Chloro{2-[(5-nitrosalicylidene)aminoethyl]-1H-benzimidazole}copper(II)

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Key indicators

Single-crystal X-ray study
$T = 293$ K
Mean σ(C–C) = 0.004 Å
R factor = 0.038
wR factor = 0.088
Data-to-parameter ratio = 14.7

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

The title compound, [Cu(C$_{16}$H$_{13}$N$_4$O$_3$)Cl], has been prepared by the reaction of 2-[(5-nitrosalicylidene)aminoethyl]-1H-benzimidazole, L, with copper(II) chloride. Ligand L coordinates to the central Cu atom through two N atoms and one O atom, and a chloride ligand completes a distorted square-planar environment at the Cu^{II} centre. The chloride ligand is trans to the central N atom of the N,N,O-tridentate ligand. There are substantial distortions from ideal geometry at the copper centre, with an O—Cu—N angle of 147.35 (11)° and an N—Cu—Cl angle of 134.89 (9)°. There are intermolecular N—H···Cl hydrogen bonds parallel to the a axis.

Comment

Schiff bases constitute an interesting class of chelating agents, capable of coordination with one or more metal ions and thus forming mononuclear as well as polynuclear metal complexes, which could find applications in analytical chemistry and serve as biochemical models (Mandal & Nag, 1984). Therefore, the synthesis of new Schiff bases and their metal complexes has become a popular theme. In this work, we have prepared a new copper(II) Schiff base complex, (I), between copper(II) chloride and the tetradentate ligand 2-[(5-nitrosalicylidene)-aminoethyl]-1H-benzimidazole and determined its crystal structure.

(I)
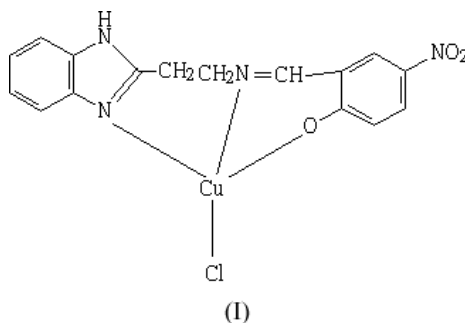
The molecular structure of (I) is shown in Fig. 1. The structure adopts a distorted square-planar geometry about the Cu atom in which atoms N1 and O1 are trans and the chloride ion is trans to N3. The Cu1—O1, Cu1—N1, Cu1—N3 and Cu1—Cl1 bond distances of 1.884 (2), 1.952 (2), 1.949 (3) and 2.2723 (10) Å, respectively, are smaller those reported for other Schiff base complexes (Bentiss et al., 2004). The trans bond angles deviate greatly from the expected value of 180°, with O1—Cu1—N1 and N3—Cu1—Cl1 being 147.35 (11) and 134.89 (9)°, respectively. The sum of the equatorial bond angles at Cu1 is not 360°, showing that the metal coordination is substantially distorted from square planar towards tetra-

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hedral. An N—H···Cl[i] hydrogen bond links the copper complex molecules in a chain parallel to the *a* axis [N2—H2 = 0.72 Å, N···Cl = 3.181 (3) Å and N—H···Cl = 149°; symmetry code: (i) $x + 1$, y, z].

Experimental

The title compound was prepared by adding a methanol solution (5 ml) of copper(II) chloride (0.1 mmol) to a dichloromethane–methanol solution (1:1 *v/v*, 10 ml) of *L* (Das & Dash, 1995; 0.1 mmol) neutralized with triethylamine. The mixture was stirred for about 2 h and filtered. The filtrate was evaporated slowly at room temperature to yield green block crystals of (I) suitable for X-ray analysis. Analysis calculated for $C_{16}H_{13}ClCuN_4O_3$: C 47.06, H 3.22, N 13.73%; found: C 46.96, H 3.16, N 13.82%.

Crystal data

$[Cu(C_{16}H_{13}N_4O_3)Cl]$	$D_x = 1.646$ Mg m^{-3}
$M_r = 408.29$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 921
$a = 8.047$ (3) Å	reflections
$b = 14.384$ (5) Å	$\theta = 2.7$–$24.9°$
$c = 14.386$ (5) Å	$\mu = 1.51$ mm^{-1}
$\beta = 98.311$ (5)°	$T = 293$ (2) K
$V = 1647.7$ (9) Å^3	Block, green
$Z = 4$	$0.28 \times 0.24 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	3311 independent reflections
	2319 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.035$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 26.3°$
	$h = -9 \rightarrow 10$
$T_{min} = 0.590$, $T_{max} = 0.739$	$k = -17 \rightarrow 9$
9165 measured reflections	$l = -17 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0374P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.038$	$+ 0.6734P]$
$wR(F^2) = 0.088$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.001$
3311 reflections	$\Delta\rho_{max} = 0.47$ e Å^{-3}
226 parameters	$\Delta\rho_{min} = -0.38$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.884 (2)	Cu1—N1	1.952 (2)
Cu1—N3	1.949 (2)	Cu1—Cl1	2.2723 (10)
O1—Cu1—N3	94.85 (9)	C16—O1—Cu1	127.29 (18)
O1—Cu1—N1	147.35 (11)	C7—N1—Cu1	125.3 (2)
N3—Cu1—N1	94.75 (10)	C1—N1—Cu1	128.30 (19)
O1—Cu1—Cl1	96.18 (7)	C10—N3—Cu1	124.5 (2)
N3—Cu1—Cl1	134.89 (9)	C9—N3—Cu1	117.32 (18)
N1—Cu1—Cl1	98.87 (7)		

H atoms were placed in calculated positions and refined with fixed displacement parameters, riding on their parent atoms, with C—H distances in the range 0.93–0.98 Å, N—H distances in the range 0.86–0.90 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.2U_{eq}(N)$.
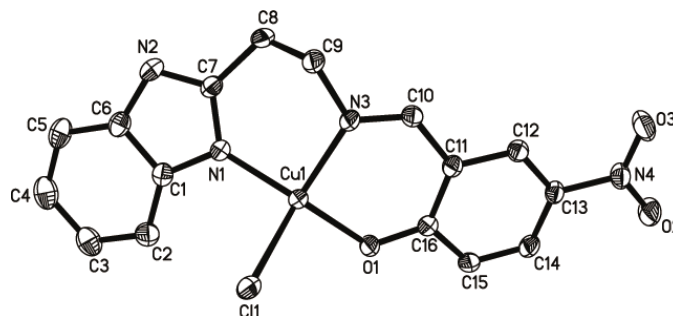

Figure 1
A view of the cation of the title compound, shown with 30% probability displacement ellipsoids. H atoms have been omitted for clarity.
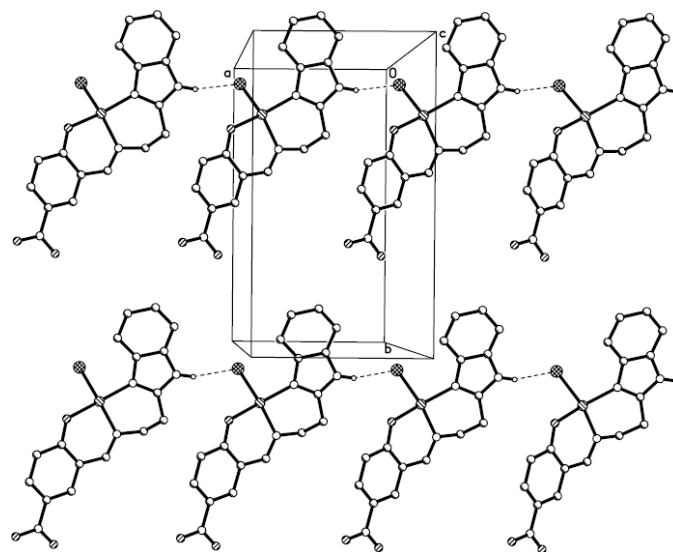

Figure 2
Packing diagram of the title compound, with N—H···Cl hydrogen bonds shown as dashed lines. H atoms have been omitted.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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