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Layered structure of *catena*-poly[[bis[1-(2-azidoethyl)-tetrazole-N^4]copper(**II**)]-di-μ-chloro]

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Key indicators

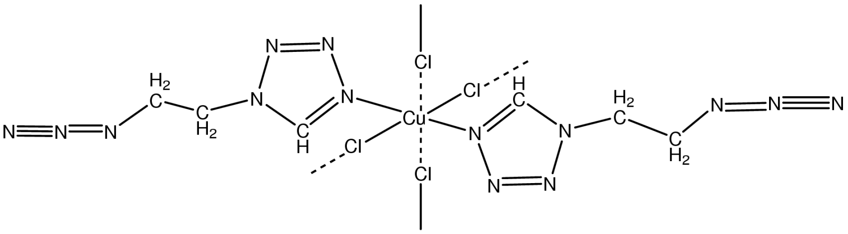
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.033
wR factor = 0.097
Data-to-parameter ratio = 16.4

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

In the title compound, $[CuCl_2(C_3H_5N_7)_2]$, the coordination polyhedron of the Cu atom is an elongated square bipyramid with $\overline{1}$ site symmetry. The equatorial positions are occupied by the two Cl atoms with Cu—Cl distances of 2.288 (1) Å and two azidoethyltetrazole ligands with Cu—N distances of 1.999 (2) Å. Two Cl atoms in axial positions are 2.956 (1) Å distant from the Cu atom. The Cl atoms play the role of non-symmetrical bridges responsible for formation of layers parallel to the *bc* plane.

Comment

It has been found in the past few years that the complexes of copper(II) chloride with 1-monosubstituted tetrazole of composition $CuCl_2L_2$, where L = 1-ethyl-, 1-hexyl-, 1-vinyl- and 1-allyltetrazole, undergo magnetic phase transition to a ferromagnetic form at T = 10–12 K (Gaponik, 1998). X-ray investigations of the complexes with L = 1-ethyltetrazole (Virovets *et al.*, 1995) and L = 1-allyltetrazole (Virovets *et al.*, 1996) showed a layered polymeric crystal structure for these compounds. This is known to be a necessary condition for ferromagnetic ordering for transition metal complexes (Ovcharenko & Sagdeev, 1999). In the present work, the crystal structure of a new complex, (I), of composition $CuCl_2L_2$ (L = 1-azidoethyltetrazole), is reported.



(I)

In the title compound, the coordination polyhedron of the Cu atom is an elongated square bipyramid with $\overline{1}$ site symmetry. The equatorial positions are occupied by the two Cl atoms with Cu—Cl distances of 2.288 (1) Å and two N4 atoms of azidoethyltetrazole molecules with Cu—N distances of 1.999 (2) Å. Two Cl atoms in axial positions are at a distance of 2.956 (1) Å from the Cu atom.

The tetrazole ring is essentially planar, with a mean deviation of the terazole ring atoms from their least-squares plane of 0.006 (2) Å. The tetrazole plane forms a dihedral angle of 50.9 (1)° with the equatorial plane of the coordination square bipyramid of the Cu atom. In the azide fragment, the N5—N6

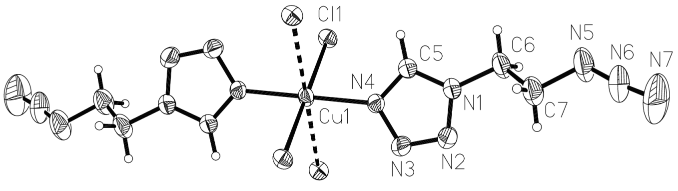


Figure 1
ORTEP-3 (Farrugia, 1997) drawing of the molecule of (I). Long intermolecular Cu···Cl interactions are shown as dashed lines. Displacement ellipsoids are plotted at the 50% probability level.

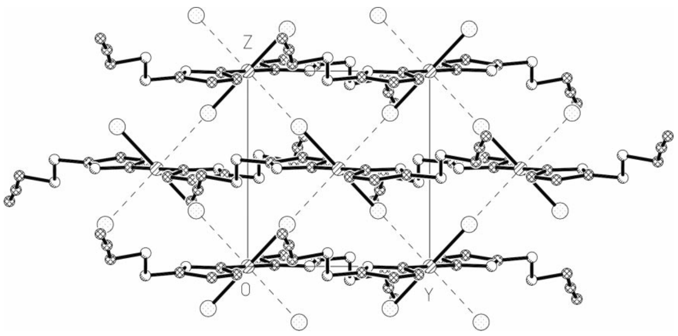


Figure 2
The packing diagram of (I) viewed along the *a* axis (H atoms have been omitted for clarity).

distance is 1.204 (4) Å and the N6—N7 distance is 1.123 (4) Å; the N5—N6—N7 and C7—N5—N6 bond angles are 173.1 (4) and 115.7 (3)°, respectively.

The analysis of the crystal packing of complex (I) reveals a couple of interesting features. The Cl atoms play the role of non-symmetrical bridges which are responsible for formation of layers parallel to the *bc* plane. They also act as acceptors of non-classic intermolecular hydrogen bonds C5—H5···Cl, with a Cl···C5 distance of 3.529 (3) Å (Steiner, 1996). Thus, the title compound has a layered polymeric crystal structure, and hence may be a candidate for magnetic properties investigations.

Experimental

The synthesis of the title compound was carried out at 425–426 K by reaction of $CuCl_2{\cdot}2H_2O$ with 1-(2-azidoethyl)tetrazole (molar ratio 1:2) by a method proposed by Degtiarik *et al.* (1985). Recrystallization of (I) was performed from aqueous solution. 1-(2-Azidoethyl)-tetrazole was prepared by heterocyclization of 1-amino-2-azidoethane with ethyl orthoformate and sodium azide in acetic acid (Gaponik *et al.*, 1985).

Crystal data

$[CuCl_2(C_3H_5N_7)_2]$
$M_r = 412.72$
Monoclinic, $P2_1/c$
$a = 15.616$ (2) Å
$b = 6.702$ (2) Å
$c = 7.208$ (6) Å
$\beta = 91.87$ (3)°
$V = 754.0$ (7) Å^3
$Z = 2$

$D_x = 1.818$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 17.2$–24.2°
$\mu = 1.83$ mm^{-1}
$T = 293$ (2) K
Plate, blue
0.80 × 0.46 × 0.02 mm

Data collection

Nicolet *R*3*m* four-circle diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.323$, $T_{\max} = 0.964$
1880 measured reflections
1734 independent reflections
1529 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.018$
$\theta_{\max} = 27.5$°
$h = -20 \rightarrow 20$
$k = -8 \rightarrow 0$
$l = 0 \rightarrow 9$
3 standard reflections every 100 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.097$
$S = 1.04$
1734 reflections
106 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0690P)^2 + 0.2230P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.47$ e Å^{-3}
$\Delta\rho_{\min} = -0.34$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—Cl1	2.288 (1)	N3—N4	1.351 (3)
Cu1—Cl1$^{\rm i}$	2.956 (1)	N4—C5	1.309 (3)
Cu1—N4	1.999 (2)	C6—C7	1.475 (4)
N1—N2	1.342 (3)	C7—N5	1.476 (3)
N1—C5	1.319 (3)	N5—N6	1.204 (4)
N1—C6	1.467 (3)	N6—N7	1.123 (4)
N2—N3	1.288 (3)		
N4—Cu1—Cl1	89.49 (5)	C5—N4—N3	106.8 (2)
N4$^{\rm ii}$—Cu1—Cl1$^{\rm i}$	89.18 (6)	C5—N4—Cu1	128.4 (1)
Cl1—Cu1—Cl1$^{\rm i}$	93.35 (5)	N3—N4—Cu1	124.4 (1)
C5—N1—N2	108.5 (2)	N4—C5—N1	108.3 (2)
C5—N1—C6	130.1 (2)	N1—C6—C7	111.4 (2)
N2—N1—C6	121.3 (2)	C6—C7—N5	106.4 (2)
N3—N2—N1	107.0 (2)	N6—N5—C7	115.7 (3)
N2—N3—N4	109.5 (2)	N7—N6—N5	173.1 (4)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···Cl1$^{\rm i}$	0.93	2.75	3.529 (3)	142

Symmetry code: (i) $-x, 2-y, 1-z$.

The H atoms were included in geometrically calculated positions and refined using a riding model with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$ of the corresponding carrier atom.

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.

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