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Dichloro[*N*,*N*-dimethyl-1-(1-methyl-1*H*-tetrazol-5-yl-κN^4)methanamine-κN]copper(II)

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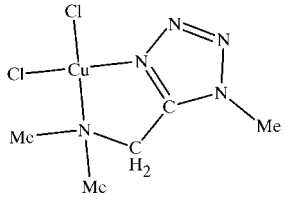
The title compound, $[CuCl_2(C_5H_{11}N_5)]$, is the first structurally characterized molecular chelate complex involving an α-aminoalkyltetrazole. There are two complex molecules in the asymmetric unit. The ligand molecules are bidentate. Both Cu atoms reveal rather distorted square-planar coordinations. The complex molecules are linked together by van der Waals interactions only.

Comment

5-(α-Aminoalkyl)-1alkyltetrazoles represent an interesting class of ligands which have various coordination abilities because of the presence of five N atoms. Moreover, the coordination chemistry of these ligands is of considerable interest due to the fact that they are isosteric with peptide units (Lodyga-Chruscinska *et al.*, 1999). However, no structures of transition metal complexes containing α-aminoalkyltetrazole ligands have been described to date. In this paper, we report the molecular and crystal structures of the copper(II) chloride complex of *N*,*N*-dimethyl-1-(1-methyl-1*H*-tetrazol-5-yl)methanamine, *i.e.* the title complex, (I).



(I)

There are two molecules of (I) in the asymmetric unit, and these are denoted *A* and *B*; molecule *A* is illustrated in Fig. 1. The *N*,*N*-dimethyl-1-(1-methyl-1*H*-tetrazol-5-yl)methanamine ligands are bidentate. Both Cu atoms reveal rather distorted square-planar coordination, with the coordination environment of the Cu atom being formed by atom N4 of the tetrazole ring, atom N5 of the *N*,*N*-dimethylmethanamine side chain and the two Cl atoms (Table 1). The mean deviation from the least-squares plane for the four atoms coordinated to the Cu atom is 0.2435 (15) Å for molecule *A* and 0.2113 (16) Å for molecule *B*. The Cu atoms are 0.0511 (13) and 0.0475 (13) Å from the corresponding least-squares plane in molecules *A* and *B*, respectively.

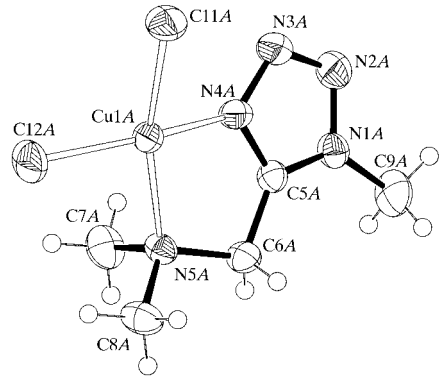


Figure 1
A view of the structure of molecule *A* of (I), showing the atom-numbering scheme; for molecule *B*, suffix *A* is replaced by *B*. Displacement ellipsoids are plotted at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

The tetrazole rings of molecules *A* and *B* have very similar geometries, close to those previously observed for 1,5-substituted tetrazole rings (Cambridge Structural Database, Version 5.23 of September 2002; Allen & Kennard, 1993). The rings are essentially planar, with mean deviations from the least-squares plane of the tetrazole ring of 0.004 (2) and 0.005 (2) Å for molecules *A* and *B*, respectively.

The chelate rings formed by atoms Cu, N4, C5, C6 and N5 are not planar. Atoms Cu, N4, C5 and C6 lie in the plane, with a mean deviation of 0.016 (2) Å for molecule *A* and 0.009 (2) Å for molecule *B*, and the dihedral angles between these planes and the C6/N5/Cu planes are 31.13 (14) and 31.91 (15)° for molecules *A* and *B*, respectively.

There are no hydrogen bonds in the structure of (I); the complex molecules are linked together by van der Waals interactions only (Fig. 2).

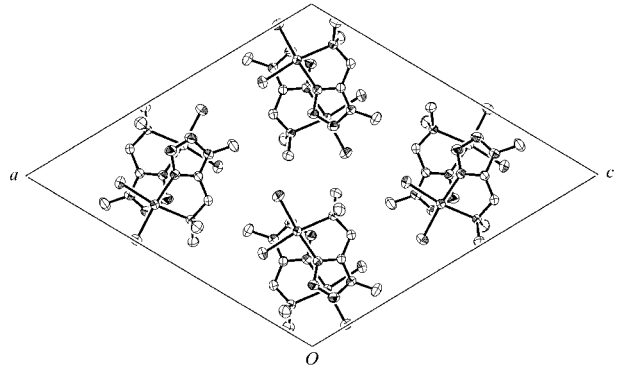


Figure 2
The crystal packing of (I), viewed along the *b* axis.

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Experimental

The *N*,*N*-dimethyl-1-(1-methyl-1*H*-tetrazol-5-yl)methanamine ligand was synthesized by aminomethylation of 1-methyltetrazole with dimethylamine hydrochloride and formaldehyde, according to the technique described by Karavai & Gaponik (1991). Green crystals of the title complex were obtained by slow evaporation in air of an equimolar solution of copper(II) chloride and *N*,*N*-dimethyl-1-(1-methyl-1*H*-tetrazol-5-yl)methanamine in a mixture of ethanol and butanol (*v*/*v* 3:1) [yield 91%; m.p. 548 K (decomposition)].

Crystal data

$[CuCl_2(C_5H_{11}N_5)]$
M_r = 275.63
Monoclinic, $P2_1/n$
a = 18.043 (3) Å
b = 7.1948 (13) Å
c = 18.048 (3) Å
β = 118.205 (13)°
V = 2064.7 (6) Å^3
Z = 8
D_x = 1.773 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 16.9–21.9°
μ = 2.60 mm^{-1}
T = 293 (2) K
Prism, green
0.60 × 0.35 × 0.10 mm

Data collection

Nicolet *R*3*m* four-circle diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.305, T_{max} = 0.781
6427 measured reflections
6052 independent reflections
4431 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 30.1°
$h = 0 \rightarrow 25$
$k = 0 \rightarrow 10$
$l = -25 \rightarrow 22$
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.122
S = 1.19
6052 reflections
235 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0320P)^2 + 4.2852P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

H atoms were included in idealized positions, with C—H distances of 0.96 Å, and refined using a riding model, with $U_{iso}(H) = 1.5U_{eq}(C)$ for the methyl groups and $1.2U_{eq}(C)$ for the methylene group.

Table 1
Selected geometric parameters (Å, °).

N4*A*—Cu1*A*	1.979 (3)	N4*B*—Cu1*B*	1.973 (3)
N5*A*—Cu1*A*	2.114 (3)	N5*B*—Cu1*B*	2.120 (3)
Cl1*A*—Cu1*A*	2.2413 (11)	Cl1*B*—Cu1*B*	2.2411 (11)
Cl2*A*—Cu1*A*	2.1922 (11)	Cl2*B*—Cu1*B*	2.1869 (11)
N4*A*—Cu1*A*—N5*A*	79.33 (11)	N4*B*—Cu1*B*—N5*B*	79.12 (11)
N4*A*—Cu1*A*—Cl2*A*	162.22 (11)	N4*B*—Cu1*B*—Cl2*B*	164.19 (11)
N5*A*—Cu1*A*—Cl2*A*	95.33 (8)	N5*B*—Cu1*B*—Cl2*B*	95.55 (8)
N4*A*—Cu1*A*—Cl1*A*	92.52 (9)	N4*B*—Cu1*B*—Cl1*B*	92.19 (9)
N5*A*—Cu1*A*—Cl1*A*	165.78 (9)	N5*B*—Cu1*B*—Cl1*B*	166.76 (9)
Cl2*A*—Cu1*A*—Cl1*A*	95.79 (4)	Cl2*B*—Cu1*B*—Cl1*B*	95.35 (5)

Data collection: *R*3*m Software* (Nicolet, 1980); cell refinement: *R*3*m Software*; data reduction: *R*3*m Software*; program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: AV1123). Services for accessing these data are described at the back of the journal.

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