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2-[(3-Aminopropyl)aminopropyliminomethyl]imidazolato-*N*,*N*′,*N*′′,*N*′′′-(methanol-*O*)copper(II) perchlorate

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{2-[(3-Aminopropyl)aminopropyliminomethyl]imidazolato-*N*,*N*′,*N*″,*N*‴}(methanol-*O*)copper(**II**) perchlorate

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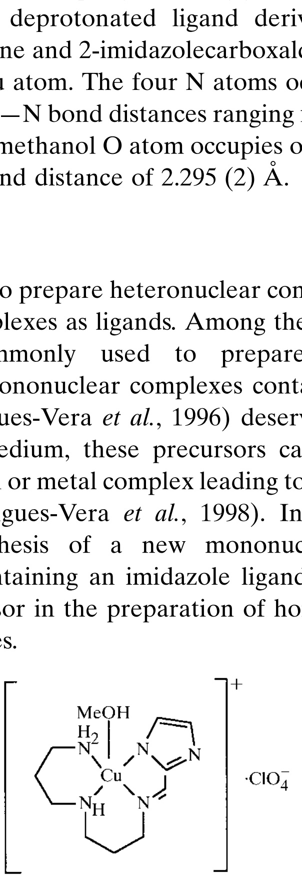
In the title compound, $[Cu(C_{10}H_{18}N_5)(CH_4O)]ClO_4$, four N atoms from the deprotonated ligand derived from bis(3-aminopropyl)amine and 2-imidazolecarboxaldehyde are coordinated to the Cu atom. The four N atoms occupy equatorial positions with Cu—N bond distances ranging from 1.998 (2) to 2.046 (3) Å. The methanol O atom occupies one axial position with a Cu—O bond distance of 2.295 (2) Å.

Comment

A good strategy to prepare heteronuclear complexes is that of using metal complexes as ligands. Among the precursors that have been commonly used to prepare heteronuclear complexes the mononuclear complexes containing imidazole ligands (Dominques-Vera *et al.*, 1996) deserve special attention. In basic medium, these precursors can coordinate to another metal ion or metal complex leading to a heteronuclear complex (Domingues-Vera *et al.*, 1998). In this paper, we report the synthesis of a new mononuclear copper(II) complex, (I), containing an imidazole ligand, which may be used as a precursor in the preparation of homo- and heteronuclear complexes.



(I)

The structure consists of a mononuclear complex cation and a perchlorate anion. Although the amine:aldehyde ratio was 1:2, the ligand is formed by condensation of only one aldehyde molecule with one amine molecule. The ligand contains two imidazole, two amine and one imino N atoms. In the title compound, the ligand coordinates by four of its five N atoms in its deprotonated form leaving the deprotonated N2 atom uncoordinated. The tetradentate behaviour of the ligand results in the formation of one five- and two six-membered chelate rings around the Cu atom. The four N atoms of the coordination plane are almost coplanar with deviations from the least-squares plane of less than 0.006 Å. The Cu atom deviates by 0.203 (1) Å from the basal plane towards the O atom of the coordinated methanol molecule at 2.295 (2) Å. The nearest atom in the direction of the sixth coordination position is N2($1-x$, $-y$, $1-z$) at 3.738 (3) Å. The five-membered chelate ring and the imidazole ring are planar, the six-membered rings adopt chair conformations. The complex cations and anions are connected by hydrogen bonds involving the methanol O—H, the three amino H atoms, the deprotonated N2 of the imidazole ring, and O1 and O2 of the perchlorate ion.

Experimental

2-Imidazolecarboxaldehyde (2 mmol) was reacted with bis(3-aminopropyl)amine (1 mmol) in 50 ml of methanol. To the yellow solution, $Cu(ClO_4).6H_2O$ (1 mmol) was added with continuous stirring. The resulting blue solution was allowed to stand at room temperature for one day, upon which blue needle-like crystals of the compound were obtained.

Crystal data

$[Cu(C_{10}H_{18}N_5)(CH_4O)]ClO_4$
$M_r = 403.33$
Monoclinic, $P2_1/c$
$a = 7.488$ (3) Å
$b = 12.475$ (5) Å
$c = 18.176$ (6) Å
$\beta = 97.15$ (3)°
$V = 1684.7$ (11) Å^3
$Z = 4$

$D_x = 1.590$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 6.38$–10.08°
$\mu = 1.486$ mm^{-1}
$T = 193$ (2) K
Needle, blue
0.45 × 0.30 × 0.30 mm

Data collection

Rigaku AFC-7*S* diffractometer
$2\theta/\omega$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.565$, $T_{max} = 0.640$
3676 measured reflections
3501 independent reflections
3122 reflections with $I > 2\sigma(I)$

$R_{int} = 0.022$
$\theta_{max} = 26.51°$
$h = 0 \rightarrow 9$
$k = 0 \rightarrow 15$
$l = -22 \rightarrow 22$
3 standard reflections every 200 reflections intensity decay: −0.1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.111$
$S = 1.089$
3501 reflections
208 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0541P)^2 + 2.3975P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.726$ e Å^{-3}
$\Delta\rho_{min} = -0.702$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu—N1	1.998 (2)	Cu—N4	2.037 (3)
Cu—N5	2.020 (3)	Cu—N3	2.046 (3)

Cu—O5	2.295 (2)	N2—C3	1.344 (4)
N1—C3	1.345 (4)	N2—C2	1.364 (4)
N1—C1	1.366 (4)	C1—C2	1.378 (5)

N5—Cu—N4	93.73 (11)	N5—Cu—O5	98.80 (10)
N1—Cu—N3	81.15 (10)	N4—Cu—O5	94.95 (10)
N4—Cu—N3	93.20 (11)	N3—Cu—O5	92.57 (9)
N1—Cu—O5	96.58 (10)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5···N2^{i}	0.85	1.95	2.789 (4)	171
N4—H41···O2	0.90	2.31	3.188 (5)	166
N5—H51···N2^{ii}	0.90	2.28	3.127 (4)	158
N5—H52···O1^{iii}	0.90	2.22	3.057 (4)	154

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

The H5 atom of the methanol molecule was refined in a riding model with an O—H bond length of 0.85 Å and all other H-atom coordinates were constrained using the *SHELXL*97 default N—H and C—H distances.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1993*a*); cell refinement: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1993*a*); data reduction: *TEXSAN PROCESS* (Molecular Structure Corporation, 1993*b*); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL*97 (Sheldrick, 1997).

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