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Poly[μ-4,4′-bipyridine-di-μ-isothiocyanato-copper(II)]

Wang-Xi Luo, Ming-Ming Yu, Lei Zheng, Ai-Li Cui* and Hui-Zhong Kou

Department of Chemistry, Tsinghua University, Beijing 100084, People's Republic of China

Correspondence e-mail: cuial@mail.tsinghua.edu.cn

In the title compound, $[Cu(NCS)_2(C_{10}H_8N_2)]_n$, the Cu^{II} ion (site symmetry 2) has an elongated octahedral coordination. Four N atoms of two thiocyanate anions and two 4,4′-bipyridine (4,4′-bipy) ligands are sited at the equatorial positions, while two S atoms of two coordinating thiocyanate anions occupy the axial positions. The complete 4,4′-bipy molecule is generated by the twofold axis and one of its pyridine rings is disordered over two sets of positions. The copper ions are bridged by the 4,4′-bipy ligands, giving rise to a one-dimensional chain. The chains are further linked by the NCS⁻ anions, through the long axial Cu—S contacts, yielding a two-dimensional network.

Comment

Within the context of crystal engineering (Batten & Robson, 1998), 4,4′-bipyridine (4,4′-bipy) is an excellent bridging ligand, which can link two metal atoms *via* the N atoms of its two pyridine rings, and a variety of networks have been reported (Blake *et al.*, 1998; Carlucci *et al.*, 1999; Dong *et al.*, 2005; Maji *et al.*, 2004; Xu *et al.*, 2006). The thiocyanate anion (NCS⁻) can serve as a terminal ligand or a bridging ligand since both the N atom and the S atom can coordinate with metal centers (Bose *et al.*, 2006; Jiang *et al.*, 2004; Zhang *et al.*, 2005). As part of our ongoing investigations of networks containing the NCS⁻ anion, we report here the crystal structure of the title compound, (I) (Fig. 1).

(I)
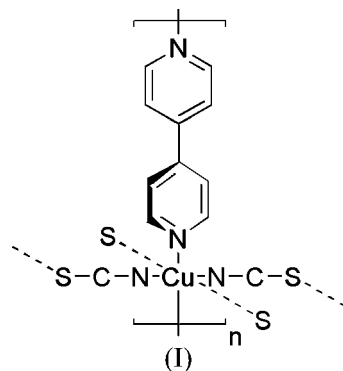
The coordination geometry of the copper(II) ion (site symmetry 2) is distorted octahedral. Two N-bonded NCS⁻ anions and two 4,4′-bipy ligands establish the equatorial plane with normal Cu—N distances (Table 1). The elongated octahedral geometry is completed by two S atoms in the axial positions with a Cu—S bond distance of 3.047 (3) Å. One pyridine ring of the 4,4′-bipyridine unit is disordered over two sets of positions. The 4,4′-bipy ligands bridge Cu^{II} ions,
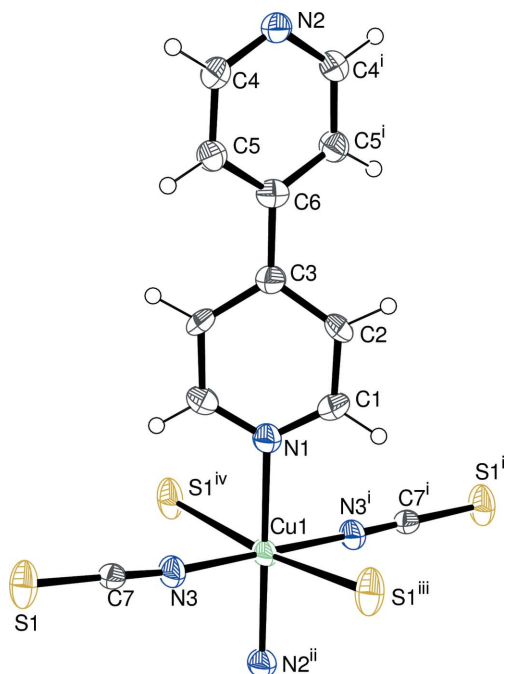
Figure 1
A segment of the polymeric structure of (I), showing 50% probability displacement ellipsoids and arbitrary spheres for the H atoms. Only one orientation of the disordered C1-pyridine ring is shown. [Symmetry codes: (i) $\frac{1}{2} - x, 1 - y, z$ (also for unlabelled atoms), (ii) $x, 1 - y, \frac{1}{2} + z$; (iii) $x, 1 + y, z$; (iv) $\frac{1}{2} - x, -y, z$.]
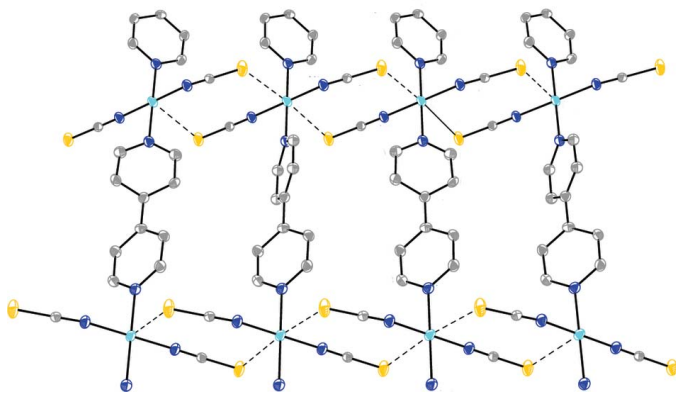
Figure 2
The two-dimensional network of (I) formed by the Cu···S contacts. Only one disorder component of each 4,4′-bipy ligand is shown. H atoms have been omitted.

forming polymeric chains along the c axis. Adjacent chains are connected by the axial Cu—S contacts, forming a two-dimensional network extending parallel to (100) (Fig. 2).

Experimental

$Cu(CH_3COO)_2 \cdot 2H_2O$ (0.1 mmol) and 4,4′-bipyridine (0.1 mmol) were dissolved in 15 ml of water and ethanol (2:1 v/v), resulting in a blue solution which was transfered to the left-hand side of an H-tube. An aqueous solution (15 ml) of KSCN (0.2 mmol) was placed in the right-hand side of the H-tube and ethanol served as the diffusion solvent. The reaction container was kept at room temperature and

three months later green needles of (I) suitable for X-ray diffraction analysis were obtained (yield 50%, based on Cu).

Table 1
Selected geometric parameters (Å, °).

Cu1—N3	1.937 (3)	Cu1—N1	2.071 (5)
Cu1—N2^i	2.040 (4)	Cu1—S1^{ii}	3.0471 (12)
C7—N3—Cu1	172.4 (3)	N3—C7—S1	179.2 (3)
C7—S1—Cu1^{iii}	94.8 (2)		

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

Atoms C1 and C2 and their attached H atoms are disordered over two positions with equal site occupancies. The H atoms were placed in calculated positions and treated using a riding-model approximation [C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$].

Data collection: $SMART$ (Bruker, 2000); cell refinement: $SAINT$ (Bruker, 2000); data reduction: $SAINT$; program(s) used to solve structure: $SHELXS97$ (Sheldrick, 1997); program(s) used to refine structure: $SHELXL97$ (Sheldrick, 1997); molecular graphics: XP in $SHELXTL$ (Sheldrick, 1998); software used to prepare material for publication: $SHELXTL$.

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