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catena-Poly[[[μ-5,5′-di-2-pyridyl-1,1′-(*p*-phenylenedimethylene)bis(1*H*-tetrazole)]-[chloridocopper(II)]-di-μ-chlorido-[chlorido-copper(II)]] acetonitrile solvate]

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In the title coordination polymer, $\{[Cu_2Cl_4(C_{20}H_{16}N_{10})]\cdot CH_3CN\}_n$, the Cu^{II} atom is five-coordinated by two N atoms from the *L* ligand (where *L* is bis{[2-pyridyl(1*H*-tetrazol-5-yl)]-1-ylmethyl}benzene) and three chloride ions to form a square-pyramidal geometry. The *L* ligands bridge adjacent Cu^{II} dinuclear units, forming a one-dimensional chain.

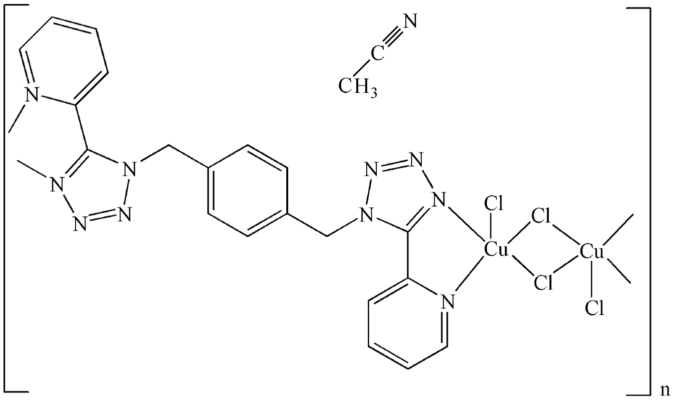
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.034
wR factor = 0.081
Data-to-parameter ratio = 13.7

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

Comment

In recent years, tetrazoles have found a wide range of applications in the area of coordination chemistry, because they can act as mono- or bidentate ligands and exhibit a strong networking ability (Wu *et al.*, 2005; Zhang *et al.*, 2006). The study of complexes containing substituted tetrazole derivatives is of interest to establish the ways in which tetrazoles bind to metal centers (Lin *et al.*, 2005). We report here the crystal structure of a copper complex, (I).



(I)

In the structure of (I) (Fig. 1), the bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987) . The

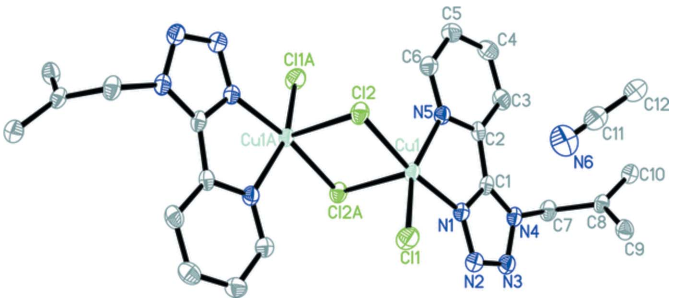


Figure 1
Part of the polymeric structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code: (A) $-x+1, -y+2, -z+1$]. H atoms have been omitted.

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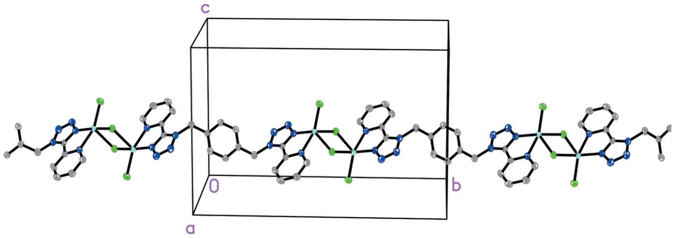

Figure 2
One-dimensional chain stucture of (I), viewed along the *a* axis. H atoms have been omitted.

Cu^{II} center is five-coordinated (Table 1) by two N atoms from the *L* ligand (where *L* is bis{[2-pyridyl(1*H*-tetrazol-5-yl)]-1-ylmethyl}benzene) and three chloride ions (Table 1) to form a square-pyramidal geometry. In fact, the chloride ions have two different coordination modes; while one chloride ion is coordinated directly to one Cu^{II} center, the remaining ones bridge the two Cu^{II} centers, separated by a relatively short distance of 3.412 (2) Å. The Cu^{II} centers are interconnected by *L* ligands and chloride ions to form a one-dimensional chain.

Experimental

A mixture of acetonitrile and chloroform (1:1, 10 ml) was carefully layered over a chloroform solution (3 ml) of *L* (0.05 mmol). A solution of $CuCl_2$ (0.1 mmol) in acetonitrile (3 ml) was then layered on top. Green block crystals, suitable for X-ray analysis, were collected after several weeks (yield 30%).

Crystal data

$[Cu_2Cl_4(C_{20}H_{16}N_{10})]\cdot C_2H_3N$
$M_r = 373.72$
Monoclinic, $P2_1/n$
$a = 7.7541$ (16) Å
$b = 17.086$ (3) Å
$c = 11.383$ (2) Å
$\beta = 98.72$ (3)°
$V = 1490.6$ (5) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 1.82$ mm^{-1}
$T = 294$ (2) K
0.20 × 0.18 × 0.16 mm

Data collection

Rigaku R-AXIS RAPID-S diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.698$, $T_{max} = 0.744$
8990 measured reflections
2625 independent reflections
2196 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.081$
$S = 1.06$
2625 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.995 (2)	Cu1—Cl2	2.2576 (9)
Cu1—N5	2.090 (2)	Cu1—Cl2^{i}	2.6955 (10)
Cu1—Cl1	2.2385 (10)		
N1—Cu1—N5	78.40 (9)	N1—Cu1—Cl2^{i}	89.48 (7)
N1—Cu1—Cl1	92.94 (7)	N5—Cu1—Cl2^{i}	91.56 (6)
N5—Cu1—Cl1	159.97 (7)	Cl1—Cu1—Cl2^{i}	106.53 (4)
N1—Cu1—Cl2	171.46 (7)	Cl2—Cu1—Cl2^{i}	93.40 (3)
N5—Cu1—Cl2	93.48 (7)	Cu1—Cl2—Cu1^{i}	86.60 (3)
Cl1—Cu1—Cl2	93.94 (3)		

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

H atoms were positioned geometrically with C—H = 0.93, 0.97 and 0.96 Å, for aromatic, methylene and methyl H atoms, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C)$, where $x = 1.5$ for methyl H and $x = 1.2$ for all other H atoms.

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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