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trans-Bis[2-(aminomethyl)-1*H*-benzimidazole-κ^2N^2,N^3]aquacopper(II) dichloride dihydrate

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.005 Å
R factor = 0.040
wR factor = 0.101
Data-to-parameter ratio = 13.4

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

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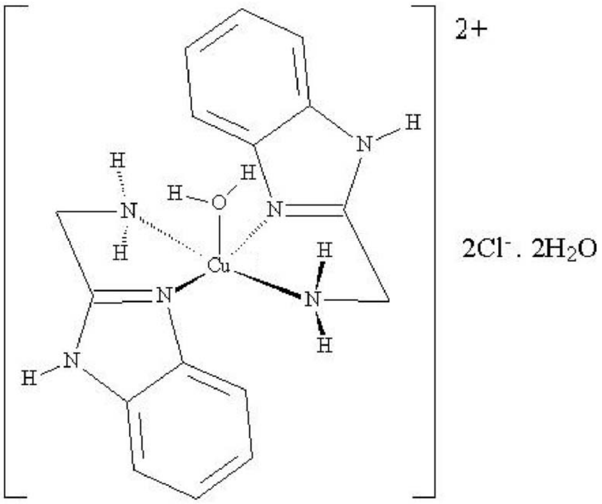
In the title compound, $[Cu(C_8H_9N_3)_2(H_2O)]Cl_2\cdot 2H_2O$, the Cu^{II} ion is coordinated in a square-pyramidal geometry, with four N atoms as basal ligands and one water O atom as an apical ligand. The complex molecule is situated on a crystallographic twofold rotation axis. The molecules are bonded to their neighbours by N—H···O, O—H···Cl and N—H···Cl hydrogen bonds. The packing is further stabilized by π–π interactions between the substituted imidazole molecules.

Comment

Hydrogen bonding and π–π interactions are two of the principal forces which determine structure, self-assembly and recognition in some chemical and biological systems (Lehn, 1990). Imidazole and benzimidazole derivatives are important heteroaromatic compounds in biochemistry, acting as polydentate ligands in many copper(II) complexes containing proteins (Brown *et al.*, 1980; Larrabee & Spiro, 1980) and nucleotide systems (Shahina Begum *et al.*, 1989; Shahina Begum & Manohar, 1992). In our ongoing research on benzimidazole derivatives as ligands in coordination compounds (García-Orozco *et al.*, 2002; Andrade-López *et al.*, 1997), we have synthesized the title compound, (I).



(I)

The complex molecule is situated on a crystallographic twofold rotation axis. The Cu^{II} ion of (I) is coordinated in a slightly distorted square-pyramidal geometry. In the basal plane, it is coordinated by four N atoms from two bidentate 2-aminomethylbenzimidazole ligands, while the apical ligand is a water molecule (Fig. 1). In addition to this coordinated water

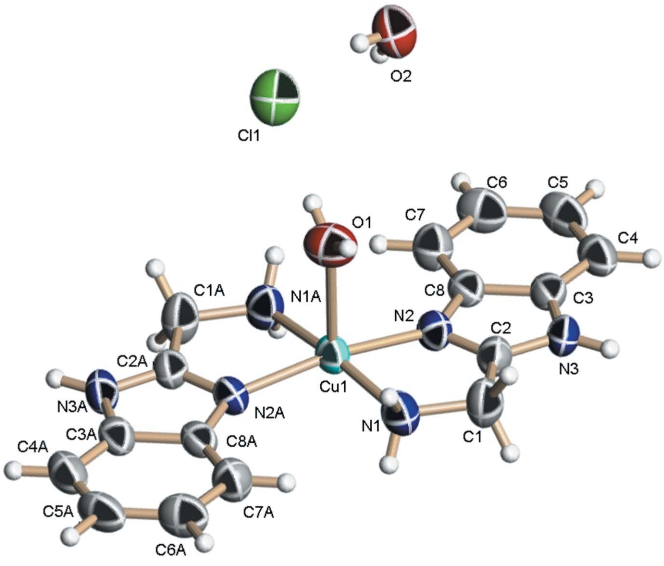


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radius. Atoms with the suffix A are generated by the symmetry operator ($1-x, y, \frac{3}{2}-z$).

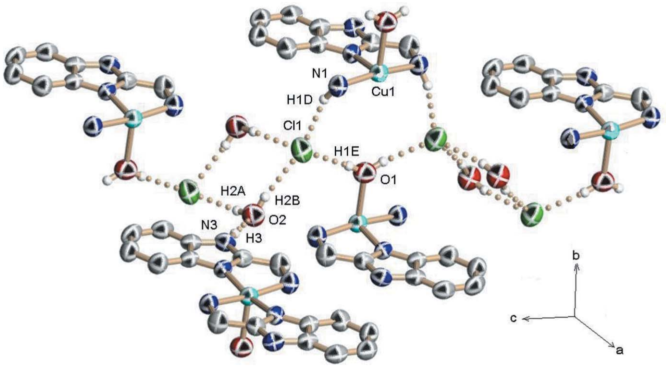


Figure 2
A view of the hydrogen bonds (dashed lines) in (I), showing the N3—H3$\cdots$O2 interactions and the $R_4^2(8)$ and $R_4^3(10)$ motifs.

molecule, there is a solvent water molecule in a general position that takes part in the hydrogen-bond network (Table 1). It is interesting that atom Cl1 is an acceptor of four H atoms (Fig. 2). Two of these H atoms are from the complex molecule, *i.e.* from the coordinated water O1 and the primary amine group. The two remaining H atoms are donated by two solvent water molecules.

In the hydrogen-bond pattern, two graph sets (Bernstein *et al.* 1995) (Fig. 2) can be distinguished: $R_4^2(8)$, involving atoms ($\cdots$H2*B*—O2—H2*A*$\cdots$Cl1$\cdots$)$_2$, and $R_4^3(10)$, involving atoms Cu1(—N1—H1*D*$\cdots$Cl1$\cdots$H1*E*)$_2$O1. Both patterns $R_4^2(8)$ and $R_4^3(10)$ generate polyspiro chains running along the *c* axis (Fig. 2). In addition, the 2-aminomethylbenzimidazoles show N3—H3$\cdots$O2 hydrogen-bonding interactions that can be described by the graph set $R_4^2(8)$ (Fig. 2). The packing is further stabilized by offset π–π interactions between two adjacent complex molecules, with a distance between the ring centroids *Cg*1 and *Cg*2 (*Cg*1 is the centroid of the imidazole ring N2/C2/N3/C3/C8 and *Cg*2 is the centroid of the benzene ring C3–C8) of 3.71 Å (Fig. 3).

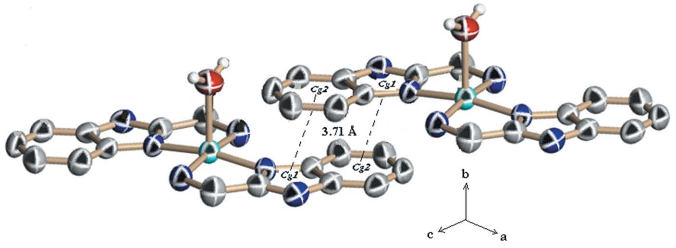


Figure 3
Two molecules of (I), showing the offset π–π interactions between the benzimidazole ring systems. Dashed lines indicate the interactions between the imidazole ring centroid (*Cg*1) and the benzene ring centroid (*Cg*2).

The Cu—O and Cu—N bond distances of (I) are in the ranges found in similar compounds (García-Orozco *et al.*, 2002; Wen-Long *et al.*, 2004). The bond distances and angles within the ligand have normal values.

Experimental

A solution of $CuCl_2$ (8.0 mg, 0.06 mmol) in H_2O (3 ml, pH 7.5) was added to 2-aminomethylbenzimidazole (17.6 mg, 0.12 mmol) dissolved in an aqueous solution (3 ml) of 0.5 *M* NaCl. The resulting clear blue solution was concentrated by evaporation at room temperature over a period of two weeks. The blue single crystals which formed were prism-shaped and these were filtered off (yield 29.5 mg, 57%; m.p. 451.2–455.2 K).

Crystal data

$[Cu(C_8H_9N_3)_2(H_2O)]Cl_2\cdot 2H_2O$
$M_r = 482.85$
Monoclinic, $C2/c$
$a = 17.765$ (4) Å
$b = 6.7233$ (13) Å
$c = 19.074$ (4) Å
$\beta = 114.03$ (3)°
$V = 2080.7$ (9) Å^3
$Z = 4$
$D_x = 1.541$ Mg m$^{-3$}
Mo *Kα* radiation
$\mu = 1.34$ mm^{-1}
$T = 292$ (2) K
Prism, blue
0.34 × 0.27 × 0.13 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.636$, $T_{max} = 0.841$
5024 measured reflections
1929 independent reflections
1384 reflections with $I > 2\sigma(I)$
$R_{int} = 0.044$
$\theta_{max} = 25.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.101$
$S = 1.03$
1929 reflections
144 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.035P)^2 + 2.9635P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}

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Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots$$A$	D—H	H$\cdots$$A$	$D\cdots A$	D—H$\cdots$$A$
N1—H1$D\cdots$Cl1^{i}	0.90	2.41	3.270 (4)	159
O1—H1$E\cdots$Cl1^{ii}	0.82 (3)	2.29 (3)	3.105 (2)	172 (4)
O2—H2$A\cdots$Cl1	0.82 (4)	2.37 (4)	3.170 (4)	170 (6)
O2—H2$B\cdots$Cl1^{iii}	0.82 (3)	2.39 (3)	3.188 (4)	165 (3)
N3—H3$\cdots$O2^{iv}	0.86 (2)	1.95 (2)	2.813 (5)	177 (2)

Symmetry codes: (i) $-x+1, y-1, -z+\frac{3}{2}$; (ii) $-x+1, y, -z+\frac{3}{2}$; (iii) $-x+1, -y+1, -z+2$; (iv) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

All H atoms were located in a difference Fourier map. The aryl, methylene and amino H atoms could be refined, resulting in C(aryl)—H, C(methylene)—H and N(amino)—H distances in the range 0.83 (4)–1.02 (4) Å. Nevertheless, the aryl, methylene and amino H atoms were constrained using a riding-model approximation, with C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) for aryl H, C—H = 0.97 Å and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C) for methylene H and N1—H1D = 0.90 Å and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(N) for amino H. For atoms H2A, H2B, H1E and H3, which are involved in hydrogen-bonding interactions, the O—H and N—H distances were restrained to 0.82 (3) and 0.86 (2) Å, respectively, and their $U_{\rm iso}$(H) values were refined.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL-NT* (Bruker, 2000); program(s) used to refine structure: *SHELXTL-NT*; molecular graphics: *SHELXTL-NT*; software used to prepare material for publication: *PLATON* (Spek, 2003).

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