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catena-Poly[[(thiocyanato-κN)copper(II)]-μ_3-[2-(2-pyridylmethylamino)ethanesulfonato-$\kappa^5 N,N',O:O':O''$]]

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The title polymer, $[\mathrm{Cu(C_8H_{11}N_2O_3S)(SCN)}]_n$ or $[\mathrm{Cu(PMT)(SCN)}]_n$, contains six-coordinate Cu$^{\mathrm{II}}$ units. The Cu$^{\mathrm{II}}$ ion is coordinated by one thiocyanate N atom, an *N*,*N*′,*O*-tridentate 2-(2-pyridylmethylamino)ethanesulfonate (PMT) anion and two axial bridging sulfonate O atoms from two adjacent PMT ligands in a distorted octahedron. The deprotonated PMT ligand acts as a μ_3-bridging ligand and forms an eight-membered $(\text{–Cu—O—S—O–})_2$ ring between two neighbouring Cu$^{\mathrm{II}}$ atoms. These rings are interconnected, generating a one-dimensional linear chain structure. These polymetric chains are connected into a three-dimensional network *via* interchain π–π stacking of the pyridine rings and intermolecular hydrogen bonds.

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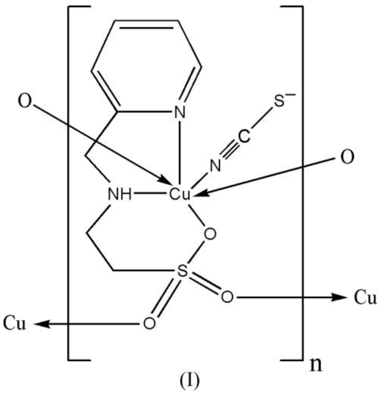
Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.004 Å
R factor = 0.030
wR factor = 0.077
Data-to-parameter ratio = 17.5

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

Comment

The investigation of Schiff base complexes containing both sulfur and amino acid functional groups (Casella & Gullotti, 1981, 1986*a*,*b*; Wang *et al.*, 1994) has received much attention because of their applications in life sciences (Casella & Gullotti, 1986*a*,*b*; Li & Li, 1993; Jiang *et al.*, 2003; Zhang *et al.*, 2003). Taurine, an amino acid containing sulfur, is indispensable to humans and plays an important role in physiological functions. Recently, we have found that Schiff bases derived from taurine have various coordination modes, as reported by Zeng *et al.* (2003) and Jiang *et al.* (2003, 2004). π–π Stacking interactions have been a topic of much interest since the 1980s (Tsuzuki *et al.*, 2002). They are one of the significant characteristics of ternary complexes and they also participate in stabilizing the DNA double helix structure (Frieden, 1975) and its complexes with anticancer drugs (Hollis *et al.*, 1989). Here, we report the synthesis and crystal structure of the title copper(II) polymer, (I) (Fig. 1).



(I)

Complex (I) is composed of $[\mathrm{Cu(C_8H_{11}N_2O_3S)(SCN)}]$ units, in which the Cu$^{\mathrm{II}}$ ion is six-coordinated in a distorted octa-

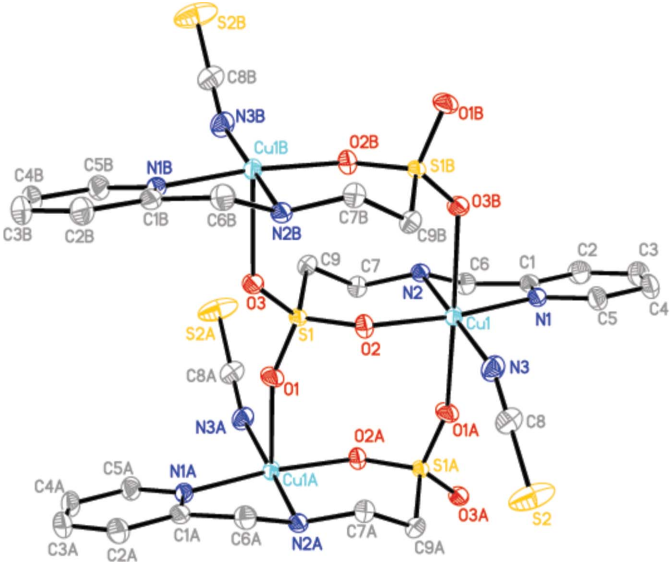


Figure 1
The structure of the building unit of the one-dimensional infinite chain of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted. [Symmetry codes: (A) $-x$, $-y + 1$, $-z + 2$; (B) $-x + 1$, $-y + 1$, $-z + 2$.]

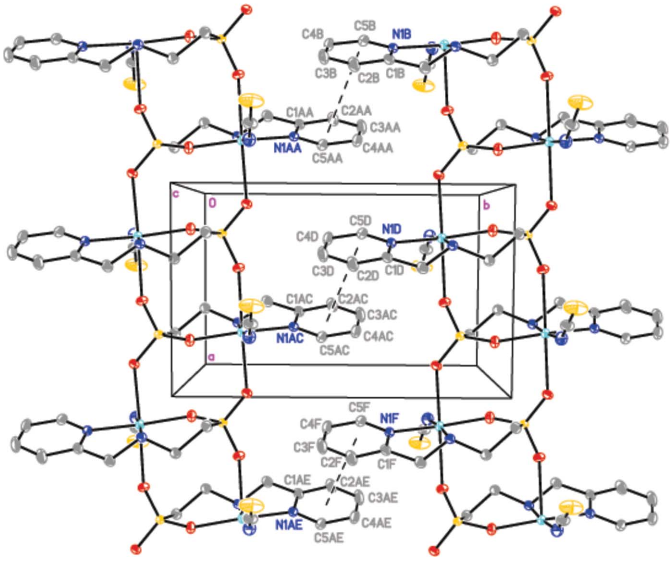


Figure 2
Packing diagram, projected on the *ab* plane, showing the π–π stacking between pyridine rings of adjacent chains of (I). All H atoms have been omitted for clarity. [Symmetry codes: (B) $-x - \frac{1}{2}$, $y + \frac{1}{2}$, $-z + \frac{3}{2}$; (D) $-x + \frac{1}{2}$,$y + 1/2$, $-z + \frac{3}{2}$; (F) $-x + \frac{3}{2}$,$y + 1/2$, $-z + \frac{3}{2}$; (AA) $x - \frac{1}{2}$, $-y + \frac{1}{2}$, $z - \frac{1}{2}$; (AC) $x + \frac{1}{2}$,$-y + \frac{1}{2}$, $z - \frac{1}{2}$; (AE) $x + \frac{3}{2}$,$-y + \frac{1}{2}$, $z - \frac{1}{2}$.]

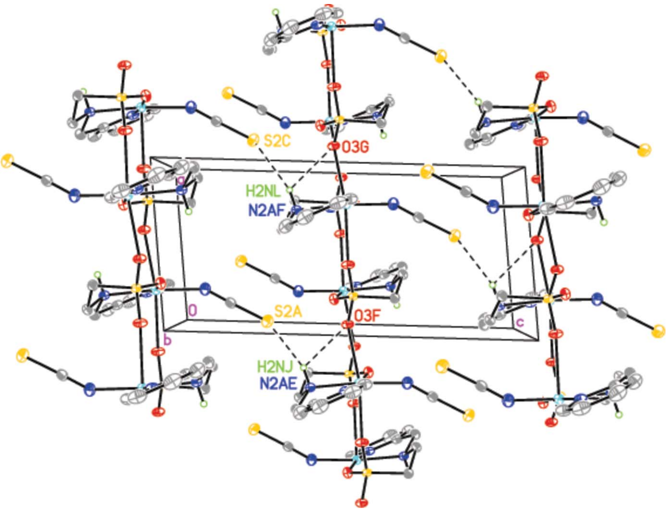


Figure 3
The hydrogen bonds in the crystal packing of (I), shown as dashed lines. H atoms bound to C atoms have been omitted.

hedral geometry (Table 1) by one N atom from thiocyanate, two N and one O atoms from the tridentate chelating PMT anion, and two different sulfonate O atoms from two adjacent ligands. The deprotonated PMT ligand acts as a μ_3-bridging ligand, linking three neighbouring Cu^{II} ions, and it forms an eight-membered (–Cu—O—S—O–)$_2$ ring. These interconnected rings create a one-dimensional linear chain propagating along the *a* axis in the monoclinic unit cell, with Cu1$\cdots$Cu1($-x$, $1 - y$, $2 - z$) and Cu1$\cdots$Cu1($1 - x$, $1 - y$, $2 - z$) distances of 5.310 (2) and 5.389 (6) Å, respectively.

In the crystal structure of (I), there is a strong π–π stacking interaction between the parallel pyridine rings of neighbouring chains along the *a* axis (Fig. 2). The interplanar average distance and ring-centroid separation distance are 3.411 (2) Å and 3.661 (4) Å, respectively. The chain structure is expanded into two-dimensional layers in the *ab* plane by π–π stacking. A pair of weak intermolecular N—H$\cdots$O and N—H$\cdots$S hydrogen bonds (Table 2 and Fig. 3) are observed and they join the layers into a three-dimensional network.

Experimental

The ligand 2-(2-pyridylmethylamino)ethanesulfonic acid (HPMT) was prepared according to the method of Li *et al.* (2006). A solution of $CuCl_2 \cdot 2H_2O$ (0.171 g, 1.0 mmol) in methanol (7 ml) was added dropwise to a solution (8 ml) of the HPMT ligand (1.0 mmol, 0.216 g) in water with stirring and refluxing at 373 K for 2 h. Potassium thiocyanate (1.0 mmol, 0.097 g) in water (10 ml) was then gradually added to the above solution. The resulting mixture was stirred for another 4 h, filtered and kept at room temperature to yield green block-shaped crystals of (I) after several days. Analysis, found: C 32.02, H 3.22, N 12.51, S, 9.53%; calculated for $C_9H_{11}CuN_3O_3S_2$: C 32.06, H 3.26, N 12.47, S 9.50%. IR (KBr,ν, cm^{-1}): 771.5 [γ (C═C—H)], 756.1(γ CH$_2$), 1230.8, 1175.3, 1049.0 (ν SO$_3^-$), 1610.5, 1574.6 (ν C═C + C═N), 2084.8 (ν NCS$^-$), 3224.9 (ν N—H).

Crystal data

$[Cu(C_8H_{11}N_2O_3S)(NCS)]$
$M_r = 336.87$
Monoclinic, $P2_1/n$
$a = 7.2245$ (9) Å
$b = 11.4470$ (14) Å
$c = 15.5537$ (19) Å
$\beta = 95.970$ (1)°
$V = 1279.3$ (3) Å^3

$Z = 4$
$D_x = 1.749$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 2.04$ mm^{-1}
$T = 291$ (2) K
Block, green
0.25 × 0.20 × 0.17 mm

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Data collection

Bruker APEXII CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\rm min} = 0.631$, $T_{\rm max} = 0.720$
10694 measured reflections
2923 independent reflections
2541 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.023$
$\theta_{\rm max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.077$
$S = 1.04$
2923 reflections
167 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0345P)^2 + 1.2013P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.002$
$\Delta\rho_{\rm max} = 1.01$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.77$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N3	1.958 (2)	Cu1—N2	2.024 (2)
Cu1—O2	2.0032 (16)	Cu1—O3$^{\rm i}$	2.4260 (16)
Cu1—N1	2.011 (2)	Cu1—O1$^{\rm ii}$	2.4306 (17)
N3—Cu1—O2	89.43 (8)	N3—Cu1—O3$^{\rm i}$	99.57 (8)
N3—Cu1—N1	95.39 (9)	N2—Cu1—O3$^{\rm i}$	85.10 (7)
O2—Cu1—N1	173.79 (7)	N3—Cu1—O1$^{\rm ii}$	89.01 (8)
N3—Cu1—N2	174.33 (9)	N2—Cu1—O1$^{\rm ii}$	86.19 (7)
O2—Cu1—N2	93.98 (7)	O3$^{\rm i}$—Cu1—O1$^{\rm ii}$	171.06 (6)
N1—Cu1—N2	81.52 (8)		

Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $-x, -y+1, -z+2$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2N···O3$^{\rm i}$	0.86 (3)	2.54 (3)	3.024 (3)	116 (2)
N2—H2N···S2$^{\rm iii}$	0.86 (3)	2.79 (3)	3.560 (2)	150 (2)

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

H atoms bonded to C were positioned geometrically, with C—H distances in the range 0.93–0.97 Å, and treated as riding atoms, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. The N-bound H atom was located in a difference Fourier map and refined isotropically. The highest residual electron density peak is located 1.01 Å from atom S2.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); software used to prepare material for publication: *SHELXTL*.

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