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catena-Poly[[bis(*cis*-1-*tert*-butyltetrazole-κN^4)copper(II)]-di-μ-chloro]

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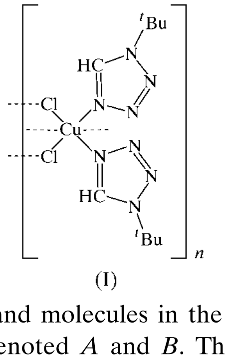
The title polymeric compound, $[CuCl_2(C_5H_{10}N_4)_2]_n$, is the first structurally characterized complex with a bulky 1-alkyltetrazole ligand. The coordination polyhedron of the Cu atom is an elongated octahedron. The equatorial positions of the octahedron are occupied by the two Cl atoms, with Cu—Cl distances of 2.2920 (8) and 2.2796 (9) Å, and by the two N-4 atoms of the tetrazole ligands, with Cu—N distances of 2.023 (2) and 2.039 (2) Å. Two symmetry-related Cl atoms occupy the axial positions, at distances of 2.8244 (8) and 3.0174 (8) Å from the Cu atom. The $[CuCl_2(C_5H_{10}N_4)_2]$ units form infinite chains extended along the *b* axis, linked together only by van der Waals interactions. The skeleton of each chain consists of Cu and Cl atoms.

Comment

It has been found that complexes of copper(II) chloride with 1-substituted tetrazoles, of composition $CuCl_2L_2$, undergo magnetic phase transition to a ferromagnetic form at T = 10–12 K (Gaponik, 1998). X-ray investigations of such complexes are important for correlating their structures and magnetic properties. The present work is concerned with the crystal structure investigation of a new complex of composition $CuCl_2L_2$, namely the title complex, (I) (Fig. 1).



(I)

There are two ligand molecules in the asymmetric unit of (I), and these are denoted *A* and *B*. The tetrazole rings of molecules *A* and *B* have very similar geometries, close to those previously observed for these rings (Cambridge Structural Database; Version 5.22 of October 2001; Allen & Kennard, 1993). The rings are essentially planar, with mean deviations of the tetrazole ring atoms from the least-squares plane of 0.0084 (3) and 0.0041 (3) Å for ligands *A* and *B*, respectively.

In (I), the coordination polyhedron of the Cu atom is an elongated octahedron (Table 1). The equatorial positions of the octahedron are occupied by two Cl atoms, with distances Cu—Cl1 2.2920 (8) Å and Cu—Cl2 2.2796 (9) Å, and by the two N-4 atoms of the 1-*tert*-butyltetrazole ligands, with distances Cu—N4*A* 2.023 (2) Å and Cu—N4*B* 2.039 (2) Å. The dihedral angle between the planes of the tetrazole rings of ligands *A* and *B* is 81.88 (14)°. The Cu—Cl distances for the axial bridging Cl atoms are 2.8244 (8) Å for Cl1^{i} and 3.0174 (8) Å for Cl2^{ii} [symmetry codes: (i) $-x, 1-y, -z$; (ii) $-x, -y, -z$].

With regard to the packing structure of (I), the following may be noted. The $[CuCl_2(C_5H_{10}N_4)_2]$ units form infinite chains extended along the *b* axis, linked together only by van der Waals interactions. The skeleton of each chain consists of Cu and Cl atoms. There are no classical hydrogen bonds in the

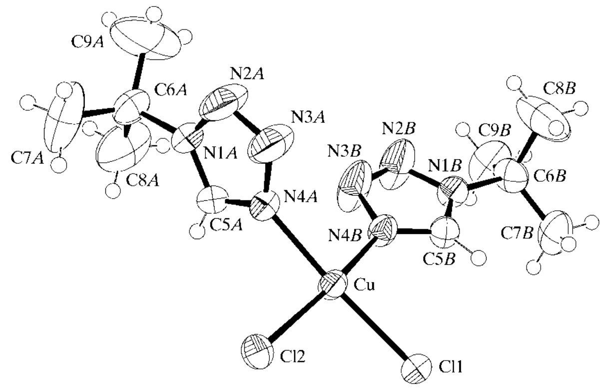


Figure 1
A view of the asymmetric unit of (I), showing the atom-numbering scheme. Displacement ellipsoids are plotted at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

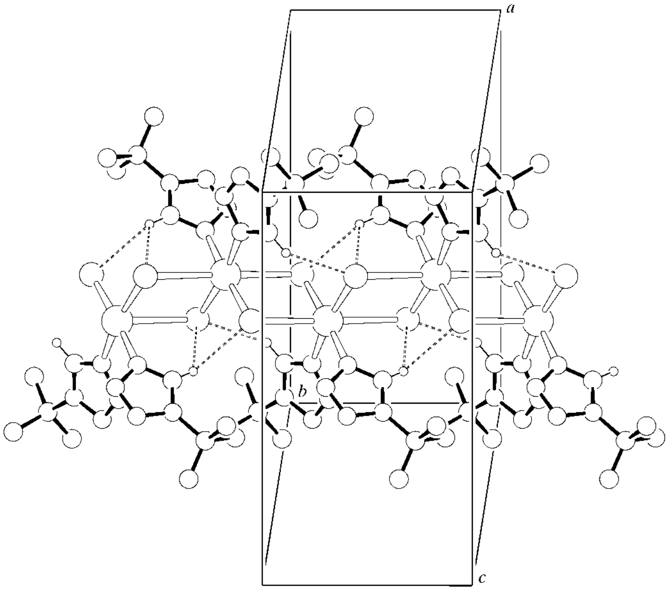


Figure 2
A fragment of the structure of (I) showing the chlorine-bridged chain.

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structure, but the following intermolecular contacts are noteworthy: C5*B*—H5*B*···Cl2^{i} = 3.369 (3) Å, C5*A*—H5*A*···Cl1^{ii} = 3.369 (3) Å and C5*A*—H5*A*···Cl2^{ii} = 3.343 (3) Å (Steiner, 1996). These long contacts are additional interactions in the polymeric chains.

Experimental

1-*tert*-Butyltetrazole was prepared by heterocyclization of *tert*-butylamine with triethyl orthoformate and trimethylsilyl azide (Grigoriev *et al.*, 1997). Single crystals of (I) were grown by slow crystallization from a solution in methanol–2-propanol–butanol (molar ratio 2:1.5:1) of a mixture containing $CuCl_2·2H_2O$ and 1-*tert*-butyltetrazole in a 1:2.1 molar ratio over a period of one week at 288–291 K.

Crystal data

$[CuCl_2(C_5H_{10}N_4)_2]$
M_r = 386.78
Monoclinic, $P2_1/n$
a = 13.389 (3) Å
b = 7.1460 (10) Å
c = 19.473 (4) Å
β = 108.57 (3)°
V = 1766.1 (6) Å^3
Z = 4

D_x = 1.455 Mg m^{-3}
Mo *K*α radiation
Cell parameters from 25 reflections
θ = 12.9–23.5°
μ = 1.55 mm^{-1}
T = 293 (2) K
Prism, green
0.64 × 0.42 × 0.30 mm

Data collection

Nicolet *R*3*m* four-circle diffractometer
ω/2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.438, T_{max} = 0.654
5383 measured reflections
5183 independent reflections
4063 reflections with $I > 2\sigma(I)$

R_{int} = 0.039
θ_{max} = 30.1°
h = 0 → 18
k = 0 → 10
l = −27 → 26
3 standard reflections every 100 reflections intensity decay: none

Table 1
Selected geometric parameters (Å, °).

Cu—N4*A*	2.023 (2)	Cu—Cl1	2.2920 (8)
Cu—N4*B*	2.039 (2)	Cu—Cl1^{i}	2.8244 (8)
Cu—Cl2	2.2796 (9)	Cu—Cl2^{ii}	3.0174 (8)
N4*A*—Cu—N4*B*	86.07 (9)	Cl2—Cu—Cl1^{i}	98.10 (3)
N4*A*—Cu—Cl2	89.95 (7)	Cl1—Cu—Cl1^{i}	83.85 (2)
N4*B*—Cu—Cl2	170.30 (7)	N4*A*—Cu—Cl2^{ii}	87.98 (7)
N4*A*—Cu—Cl1	175.38 (6)	N4*B*—Cu—Cl2^{ii}	87.81 (7)
N4*B*—Cu—Cl1	89.61 (6)	Cl2—Cu—Cl2^{ii}	83.21 (3)
Cl2—Cu—Cl1	94.57 (3)	Cl1—Cu—Cl2^{ii}	93.51 (2)
N4*A*—Cu—Cl1^{i}	94.57 (7)	Cl1^{i}—Cu—Cl2^{ii}	177.130 (18)
N4*B*—Cu—Cl1^{i}	91.03 (7)		

Symmetry codes: (i) −*x*, 1 − *y*, −*z*; (ii) −*x*, −*y*, −*z*.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5*B*—H5*B*···Cl2^{i}	0.94 (3)	2.59 (3)	3.369 (3)	140 (2)
C5*A*—H5*A*···Cl1^{ii}	0.89 (3)	2.72 (3)	3.369 (3)	130 (2)
C5*A*—H5*A*···Cl2^{ii}	0.89 (3)	2.70 (3)	3.343 (3)	130 (2)

Symmetry codes: (i) −*x*, 1 − *y*, −*z*; (ii) −*x*, −*y*, −*z*.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.127
S = 1.05
5183 reflections
196 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0610P)^2 + 1.2623P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}

The positions of atoms H5*A* and H5*B*, on atoms C5*A* and C5*B*, respectively, were refined, with U_{iso}(H) = 0.05 Å^2. The remaining H atoms were included in their idealized positions, with C—H = 0.96 Å, and refined using a riding model, with $U_{iso}(H) = 1.5U_{eq}(C)$.

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: *SHELXS*97 (Sheldrick, 1997); 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: SK1540). Services for accessing these data are described at the back of the journal.

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