Bis(2-aminoethyl-1*H*-benzimidazole-κN^3)-chlorocopper(II) perchlorate

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Key indicators

Single-crystal X-ray study

$T = 293$ K

Mean σ(C–C) = 0.004 Å

R factor = 0.030

wR factor = 0.079

Data-to-parameter ratio = 15.1

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

The title compound, [CuCl(C$_9$H$_{11}$N$_3$)]ClO$_4$, was prepared by reaction of 2-aminoethylbenzimidazole dihydrochloride with copper(II) perchlorate. The crystal structure is built of bis(2-aminoethylbenzimidazole)chlorocopper(II) cations and perchlorate anions. Both cation and anion occupy special positions on a twofold axis. Each of the aminoethylbenz-imidazole ligands coordinates the Cu atom through one cyclic imine and one exocyclic amine group. The chloro ligand occupies the fifth coordination site in the Cu-atom environment, thus forming a trigonal bipyramid, with the Cl atom and amine N atoms in the equatorial and both cyclic imine atoms in the axial positions [the N—Cu—N angle formed by the axial bonds is 179.61 (10)°]. N—H···Cl and N—H···O hydrogen-bonding interactions link cations and anions into layers normal to the *b* axis.

Comment

The copper(II) ion has been found to be essential for almost all forms of life. It has been generally accepted that imidazole groups play an important role in the coordination chemistry of the copper(II) ion, as in many copper(II)-containing metalloenzymes and proteins, the Cu centers are bound by the imidazole N atom of histidines, *e.g.* in tyrosinase, catechol oxidase (Gupta *et al.*, 2001) and hemocyanin (Hendriks *et al.*, 1982). On the other hand, low molecular weight coordination compounds are used to study correlations between structure and magnetic and spectroscopic properties (Helis *et al.*, 1977). A new copper(II) complex with 2-aminoethylbenzimidazole, (I), which is reported in this paper, may be of interest with respect to both of the above-mentioned areas.

(I)
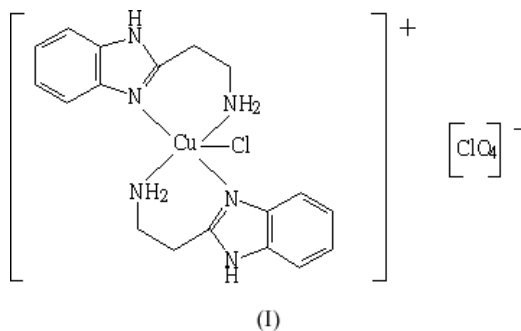
The crystal structure of (I) is composed of bis(2-amino-ethylbenzimidazole)chlorocopper cations and perchlorate anions. Both cation and anion occupy special positions on a twofold axis. The structure of the cation is shown in Fig. 1.

Atom Cu1 has a trigonal–bipyramidal coordination, with the cyclic imine atoms N2 and N2^i in the axial positions [N2—Cu1—N2^i = 179.61 (10)°; symmetry code: (i) $\frac{1}{2} - x$, $\frac{1}{2} - y$, z],
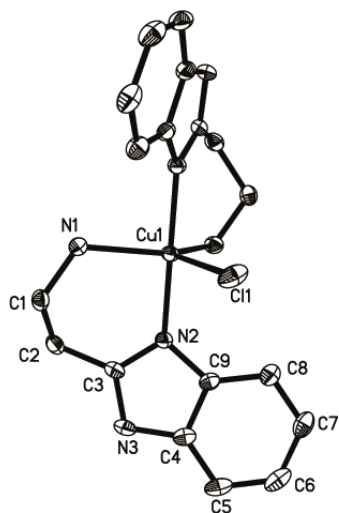
Figure 1
A view of the cation of the title compound, shown with 30% probability displacement ellipsoids. H atoms have been omitted.

and atoms Cl1, N1 and N1^i in the equatorial sites [Cl1—Cu1—N1 = 116.89 (6)° and N1—Cu1—N1^i = 126.22 (11)°]. The Cu—N bond distances [Cu1—N1 = 2.0803 (19) Å and Cu1—N2 = 2.0095 (18) Å] are slightly longer than those found for similar copper complexes with benzimidazole (Gupta *et al.*, 2001) and imidazole ligands (Colacio *et al.*, 2000). The Cu1—Cl1 bond distance of 2.4468 (12) Å is also longer than that reported in the literature in similar chlorocopper complexes, *e.g.* by Gupta *et al.* (2001).

There are two symmetry-independent hydrogen bonds in the crystal structure. One of the hydrogen bonds links the exocyclic amine group to the chloro ligand of the adjacent cation, while the other involves the imidazole NH group and one of the O atoms of the perchlorate anion (Table 2 and Fig. 2). The hydrogen bonds of the first type are responsible for the formation of infinite cationic chains along the *c* axis; bonds of the second type join anions and cations along the *a* direction, producing layers orthogonal to the *b* axis of the crystal.

Experimental

The title compound was prepared by adding an aqueous solution (3 ml) of copper(II) 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. The filtrate was evaporated slowly at room temperature and blue block-shaped crystals suitable for X-ray analysis were obtained. Analysis calculated for $C_{18}H_{22}Cl_2CuN_6O_4$: C 41.51, H 4.26, N 10.76%; found: C 41.49, H 4.25, N 10.74%.

Crystal data

[CuCl(C$_9$H$_{11}$N$_3$)]ClO$_4$
$M_r = 520.86$
Orthorhombic, *Pccn*
$a = 15.202$ (5) Å
$b = 11.241$ (4) Å
$c = 12.268$ (4) Å
$V = 2096.4$ (11) Å^3
$Z = 4$
$D_x = 1.650$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 788 reflections
$\theta = 2.2–26.2°$
$\mu = 1.34$ mm^{-1}
$T = 293$ (2) K
Block, blue
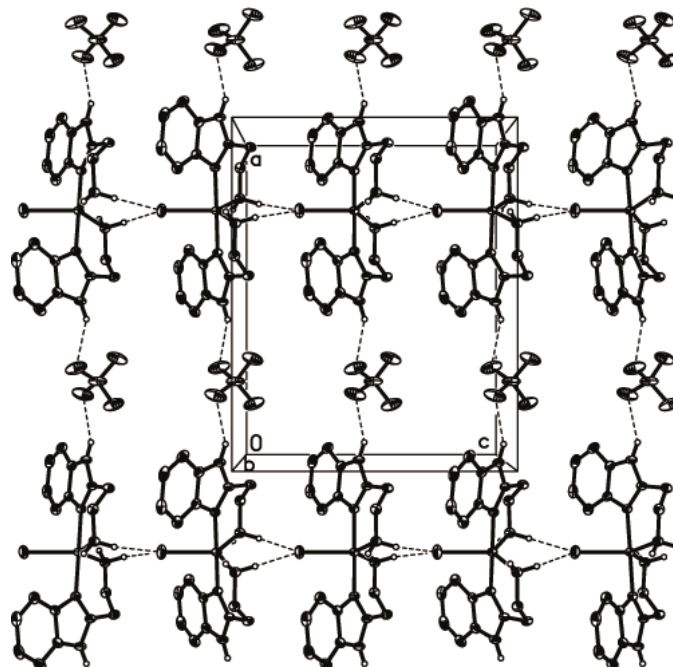$0.20 \times 0.18 \times 0.16$ mm

Figure 2
The packing of the title compound, viewed down the *b* axis. Only H atoms bonded to the N atoms are shown. Hydrogen bonds are represented as dashed lines.

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.665$, $T_{max} = 0.807$
11 264 measured reflections

2145 independent reflections
1541 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 26.4°$
$h = -18 \rightarrow 18$
$k = -14 \rightarrow 5$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.079$
$S = 1.02$
2145 reflections
142 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0359P)^2 + 1.0483P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.0803 (19)	Cu1—Cl1	2.4468 (12)
Cu1—N2	2.0095 (18)		
N2—Cu1—N2^i	179.61 (10)	N1^i—Cu1—N1	126.22 (11)
N2—Cu1—N1^i	88.57 (7)	N2—Cu1—Cl1	89.81 (5)
N2—Cu1—N1	91.60 (7)	N1—Cu1—Cl1	116.89 (6)

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

Table 2
Hydrogen-bonding geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$B\cdots$Cl1^{ii}	0.90	2.56	3.314 (2)	142
N3—H3$\cdots$O1	0.86	2.22	2.960 (4)	145

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

H atoms were placed in calculated positions and included in the refinement in the riding-model approximation, with C—H distances in the range 0.93–0.98 Å, N—H distances in the range 0.86–0.90 Å and $U_{iso}(H) = 1.2U_{eq}$ of the carrier atom.

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

References

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