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[*N*-(2-Aminoethyl)-*N*-(3-aminopropyl)amine]-(2-aminopyrimidine)chlorocopper(II) perchlorate

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Key indicators

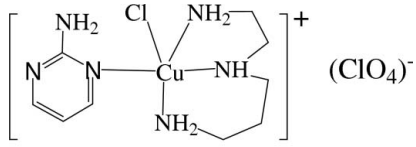
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.015 Å
R factor = 0.063
wR factor = 0.148
Data-to-parameter ratio = 14.1

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

In the title complex, $[CuCl(C_4H_5N_3)(C_5H_{15}N_3)](ClO_4$, the Cu^{II} ion assumes a distorted square-pyramidal CuN_4Cl coordination geometry. Extensive hydrogen bonding occurs, which helps to stabilize the crystal structure.

Comment

The pyrimidine substructure plays a vital role in physiological systems (Dimitra, 1991; Ramesh *et al.*, 2004). We report here the crystal structure of the title aminopyrimidine Cu^{II} complex, (I).



(I)

The molecule of (I) consists of Cu^{II} complex cations and perchlorate anions (Fig. 1). The Cu^{II} atom assumes a distorted square-pyramidal coordination geometry, with four N atoms in the basal plane and one Cl^- ion at the apical position. The Cu1 atom is displaced by 0.279 (4) Å from the basal plane towards the atom Cl1. The Cu—N bond lengths range from 1.969 (7) to 2.082 (7) Å. The longer axial Cu—Cl1 bond distance shows Jahn–Teller distortion (Table 1), as found in five-coordinate Cu^{II} complexes reported previously (Lundin *et al.*, 2004; Yamada *et al.*, 2002).

Extensive hydrogen bonding occurs in the crystal structure (Table 2). The Cu^{II} complex cation is linked to the perchlorate anion *via* N—H···O hydrogen bonds. Hydrogen bonding also occurs between Cu^{II} complex cations.

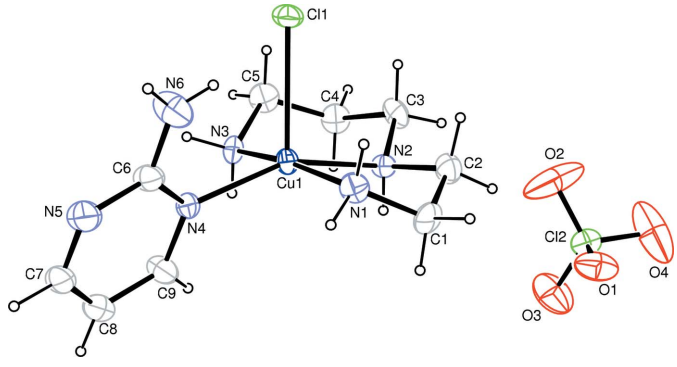


Figure 1
The asymmetric unit of (I) with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

Experimental

A methanol solution (15 ml) of $CuCl_2{\cdot}4H_2O$ (0.5 mmol) was mixed with a methanol solution (15 ml) of (2-aminoethyl)(3-aminopropyl)amine (0.5 mmol). After stirring for 15 min, another methanol solution (20 ml) of 2-aminopyrimidine (0.5 mmol) was added dropwise to the above solution. The resulting solution was refluxed for 2 h. After adding small amount of $NaClO_4$, the solution was filtered. Single crystals of (I) were obtained from the solution after two weeks.

Crystal data

$[CuCl(C_4H_5N_3)(C_5H_{15}N_3)](ClO_4$
M_r = 410.75
Orthorhombic, $Pna2_1$
a = 12.019 (2) Å
b = 15.450 (3) Å
c = 8.8057 (16) Å
V = 1635.2 (5) Å^3
Z = 4
D_x = 1.668 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.69 mm^{-1}
T = 298 (2) K
Block, blue
0.35 × 0.32 × 0.30 mm

Data collection

Bruker Smart 1000 detector diffractometer
φ and ω scans
Absorption correction: multi-scan *SADABS* (Sheldrick, 2002)
T_{min} = 0.540, T_{max} = 0.606
8212 measured reflections
2799 independent reflections
2500 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.148
S = 1.16
2799 reflections
199 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0315P)^2 + 11.4496P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}
Absolute structure: Flack (1983), 1249 Friedel Pairs
Flack parameter: 0.43 (4)

Table 1
Selected bond lengths (Å).

Cu1—N1	2.050 (8)	Cu1—N4	2.082 (7)
Cu1—N2	2.029 (6)	Cu1—Cl1	2.593 (2)
Cu1—N3	1.969 (7)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1B···O3^{i}	0.90	2.20	3.102 (13)	177
N2—H2···Cl1^{ii}	0.91	2.50	3.279 (6)	143
N3—H3B···N5^{iii}	0.90	2.17	3.036 (12)	161
N6—H6A···Cl1	0.86	2.38	3.198 (10)	160
N6—H6B···O1^{iv}	0.86	2.42	3.136 (13)	142

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

H atoms were placed in calculated positions with C—H = 0.93 − 0.97 Å and N—H = 0.86 − 0.91 Å, and refined in riding mode with U_{iso}(H) = 1.2U_{eq}(C,N). The highest peak is 0.96 Å from atom Cu1. The value of the Flack parameer, 0.43 (4) suggests that the crystal is an inversion twin.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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