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Poly[μ-azido-κ^2N^1:N^3-μ-2-(2-pyridylmethylamino)ethanesulfonato-κ^4N,N',O:O'-copper(II)]

Jun-Xia Li,[a] Yi-Min Jiang[a]* and Jian-Ge Wang[b]

[a]College of Chemistry and Chemical Engineering, Guangxi Normal University, Guilin, Guangxi 541004, People's Republic of China, and [b]Department of Chemistry, Luoyang Normal University, Luoyang, Henan 471022, People's Republic of China

Correspondence e-mail: ljx6281@126.com

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Key indicators

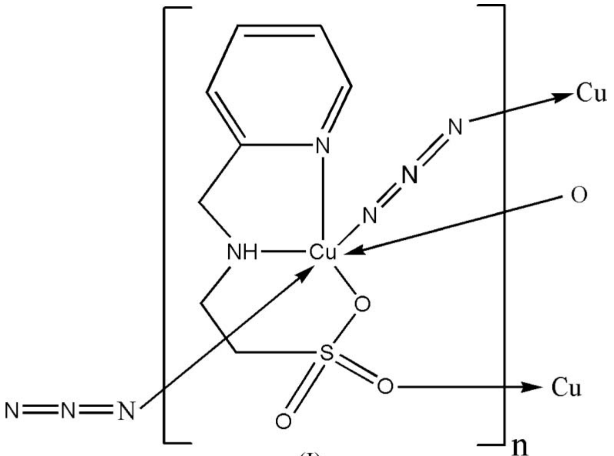
Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.005 Å
R factor = 0.030
wR factor = 0.080
Data-to-parameter ratio = 16.5

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

In the title compound, $[Cu(C_8H_{11}N_2O_3S)(N_3)]_n$, the Cu^{II} center is six-coordinated by two N and two sulfonate O atoms from two different 2-(2-pyridylmethylamino)ethanesulfonate ligands together with two N atoms from two different azide anions in a distorted octahedral geometry. The azide anions act as μ-(1,3) bridges, giving rise to a two-dimensional coordination polymer parallel to the *bc* plane of the monoclinic unit cell.

Comment

The investigation of coordination complexes has been expanded rapidly in recent decades (Subramanian & Zaworotko, 1995) in view of their applications (Zhao *et al.*, 2001). Taurine, a β-amino acid containing sulfur, plays a significant part in human life and has important physiological functions. Recently, we have observed that the sulfonate group in both taurine and its Schiff bases have diverse coordination modes, such as non-coordinate (Jiang *et al.*, 2004; Zhang *et al.*, 2004), monodentate (Cai, Jiang & Ng, 2006; Cai, Jiang, Yin *et al.*, 2006; Jiang *et al.*, 2006; Li *et al.*, 2005, 2006; Zeng *et al.*, 2003; Zhang, Jiang & Yu, 2005; Zhang, Jiang, Liu & Yu, 2005), μ_2-bridging (Cai *et al.*, 2004) and μ_3-bridging (Jiang *et al.*, 2005). Another new complex in which the sulfonate group is μ_2-bridging, (I), is described here (Fig. 1).



(I)

The Cu^{II} ion is six-coordinate in a distorted octahedral configuration formed by the pyridyl N atom, amino N atom and sulfonate O atom of the tridentate chelating 2-(2-pyridylmethylamino)ethanesulfonate ligand, another sulfonate O atom from another ligand, and two N atoms from two different azide anions. The Cu^{II} atoms are bridged by two sulfonate O atoms, forming an eight-membered (—Cu—O—

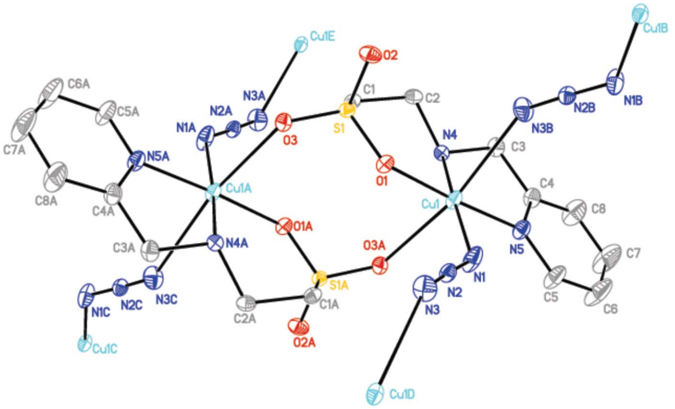


Figure 1
A segment of the polymeric structure of (I), showing the atom-numbering scheme. H atoms have been omitted for clarity. [Symmetry codes: (A) $1 - x, 1 - y, -z$; (B) $x, \frac{1}{2} - y, \frac{1}{2} + z$; (C) $1 - x, \frac{1}{2} + y, -\frac{1}{2} - z$; (D) $x, \frac{1}{2} - y, -\frac{1}{2} + z$; (E) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$.]

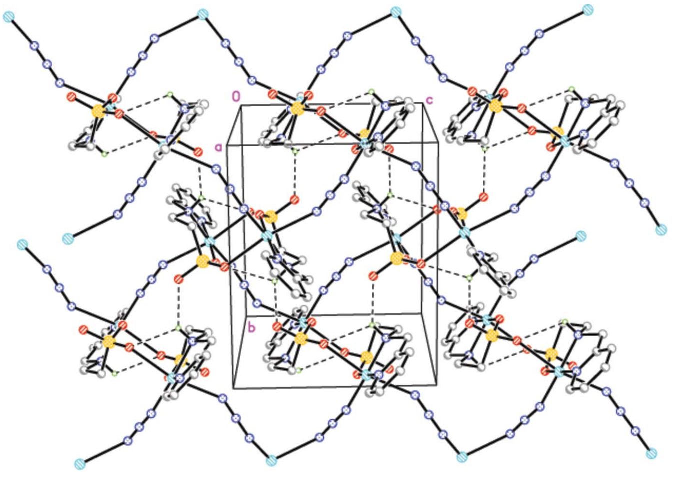


Figure 2
Hydrogen bonds in (I), shown as dashed lines. H atoms bound to C atoms have been omitted.

S—O—)$_2$ ring, with a Cu$\cdots$Cu distance of 5.453 (3) Å, that is similar to other eight-membered rings reported earlier for another copper complex (Cai *et al.*, 2004; Jiang & Zhang, 2003). Two azide anion function as a pair of μ-(1,3) bridging ligands and link the adjacent Cu^{II} atoms together, to form the title coordination polymer in the *bc* plane. The NH H atoms are involved in weak hydrogen bonding to the O atoms of S═O groups within this sheet structure (Fig. 2 and Table 2).

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 (8 ml) was added dropwise to a solution (7 ml) of ligand HPMT (1.0 mmol, 0.216 g) in water, with stirring and refluxing at 353 K for 4 h. After that, sodium azide (1.0 mmol, 0.065 g) in 10 ml of water was gradually added to the solution. The resulting mixture was stirred for another 6 h, filtered, and kept at room temperature to obtain dark-blue, block-shaped crystals several days later. Analysis found: C 29.96, H 3.39, N 21.85, S 9.92%; $C_8H_{11}CuN_5O_3S$ requires: C29.92, H 3.43, N 21.82, S 9.97%. IR (KBr, ν, cm^{-1}): 773.7 [γ(C═C—H)], 758.1 (γ CH$_2$); 1226.8, 1177.6, 1048.6 (ν SO3$^-$); 1610.7, 1573.4 (ν C═C + C═N); 2048.5 (νN$_3^-$); 3224.0 (v N—H).

Crystal data

$[Cu(C_8H_{11}N_2O_3S)(N_3)]$
$M_r = 320.81$
Monoclinic, $P2_1/c$
$a = 11.4260\ (13)$ Å
$b = 11.2920\ (13)$ Å
$c = 9.3237\ (10)$ Å
$\beta = 91.239\ (1)^\circ$
$V = 1202.7\ (2)$ Å^3
$Z = 4$
$D_x = 1.766$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 2.00$ mm^{-1}
$T = 291\ (2)$ K
Block, dark blue
0.33 × 0.17 × 0.11 mm

Data collection

Bruker APEX-II CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.560$, $T_{max} = 0.806$
10287 measured reflections
2748 independent reflections
2192 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 27.5^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.080$
$S = 1.03$
2748 reflections
167 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.04P)^2 + 0.3558P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.960 (2)	Cu1—N4	2.0160 (18)
Cu1—O1	1.9826 (15)	Cu1—O3^{i}	2.568 (2)
Cu1—N5	2.014 (2)	Cu1—N3^{ii}	2.610 (3)
N1—Cu1—O1	92.26 (8)	N1—Cu1—N4	170.89 (9)
N1—Cu1—N5	90.49 (9)	O1—Cu1—N4	95.77 (7)
O1—Cu1—N5	176.57 (7)	N5—Cu1—N4	81.65 (8)

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

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

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
N4—H1*N*$\cdots$O3^{i}	0.94 (3)	2.52 (2)	3.039 (3)	115.3 (18)
N4—H1*N*$\cdots$O2^{iii}	0.94 (3)	2.38 (2)	3.097 (3)	133.1 (19)

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

H atoms bonded to C were positioned geometrically with C—H = 0.93–0.97 Å, and treated as riding atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$. The NH H atom was located in a difference Fourier map and refined isotropically.

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

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structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); software used to prepare material for publication: *SHELXTL*.

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