4317 (2)	0.67665 (11)	0.0420 (5)
O1	0.4771 (2)	0.4484 (2)	0.80495 (10)	0.0632 (6)
O2	0.5291 (2)	0.5823 (2)	0.68545 (11)	0.0637 (6)
Zn1	0.46723 (3)	0.42824 (3)	0.72054 (2)	0.04662 (14)

ligands to the Zn ion results in the formation of two six-membered rings.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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