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Poly[[*trans*-dibromocopper(II)]-di-μ-3-pyridinecarbonitrile-κ^4N^1:N^3]

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In the title centrosymmetric compound, $[CuBr_2(C_6H_4N_2)_2]$, each Cu^{II} atom is 4 + 2-coordinated by two pyridine N atoms from two 3-pyridinecarbonitrile ligands, two Br^- anions and two semicoordinated cyano N atoms from two symmetry-related 3-pyridinecarbonitrile ligands. The 3-pyridinecarbonitrile ligands link molecules into chains running parallel to the *c* axis.

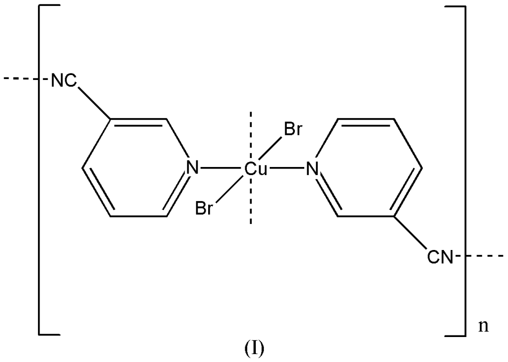
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.027
wR factor = 0.079
Data-to-parameter ratio = 13.2

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

Comment

In recent years, interest has been shown in the preparation and properties of molecular-based magnets (Galteschi *et al.*, 1991; Kahn, 1993; Miller & Epstein, 1994). A major subfield within molecular magnetism has been the construction of molecular ferrimagnets, and some excellent work has been performed in this area (Pei *et al.*, 1986). It was found that the cyanide anion can be used to construct specific dimensional crystal lattices with high magnetic ordering (Mallah *et al.*, 1993; Entley & Girolami, 1995). 4-Pyridinecarbonitrile, as a bridging ligand, has been investigated and the synthesis, crystal structures and magnetic properties of linear-chain 4-pyridinecarbonitrile compounds have already been reported (Vasilevesky *et al.*, 1991; Zhang *et al.*, 1993, 1997), but the 3-pyridinecarbonitrile compounds have rarely been considered. We report here the preparation and crystal structure of a complex of copper(II) bridged by 3-pyridinecarbonitrile, namely poly[[*trans*-dibromocopper(II)]-di-μ-3-pyridinecarbonitrile-κ^2N^1:N^3], (I).



(I)

The structural unit of the title compound, (I), consists of a Cu^{II} center, two Br^- anions and two 3-pyridinecarbonitrile molecules. The Cu^{II} atom lies on an inversion center. The geometry around the Cu^{II} atom is distorted octahedral, with bonds to two pyridine N atoms from two 3-pyridinecarbonitriles [Cu—N = 2.011 (3) Å] and two Br^- anions [Cu—Br = 2.4185 (4) Å] occupying the equatorial plane. The pyridine rings are tilted out of the equatorial plane by 58.6 (3)° (Table 1

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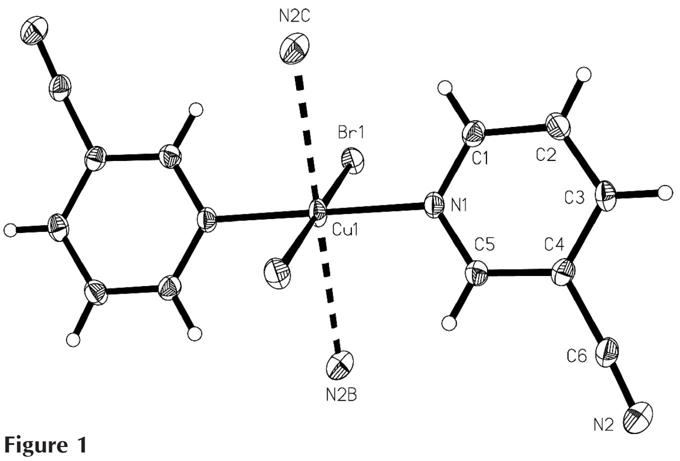

Figure 1
View of the structure of (I), with atom numbering (50% probability displacement ellipsoids). The two long bonds from the copper to the semicoordinated nitrile N atom are shown as dashed lines and the suffixes B and C refer to the symmetry codes ($x, y, z - 1$) and ($-x, -y, 1 - z$), respectively.

and Fig. 1). The axial sites are occupied by two semicoordinated cyano N atoms [Cu—N = 2.854 (4) Å] from the cyano N atoms of two symmetry-related 3-pyridinecarbonitrile ligands. This gives the copper ion a 4 + 2-coordination geometry and links the units into chains running parallel to the *c* axis (Fig. 2), with an intrachain Cu···Cu separation of 8.067 (4) Å. Deviations from ideal D_{2h} symmetry around the copper site are very small. The N—Cu—Br and N—Cu—N angles are within experimental uncertainty of being exactly 90° (see Table 1).

Experimental

Copper(I) bromide (0.45 g, 2 mmol) was dissolved in water (10 ml) and the solution was mixed with a dimethylformamide solution (10 ml) of 3-pyridinecarbonitrile (0.42 g, 4 mmol) and 1,2,4-benzenetricarboxylic acid (0.42 g, 2 mmol). The reaction mixture was filtered; green block-shaped crystals were separated from the filtrate after about a month. As shown by the crystal structure analysis, the 1,2,4-benzenetricarboxylic acid was not incorporated into the product.

Crystal data

$[CuBr_2(C_6H_4N_2)_2]$
M_r = 431.58
Triclinic, $P\overline{1}$
a = 7.0410 (10) Å
b = 7.2791 (10) Å
c = 8.0673 (11) Å
α = 116.563 (2)°
β = 107.909 (2)°
γ = 98.437 (3)°
V = 331.70 (8) Å^3
Z = 1
D_x = 2.161 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1171 reflections
θ = 3.1–25.1°
μ = 7.66 mm^{-1}
T = 298 (2) K
Block, green
0.24 × 0.17 × 0.13 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{\min}$ = 0.23, $T_{\max}$ = 0.37
1758 measured reflections
1171 independent reflections
1098 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.016
$\theta_{\max}$ = 25.1°
$h = -8 \rightarrow 8$
$k = -5 \rightarrow 8$
$l = -9 \rightarrow 9$

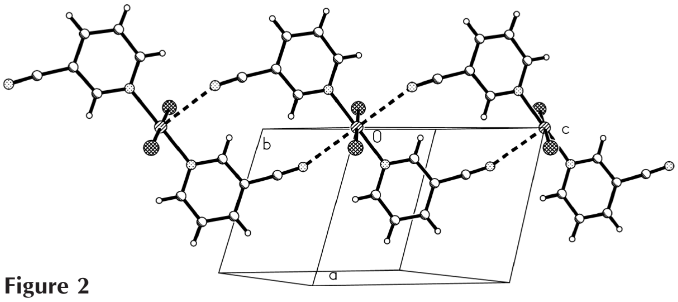

Figure 2
The linear structure of (I), bridged by 3-pyridinecarbonitrile. Dashed lines indicate the semicoordination of Cu by N atoms.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.080
S = 1.10
1171 reflections
89 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.043P)^2 + 0.2371P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max}$ = 0.65 e Å^{-3}
$\Delta\rho_{\min}$ = −0.53 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.022 (4)

Table 1
Selected geometric parameters (Å, °).

N1—Cu1	2.011 (3)	Cu1—Br1	2.4185 (4)
C5—N1—Cu1	120.1 (2)	N1—Cu1—Br1^{i}	90.10 (9)
C1—N1—Cu1	121.4 (2)	N1—Cu1—Br1	89.90 (9)
N1—Cu1—N1^{i}	180	Br1^{i}—Cu1—Br1	180
C2—C1—N1—Cu1	−178.7 (3)	C5—N1—Cu1—Br1	−118.7 (3)
C5—N1—Cu1—Br1^{i}	61.3 (3)	C1—N1—Cu1—Br1	58.6 (3)
C1—N1—Cu1—Br1^{i}	−121.4 (3)		

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

The H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of 0.93 Å (C—H), with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(parent atom).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXL*97.

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