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The chain structure of *catena*-poly[[(2-*tert*-butyltetrazole-κN^4)copper(II)]-di-μ-chloro]

Alexander S. Lyakhov, Pavel N. Gaponik, Michail M. Degtyarik and Ludmila S. Ivashkevich*

Physico-Chemical Research Institute, Belarusian State University, Leningradskaya Str. 14, Minsk 220050, Belarus

Correspondence e-mail: iva@bsu.by

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The title compound, $[\mathrm{CuCl_2(C_5H_{10}N_4)}]_n$, is the first structurally characterized complex of a transition metal halide with a 2-monosubstituted tetrazole. The Cu atom is five-coordinated and has a distorted square-pyramidal coordination geometry. One of the basal sites of the pyramid is occupied by an N atom of the tetrazole ligand [Cu—N = 2.0131 (19) Å]. A Cl atom occupies the apical position [Cu—Cl = 2.6438 (8) Å] and belongs to the basal plane of the coordination pyramid of the neighbouring Cu atom. In fact, all the Cl atoms act as bridging ligands and the Cu atom coordination polyhedron shares both Cl—Cl edges with the polyhedra of two neighbouring Cu atoms, thus giving rise to polymeric chains running along the *a* axis of the crystal.

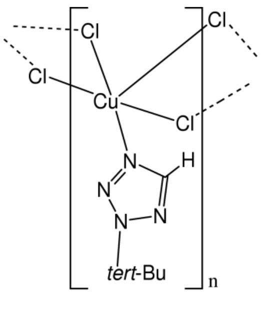
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.035
wR factor = 0.098
Data-to-parameter ratio = 26.4

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

Comment

Polynuclear chloride-bridged copper(II) compounds with N-substituted tetrazole ligands are of considerable interest, because they may undergo magnetic phase transition to a ferromagnetic form (Gaponik, 1998). However, structural studies were limited almost exclusively to complexes with 1-monosubstituted tetrazoles. A search of the Cambridge Structural Database (Version 5.23, September 2002 release; Allen, 2002) retrieved only one complex of 2-substituted tetrazole, *viz*. the nickel(II) complex $[\mathrm{Ni(2\text{-}MeTz)_6}](\mathrm{BF_4})_2$, where 2-MeTz is 2-methyltetrazole (van den Heuvel *et al.*, 1983). No structural data for complexes of transition metal halides with 2-monosubstituted tetrazoles were found.



(I)

In this paper, we report the crystal structure of the copper(II) complex $[\mathrm{CuCl_2(2\text{-}^t BuTz)}]_n$, (I), where 2-^{t}BuTz is 2-*tert*-butyltetrazole (Fig. 1).

The tetrazole ring of the ligand is planar within 0.007 (2) Å; its geometry is in good agreement with that of 2-MeTz, reported by van den Heuvel *et al.* (1983).

The coordination polyhedron of the Cu atom in (I) is a distorted square pyramid, as is apparent from the observed τ value of 0.2 (values of 0 and 1 are indicative of ideal square-pyramidal and trigonal-bipyramidal geometries, respectively;

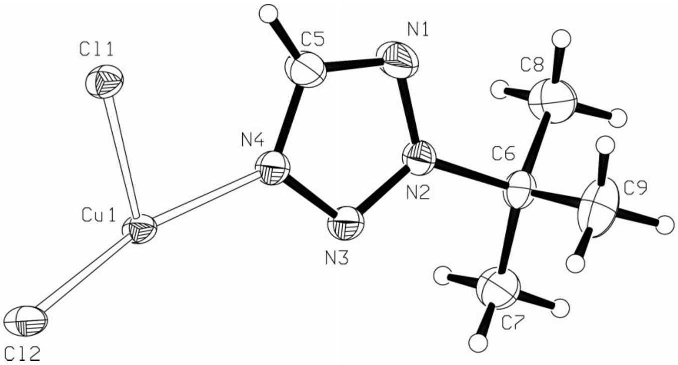


Figure 1
ORTEP-3 (Farrugia, 1997) plot of the asymmetric unit of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as spheres of arbitrary radii.

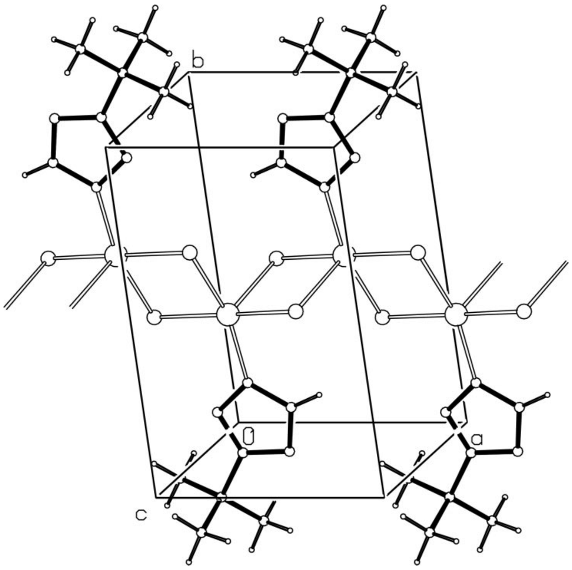


Figure 2
Fragment of the crystal structure of (I), showing a polymeric chain of chloride-bridged Cu atoms running along the *a* axis.

Addison *et al.*, 1984). The basal positions of the pyramid are occupied by three Cl atoms [Cu1—Cl1 2.2661 (9), Cu1—Cl2 2.2931 (9) and Cu1—Cl2$^{\rm i}$ 2.2892 (9) Å; symmetry code: (i) $-x$, $1-y$, $1-z$] and the N4 atom of the tetrazole ligand [Cu1—N4 2.0131 (19) Å]. The atom Cl1$^{\rm ii}$ [symmetry code: (ii) $1-x$, $1-y$, $1-z$] lies in the axial position of the pyramid [Cu1—Cl1$^{\rm ii}$ 2.6438 (8) Å]. As can be seen from Fig. 2, adjacent copper polyhedra share their Cl···Cl edges, thus forming a polymeric chain running along the *a* axis. The distances between neighbouring Cu atoms in the chain are 3.3831(10) Å for Cu1···Cu1$^{\rm i}$ [symmetry code: (i) $-x$, $1-y$, $1-z$] and 3.5041 (11) Å for Cu1···Cu1$^{\rm ii}$ [symmetry code: (ii) $1-x$, $1-y$, $1-z$]. Together with the tetrazole ligands, the chains of chloride-bridged Cu atoms form $[\mathrm{CuCl_2(2\text{-}^{\it t}BuTz)}]_n$ ribbons (Fig. 3), with only van der Waals interactions between them.

Experimental

2-*tert*-Butyltetrazole was prepared by regioselective alkylation of tetrazole with *tert*-butyl alcohol in sulfuric acid (Koren' & Gaponik, 1990). A mixture of $\mathrm{CuCl_2{\cdot}2H_2O}$ (0.008 mol) and 2-*tert*-butyltetrazole (0.008 mol) in ethyl alcohol (15 ml) was heated to 343 K, kept at this temperature for 30 min, and then cooled to 253 K. The crystalline complex was filtered off, washed with diethyl ether and air dried. Crystals suitable for single-crystal X-ray analysis were grown by slow evaporation from a methanol–ethanol–butanol–hexane solution (equal volumes of solvent components) at room temperature over a period of two weeks.

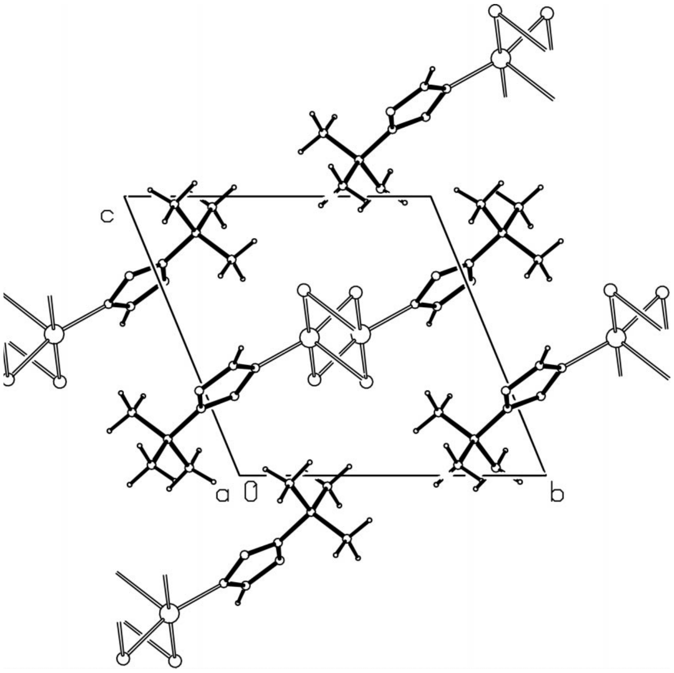


Figure 3
The crystal packing of (I), viewed along the *a* axis.

Crystal data

$[\mathrm{CuCl_2(C_5H_{10}N_4)}]$
$M_r = 260.61$
Triclinic, $P\overline{1}$
$a = 6.1054$ (15) Å
$b = 9.598$ (3) Å
$c = 9.813$ (3) Å
$\alpha = 108.92$ (2)°
$\beta = 106.899$ (19)°
$\gamma = 97.39$ (2)°
$V = 504.5$ (2) Å^3
$Z = 2$
$D_x = 1.716$ Mg m^{-3}
Mo *K*α radiation
Cell parameters from 25 reflections
$\theta = 19.2$–22.1°
$\mu = 2.65$ mm^{-1}
$T = 293$ (2) K
Prism, green
0.60 × 0.42 × 0.10 mm

Data collection

Nicolet *R*3*m* four-circle diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\rm min} = 0.299$, $T_{\rm max} = 0.778$
3216 measured reflections
2961 independent reflections
2663 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.028$
$\theta_{\rm max} = 30.1°$
$h = -8 \rightarrow 8$
$k = -13 \rightarrow 12$
$l = 0 \rightarrow 13$
3 standard reflections every 100 reflections intensity decay: 0.6%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.098$
$S = 1.06$
2961 reflections
112 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0593P)^2 + 0.2094P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 1.04$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.87$ e Å^{-3}

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Table 1
Selected geometric parameters (Å,).

Cu1—Cl1	2.2661 (9)	N1—N2	1.327 (3)
Cu1—Cl2^{i}	2.2892 (9)	N1—C5	1.316 (3)
Cu1—Cl2	2.2931 (9)	N2—N3	1.300 (2)
Cu1—Cl1^{ii}	2.6438 (8)	N3—N4	1.324 (2)
Cu1—N4	2.0131 (19)	N4—C5	1.339 (3)

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

H atoms were placed in geometrically calculated positions, with C—H = 0.93–0.96 Å, and included in the refinement in a riding-model approximation, with $U_{\rm iso}$(H) equal to $1.2U_{\rm eq}$(carrier atom) for the tetrazole ring H atom and $1.5U_{\rm eq}$(carrier atom) for the other H atoms. The maximum residual electron-density peak is 0.88 Å from the Cu 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) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL*97.

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