

Chain structure of *catena*-poly[[bis-  
[*cis*-1-(2,4,6-trimethylphenyl)tetrazole-  
 $\kappa$ N<sup>4</sup>]]copper(II)]-di- $\mu$ -chloro]Dmitry O. Ivashkevich,\*  
Alexander S. Lyakhov,  
Mikhail M. Degtyarik and  
Pavel N. GaponikBelarusian State University, Physico-Chemical  
Research Institute, Leningradskaya str. 14, Minsk  
220050, Belarus

Correspondence e-mail: ivashkevichdo@bsu.by

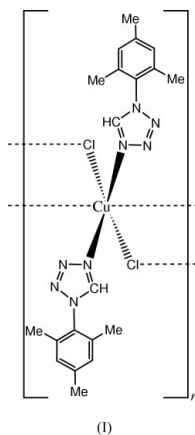
## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.038  
 $wR$  factor = 0.121  
Data-to-parameter ratio = 19.4For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

In the title compound,  $[\text{CuCl}_2(\text{C}_{10}\text{H}_{12}\text{N}_4)_2]_n$ , the coordination polyhedron of the Cu atom is an elongated octahedron. Its equatorial positions are occupied by two Cl atoms [Cu—Cl 2.2767 (8) and 2.2669 (8) Å] and two N<sup>4</sup> atoms of substituted tetrazole ligands [Cu—N<sup>4</sup> 2.016 (2) and 2.038 (2) Å]. The axial positions are occupied by two Cl atoms [Cu—Cl 2.9769 (11) and 2.8995 (11) Å], which belong to the equatorial planes of two neighbouring Cu atoms. Thus, the  $[\text{CuCl}_2(\text{C}_{10}\text{H}_{12}\text{N}_4)_2]$  units form infinite chains, extended along the  $a$  axis, which are linked together only by van der Waals interactions. The skeleton of each chain consists of Cu and Cl atoms.

## Comment

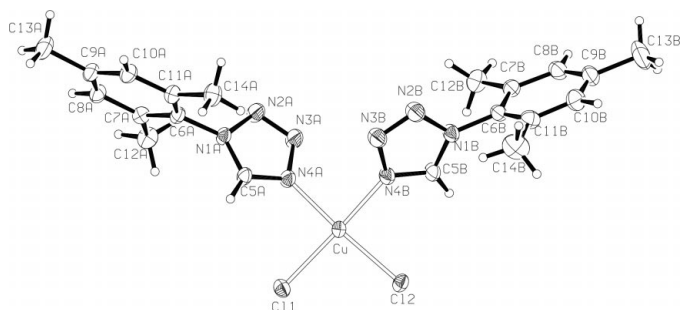
This work continues our X-ray studies of transition metal complexes with bulky 1-alkyltetrazole ligands. In an earlier paper (Ivashkevich *et al.*, 2002) we reported the structure of a complex of  $\text{CuCl}_2$  with 1-*tert*-butyltetrazole. The present paper is concerned with the crystal structure of the new title complex, (I) (Fig. 1). The structure of 2,4,6-trimethylphenyltetrazole was determined previously (Lyakhov *et al.*, 2000).



There are two substituted tetrazole ligands in the asymmetric unit of (I), and these are denoted as *A* and *B* in Fig. 1. The tetrazole rings of molecules *A* and *B* have very similar geometries, close to those previously observed for 1-substituted tetrazoles (Cambridge Structural Database; Version 5.23 of September 2002; Allen, 2002). The rings are essentially planar, with mean deviations of tetrazole ring atoms from their least-squares planes of 0.0023 (17) and 0.0023 (19) Å for ligands *A* and *B*, respectively. The dihedral angle between the planes of the tetrazole rings of the *A* and *B* ligands is 63.27 (12)°.

The tetrazole and benzene rings in each of the ligands are not coplanar, the dihedral angles formed by the least-squares planes of the benzene and tetrazole rings being equal to

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**Figure 1**

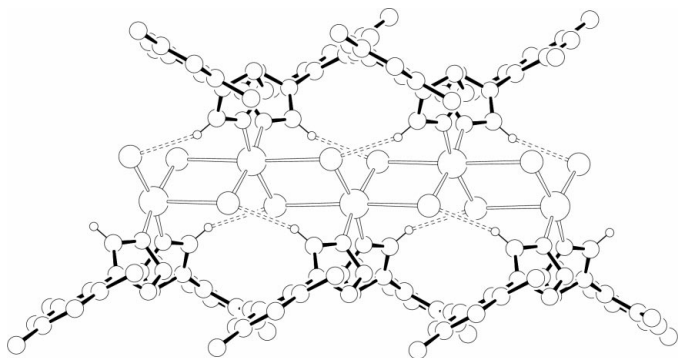
A view of the asymmetric unit of (I), showing the atom-numbering scheme. Displacement ellipsoids are plotted at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

74.74 (8) and 76.51 (10)° for ligands *A* and *B*, respectively. The N1–C6 bond lengths in both ligands are identical [1.438 (3) Å]; this value is typical for a normal N–C(benzene) single bond.

The ligand geometries are close to that of the uncoordinated 2,4,6-trimethylphenyltetrazole molecule (Lyakhov *et al.*, 2000).

In the title compound, (I), the coordination polyhedron of the Cu atom is an elongated octahedron (Table 1). Its equatorial positions are occupied by two Cl atoms [Cu–Cl1 2.2767 (8) Å and Cu–Cl2 2.2669 (8) Å] and two N<sup>4</sup> atoms of 2,4,6-trimethylphenyltetrazole ligands [Cu–N4*A* 2.016 (2) Å and Cu–N4*B* 2.038 (2) Å]. The Cu–Cl distances for the axial Cl1<sup>i</sup> and Cl2<sup>ii</sup> atoms are 2.9769 (11) and 2.8995 (11) Å, respectively [symmetry codes: (i) 1–*x*, 1–*y*, 2–*z*; (ii) –*x*, 1–*y*, 2–*z*].

The coordination polyhedra of the adjacent Cu atoms in crystal share edges, forming a one-dimensional polymeric structure composed of [CuCl<sub>2</sub>(C<sub>10</sub>H<sub>12</sub>N<sub>4</sub>)<sub>2</sub>] units. These infinite chains are extended along the *a* axis (Fig. 2) and linked together only by van der Waals interactions. There are no classical hydrogen bonds in the structure of (I), but the intermolecular contacts C5*A*–H5*A*···Cl2<sup>i</sup> and C5*B*–H5*B*···Cl1<sup>ii</sup> are noteworthy (Table 2) (Steiner, 1996). Remarkably, these contacts are within the chain, and therefore may not account for holding the chains together in the crystal.



**Figure 2**

Fragment of the structure of (I), showing a chloro-bridged chain extended along the *a* axis. The dashed lines show C–H···Cl contacts presented in Table 2.

Thus, the structure of (I) is similar to that of the CuCl<sub>2</sub>L<sub>2</sub> complex, where *L* is 1-*tert*-butyltetrazole (Ivashkevich *et al.*, 2002). However, they are both different from the structures of the complexes of this composition, but with non-bulky 1-alkyltetrazole ligands *L* = 1-ethyl- (Virovets *et al.*, 1995), 1-allyl- (Virovets *et al.*, 1996) and 1-azidoethyltetrazole (Ivashkevich *et al.*, 2001), which were found to have layered polymeric structures. The difference is probably due to steric effects.

## Experimental

2,4,6-Trimethylphenyltetrazole (m.p. 400–401 K, uncorrected) was prepared by the method described by Grigoriev *et al.* (1997). Single crystals of (I) were grown by slow crystallization from a solution in methanol–butanol–2-propanol–triethyl orthoformate–hexane (*v/v* 8:2:1:0.1:0.3) of a mixture containing CuCl<sub>2</sub>·2H<sub>2</sub>O and 2,4,6-trimethylphenyltetrazole in a 1:2.1 molar ratio over a period of 8–10 d at 293 K.

### Crystal data

[CuCl<sub>2</sub>(C<sub>10</sub>H<sub>12</sub>N<sub>4</sub>)<sub>2</sub>]  
*M<sub>r</sub>* = 510.91  
 Triclinic, *P*1̄  
*a* = 7.283 (2) Å  
*b* = 12.032 (3) Å  
*c* = 13.912 (3) Å  
 $\alpha$  = 85.97 (2)°  
 $\beta$  = 84.19 (2)°  
 $\gamma$  = 75.82 (2)°  
*V* = 1174.6 (5) Å<sup>3</sup>

*Z* = 2  
*D<sub>x</sub>* = 1.445 Mg m<sup>−3</sup>  
 Mo *K*α radiation  
 Cell parameters from 25 reflections  
 $\theta$  = 15.5–17.9°  
 $\mu$  = 1.18 mm<sup>−1</sup>  
*T* = 293 (2) K  
 Prism, green  
 0.60 × 0.10 × 0.10 mm

### Data collection

Nicolet R3m four-circle diffractometer  
 $\omega/2\theta$  scans  
 Absorption correction:  $\psi$  scan (North *et al.*, 1968)  
*T<sub>min</sub>* = 0.537, *T<sub>max</sub>* = 0.891  
 6068 measured reflections  
 5445 independent reflections  
 4277 reflections with *I* > 2σ(*I*)

*R<sub>int</sub>* = 0.014  
 $\theta_{\max}$  = 27.6°  
*h* = −2 → 9  
*k* = −15 → 15  
*l* = −18 → 18  
 3 standard reflections every 100 reflections  
 intensity decay: none

### Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.038  
*wR*(*F*<sup>2</sup>) = 0.121  
*S* = 1.05  
 5445 reflections  
 280 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0674P)^2 + 0.5007P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.49 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.53 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

Cu–N4 <i>A</i>	2.016 (2)	Cu–Cl2	2.2669 (8)
Cu–N4 <i>B</i>	2.038 (2)	Cu–Cl1 <sup>i</sup>	2.9769 (11)
Cu–Cl1	2.2767 (8)	Cu–Cl2 <sup>ii</sup>	2.8995 (11)
N4 <i>A</i> –Cu–N4 <i>B</i>	89.29 (9)	Cl2–Cu–Cl2 <sup>ii</sup>	85.08 (3)
N4 <i>A</i> –Cu–Cl1	90.55 (6)	Cl1–Cu–Cl2 <sup>ii</sup>	97.49 (3)
N4 <i>A</i> –Cu–Cl2	170.21 (6)	N4 <i>A</i> –Cu–Cl1 <sup>i</sup>	88.56 (6)
N4 <i>B</i> –Cu–Cl1	167.31 (7)	N4 <i>B</i> –Cu–Cl1 <sup>i</sup>	87.14 (7)
N4 <i>B</i> –Cu–Cl2	89.16 (6)	Cl2–Cu–Cl1 <sup>i</sup>	101.02 (3)
Cl2–Cu–Cl1	93.07 (3)	Cl1–Cu–Cl1 <sup>i</sup>	80.16 (3)
N4 <i>A</i> –Cu–Cl2 <sup>ii</sup>	85.43 (6)	Cl2 <sup>ii</sup> –Cu–Cl1 <sup>i</sup>	173.539 (19)
N4 <i>B</i> –Cu–Cl2 <sup>ii</sup>	95.15 (7)		

Symmetry codes: (i) 1–*x*, 1–*y*, 2–*z*; (ii) –*x*, 1–*y*, 2–*z*.

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$C5A-H5A \cdots Cl2^i$	0.93	2.58	3.458 (3)	159
$C5B-H5B \cdots Cl1^{ii}$	0.93	2.63	3.458 (3)	148

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

H atoms were included in their idealized positions, with  $C-H = 0.96$  Å, and refined using a riding model with  $U_{iso}(H) = 1.5U_{eq}(C)$  for methyl H atoms and with  $U_{iso}(H) = 1.2U_{eq}(C)$  for other H atoms.

Data collection: *R3m* Software (Nicolet, 1980); cell refinement: *R3m* Software; data reduction: *R3m* Software; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* for Windows (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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