Bis(2-aminoethyl-1*H*-benzimidazole)chlorocopper(II) nitrate

Hai-Yan Zhao,* Min-Li Yang and Feng-Juan Shen

College of Science, Hebei University of Science and Technology, Shijiazhuang 050018, People's Republic of China

Correspondence e-mail: hbhaiyanzh@163.com

Key indicators

Single-crystal X-ray study

T = 293 K

Mean σ(C–C) = 0.006 Å

Disorder in solvent or counterion

R factor = 0.038

wR factor = 0.106

Data-to-parameter ratio = 14.1

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

The Cu centre in the title compound, $[CuCl(C_9H_{11}N_3)_2]NO_3$, is coordinated by a cyclic imino N atom and exocyclic amino N atoms derived from two 2-aminoethylbenzimidazole ligands, as well as a Cl atom; the Cu and Cl atoms lie on a twofold axis. The coordination geometry is based on a trigonal bipyramid.

Comment

Metalloproteins that contain Cu are widespread. Characterization of model Cu complexes that mimic Cu proteins has led to a better understanding of the chemistry of Cu in biological systems (Lewis & Tolman, 2004). The presence of Cu–imidazole interactions in diverse metalloproteins has been the focus of considerable interest in biomimetic studies of copper compounds with donor atoms similar to those present in the active sites (Gilbert *et al.*, 2004). In this context, a new copper(II) complex, (I), with copper bound to 2-aminoethyl-benzimidazole, is described here.

(I)
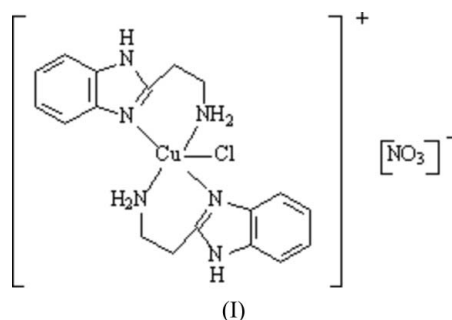
The Cu centre in (I) (Fig. 1) has a trigonal–bipyramidal coordination geometry defined by two chelating 2-aminoethylbenzimidazole ligands and a Cl atom. The cyclic imino atoms N1 and N1[i] occupy the axial positions (Table 1) and the exocyclic amino N3 and N3[i] atoms as well as the Cl atom are in equatorial sites [symmetry code: (i) $\frac{1}{2} - x, \frac{1}{2} - y, z$]. The Cu—N bond distances (Table 1) are similar to those reported in related Cu imidazole/benzimidazole complexes (Colacio *et al.*, 2000; Gupta *et al.*, 2006). By contrast, the Cu—Cl1 bond distance of 2.444 (3) Å is longer than that reported in similar chlorocopper complexes (*e.g.* Gupta *et al.* 2001).

Experimental

Complex (I) was prepared by adding 5 ml of an aqueous solution of copper perchlorate (0.1 mmol) to a methanol solution (10 ml) of 2-aminoethylbenzimidazole (0.1 mmol) neutralized by sodium hydroxide. The mixture was stirred for 2 h and then filtered. Blue crystals suitable for X-ray diffraction analysis were obtained by slow

diffusion of diethyl ether into the resulting solution over one week. Analysis calculated for $C_{18}H_{22}ClCuN_7O_3$: C 44.72, H 4.59, N 20.28%; found: C 45.27, H 4.51, N 19.19%.

Crystal data

$[CuCl(C_9H_{11}N_3)_2]NO_3$	$Z = 4$
$M_r = 483.42$	$D_x = 1.549$ Mg m^{-3}
Orthorhombic, $Pccn$	Mo $K\alpha$ radiation
$a = 11.251\ (10)$ Å	$\mu = 1.22$ mm^{-1}
$b = 14.860\ (14)$ Å	$T = 293\ (2)$ K
$c = 12.396\ (12)$ Å	Block, blue
$V = 2072\ (3)$ Å^3	$0.22 \times 0.18 \times 0.14$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	2124 independent reflections
	1320 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.054$
Absorption correction: none	$\theta_{max} = 26.4°$
11006 measured reflections	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0504P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.038$	$+ 0.8135P]$
$wR(F^2) = 0.106$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
2124 reflections	$\Delta\rho_{max} = 0.49$ e Å^{-3}
151 parameters	$\Delta\rho_{min} = -0.53$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cu1—Cl1	2.444 (3)	Cu1—N3	2.088 (3)
Cu1—N1	1.995 (3)		
Cl1—Cu1—N1	89.94 (8)	N1^i—Cu1—N1	179.87 (16)
Cl1—Cu1—N3	117.97 (9)	N1—Cu1—N3^i	88.22 (11)
N1—Cu1—N3	91.84 (12)	N3^i—Cu1—N3	124.05 (18)

Symmetry code: (i) $-x + \frac{1}{2}, -y + \frac{1}{2}, z$.

H atoms were included in the riding-model approximation, with N—H = 0.86–0.90 Å and C—H = 0.93–0.98 Å, and with $U_{iso}(H) = 1.2U_{eq}(N,C)$.

Data collection: *SMART-NT* (Bruker, 1998); cell refinement: *SMART-NT*; data reduction: *SAINT-NT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.
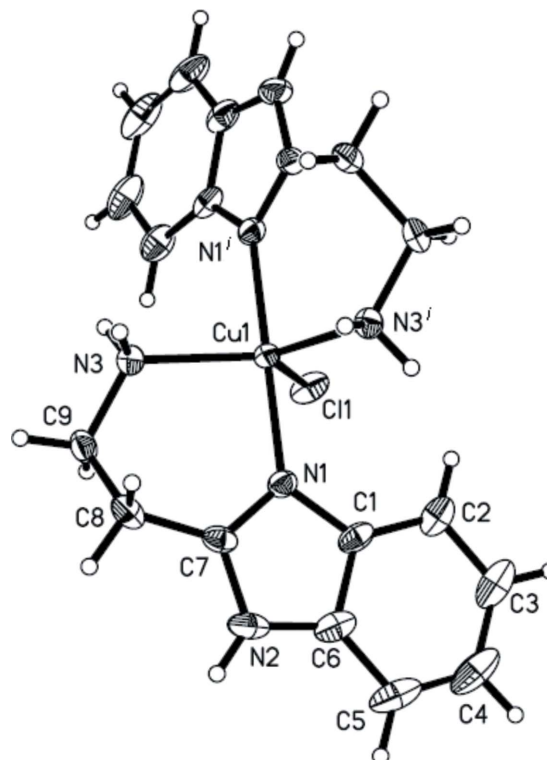

Figure 1
The molecular structure of (I), showing the atom-labelling scheme and 30% probability displacement ellipsoids. [Symmetry code: (i) $\frac{1}{2} - x, \frac{1}{2} - y, z$.]

References

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