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Poly[dipyridinecopper(II)-μ-cyano-copper(II)-tri-μ-cyano]

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.006 Å
R factor = 0.030
wR factor = 0.077
Data-to-parameter ratio = 14.4

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

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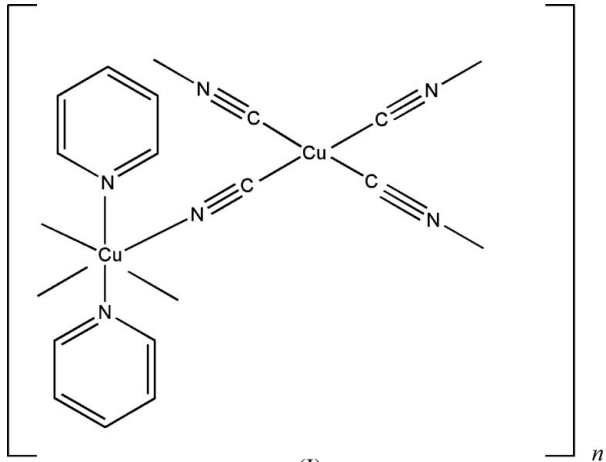
The crystal structure of the title compound, $[Cu(C_5H_5N)_2\{Cu(CN)_4\}]_n$, comprises $[Cu(py)_2]^{2+}$ (py is pyridine) and $[Cu(CN)_4]^{2-}$ subunits which are connected through bridging cyano groups to form a three-dimensional network, with Cu atoms located on sites of symmetry 2/m and 222 for the cation and anion, respectively.

Comment

The magnetic properties of low-dimensional solids are presently the subject of intense study. Tetracyanonickelates(II) are suitable model compounds for magnetic studies at low temperatures because the tetracyanonickelate anion may bridge paramagnetic ions partially coordinated with amine ligands and thus form molecular, one-, two- and three-dimensional structures. In contrast, the use of tetracyanocuprate(II) as a bridging unit in a multidimensional structure has rarely been reported. We have designed and synthesized a novel coordination polymer, poly[μ-cyano-tetracyanodipyridinedicopper(II)], $[Cu(py)_2\{Cu(CN)_4\}]_n$ (py is pyridine), (I), the structure of which is reported here.



(I)

Part of the title complex is shown in Fig. 1 and some features of the molecular geometry are listed in Table 1. The complex consists of a neutral three-dimensional network with stoichiometry $Cu(py)_2Cu(CN)_4$. The structure contains two types of copper(II) coordination environments. Atom Cu1 in the $[Cu(CN)_4]^{2-}$ unit lies on a position of crystallographic symmetry 222 and is in a slightly distorted tetrahedral coordination geometry. The briging cyano groups are all related by symmetry, with N≡C—Cu and C≡N—Cu angles of 174.6 (3) and 168.8 (3)°, respectively. Atom Cu2 of the $\{Cu(py)_2\}^{2+}$ unit, lying on a position of symmetry 2/m, is in a slightly distorted

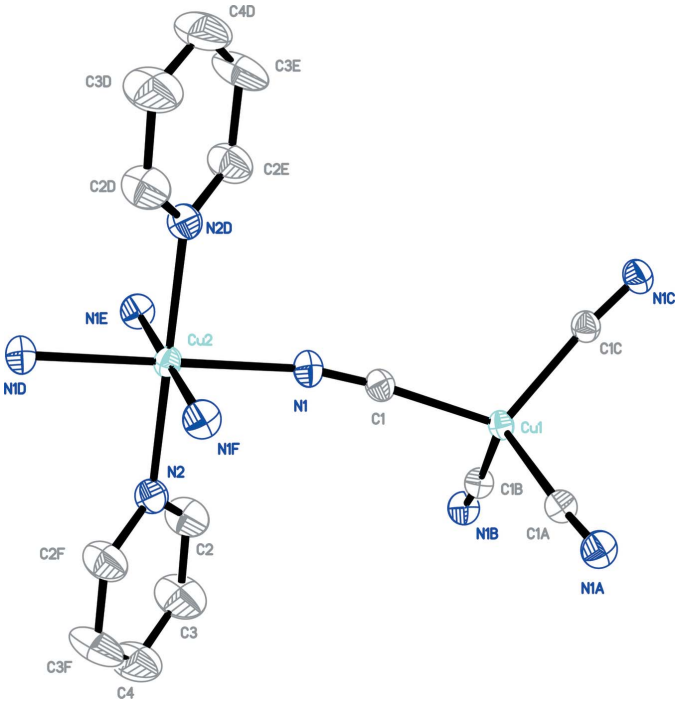


Figure 1
A view of part of the title compound. H atoms have been omitted for clarity. Ellipsoids are drawn at the 30% probability level. [Symmetry codes: (A) $-x+2, -y+1, z$; (B) $-x+2, y, -z+\frac{1}{2}$; (C) $x, -y+1, -z+\frac{1}{2}$; (D) $-x+\frac{5}{2}, -y+\frac{1}{2}, -z+1$; (E) $-x+\frac{5}{2}, -y+\frac{1}{2}, z$; (F) $x, y, -z+1$.]

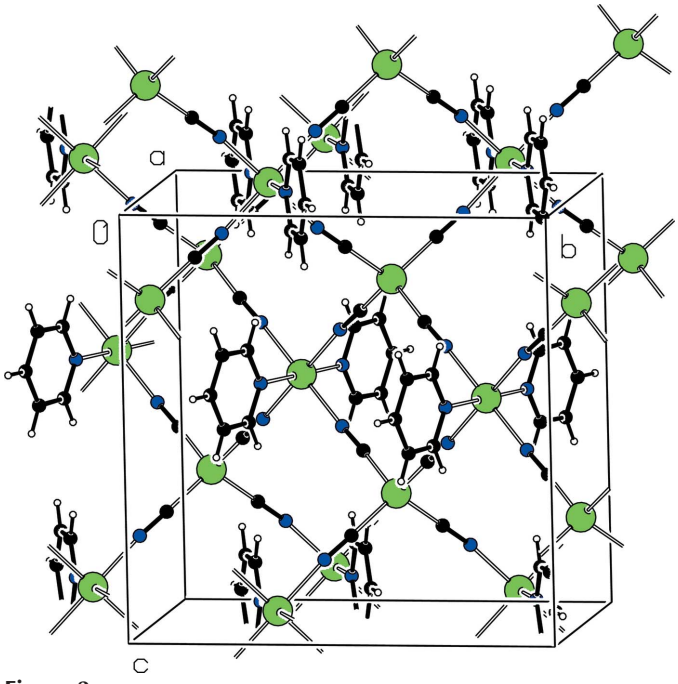


Figure 2
View of the three-dimensional structure of the title compound. Colour codes: green Cu, blue N and black C.

octahedral coordination environment. Four N atoms of the C≡N ligand lie in the equatorial plane [Cu—N = 2.144 (3) Å] and two N atoms of the pyridine ligands are in axial positions [Cu—N = 2.139 (4) Å]. An extended three-dimensional structure is formed through the cyano groups acting as bridging groups. The distance between Cu1 and Cu2 is 5.259 (4) Å. In the related cyano-bridged complex $[Cu_2(medpt)_2Ni(CN)_4(ClO_4)_2]\cdot 2.5H_2O$ [medpt = bis(3-aminopropyl)methylamine], $[Ni(CN)_4]^{2-}$ subunits coordinate through all four cyano ligands to form a criss-crossed one-dimensional chain of connected square–pyramidal Cu^{II} cations (Maji *et al.*, 2001). In the title complex, the tetrahedral $[Cu(CN)_4]^{2-}$ unit contributes to the formation of this three-dimensional network structure (Fig. 2).

Experimental

All chemicals were of reagent grade, commercially available from the Beijing Chemical Reagents Company of China, and were used without further purification. A pyridine–methanol (5 ml, 5:95 (*v*/*v*) solution of $CuCl_2\cdot 2H_2O$ (0.0511 g, 0.3 mmol) was prepared. This solution was added to a methanol solution (5 ml) of KCN (0.0384 g, 0.59 mmol). The resulting solution was stirred for 24 h, filtered and the filtrate allowed to stand at room temperature. Yellow crystals of the title compound appeared after two weeks of slow evaporation of the solution.

Crystal data

$[Cu_2(CN)_4(C_5H_5N)_2]$
$M_r = 389.36$
Orthorhombic, *Cccm*
$a = 9.231$ (3) Å
$b = 13.375$ (4) Å
$c = 13.354$ (4) Å
$V = 1648.8$ (9) Å^3
$Z = 4$
$D_x = 1.569$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4561 reflections
$\theta = 2.7$–$26.7°$
$\mu = 2.58$ mm^{-1}
$T = 273$ (2) K
Block, yellow
0.40 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
$T_{min} = 0.404$, $T_{max} = 0.595$
3933 measured reflections
806 independent reflections
726 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 25.5°$
$h = -11 \rightarrow 10$
$k = -9 \rightarrow 16$
$l = -13 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.077$
$S = 1.00$
806 reflections
56 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0459P)^2 + 1.7229P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—C1	2.011 (3)	Cu2—N1	2.144 (3)
Cu2—N2	2.139 (4)	N1—C1	1.144 (4)
$C1^{i}$—Cu1—C1	105.29 (17)	N1—Cu2—N1	89.23 (14)
$C1^{ii}$—Cu1—C1	113.68 (17)	$N1^{v}$—Cu2—N1	90.77 (14)
$C1^{iii}$—Cu1—C1	109.55 (17)	N1—Cu2—$N1^{iv}$	180
$N2^{iv}$—Cu2—N2	180	C1—N1—Cu2	168.8 (3)
N2—Cu2—$N1^{v}$	90.67 (10)	N1—C1—Cu1	174.6 (3)
N2—Cu2—N1	89.33 (10)		

Symmetry codes: (i) $-x+2, y, -z+\frac{1}{2}$; (ii) $x, -y+1, -z+\frac{1}{2}$; (iii) $-x+2, -y+1, z$; (iv) $-x+\frac{5}{2}, -y+\frac{1}{2}, -z+1$; (v) $-x+\frac{5}{2}, -y+\frac{1}{2}, z$.

H atoms were placed in geometrically idealized positions, with Csp^2 = 0.93 Å, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2000); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2000); molecular graphics: *SHELXTL* (Sheldrick, 1999) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

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