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Key indicators

Single-crystal X-ray study
 T = 298 K
 Mean $\sigma(C-C)$ = 0.005 Å
 R factor = 0.039
 wR factor = 0.089
 Data-to-parameter ratio = 13.4

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

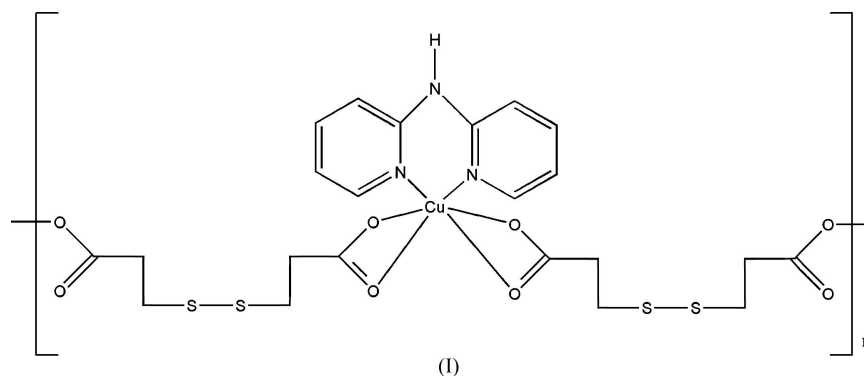
catena-Poly[[di-2-pyridylamine- $\kappa^2N^2,N^{2'}$]-copper(II)]- μ -3,3'-dithiodipropionato- $\kappa O,O':\kappa O''$]

In the title compound, $[Cu(C_6H_8O_4S_2)(C_{10}H_9N_3)]_n$, the 3,3'-dithiodipropionate anion, which acts as a bridge, is tetradentate to di-2-pyridylamine-coordinated copper(II) ions, forming a polymeric helical chain. The geometry of the copper(II) ion is that of a distorted octahedron. There are hydrogen bonds between two adjacent helical chains.

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Comment

Structural studies on compounds with disulfide bonds are helpful in understanding the mechanisms of how proteins fold (Ganesh *et al.*, 1990; Toby *et al.*, 1981). In this work, we report the structure of the title polymeric copper complex, (I).



In (I), each copper ion is coordinated by four O atoms from two carboxylate groups of two 3,3'-dithiodipropionate anions and two N atoms from di-2-pyridylamine (Fig. 1). O1 and O3 coordinate to copper atoms with typical Cu—O(carboxylate) bond lengths ranging from 1.953 (2) to 1.975 (2) Å (Yang & Li, 2005). O2 and O4 coordinate to the Cu atoms with significantly longer bond lengths of 2.777 (3) and 2.530 (2) Å, respectively, resulting in considerable distortion of the geometry of the copper(II) coordination sphere. Each 3,3'-dithiodipropionate anion bridges two copper ions, forming a polymeric helical chain structure (Fig. 2).

Experimental

A solution of $CuCl_2 \cdot 2H_2O$ (0.08 g, 0.5 mmol) in water (10 ml) was mixed with a dimethylformamide solution (10 ml) of di-2-pyridylamine (0.08, 0.5 mmol) and 3,3'-dithiodipropionic acid (0.10 g, 0.5 mmol). The reaction mixture was filtered, stirred for a few minutes, and then left to stand at room temperature for a month to afford blue prismatic crystals (m.p. 480–481 K). Analysis calculated for $C_{16}H_{17}CuN_3O_4S_2$: C 43.39, H 3.84, N 9.48%; found: C 43.35, H 3.88, N 9.51%. IR (KBr disk, cm^{-1}): 3421 (s), 2975 (m), 2359 (s), 1726 (s), 1655 (m), 1482 (s), 1381 (m), 1160 (m), 960 (m), 767 (s), 592 (m).

Crystal data

[Cu(C₆H₈O₄S₂)(C₁₀H₉N₃)]
M_r = 442.99
 Monoclinic, *C*2/*c*
a = 24.1289 (18) Å
b = 8.8057 (7) Å
c = 19.9518 (15) Å
 β = 123.509 (1)°
V = 3534.6 (5) Å³
Z = 8

D_x = 1.665 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 7574 reflections
 θ = 1.9–25.1°
 μ = 1.50 mm⁻¹
T = 298 (2) K
 Prism, blue
 0.27 × 0.25 × 0.22 mm

Data collection

Bruker APEX area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2002)
T_{min} = 0.671, *T_{max}* = 0.720
 9071 measured reflections

3152 independent reflections
 2880 reflections with *I* > 2σ(*I*)
R_{int} = 0.025
 θ_{\max} = 25.1°
h = −21 → 28
k = −10 → 9
l = −23 → 19

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.039
wR (*F*²) = 0.089
S = 1.08
 3152 reflections
 235 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0331P)^2 + 7.1784P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.39 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.22 \text{ e } \text{Å}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Cu1—O1	1.953 (2)	C15—S1	1.812 (3)
Cu1—N2	1.960 (2)	C16—S2	1.817 (3)
Cu1—O3	1.975 (2)	S1—S2	2.0320 (12)
Cu1—N1	1.996 (2)		
O1—Cu1—N2	158.50 (10)	O3—Cu1—N1	149.40 (10)
O1—Cu1—O3	89.83 (10)	C14—C15—S1	114.2 (2)
N2—Cu1—O3	95.37 (10)	C12 ⁱ —C16—S2	114.8 (2)
O1—Cu1—N1	92.96 (10)	C15—S1—S2	103.75 (13)
N2—Cu1—N1	93.08 (9)	C16—S2—S1	106.87 (12)
C15—S1—S2—C16	−91.11 (16)		

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

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N3—H3N...O4 ⁱⁱ	0.86	1.98	2.831 (3)	173

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

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with N—H = 0.86 Å, *Csp*²—H = 0.93 Å and *Csp*³—H = 0.97 Å, and with *U*_{iso}(H) = 1.2*U*_{eq}(parent atom).

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPII (Johnson, 1976); software used to prepare material for publication: SHELXL97.

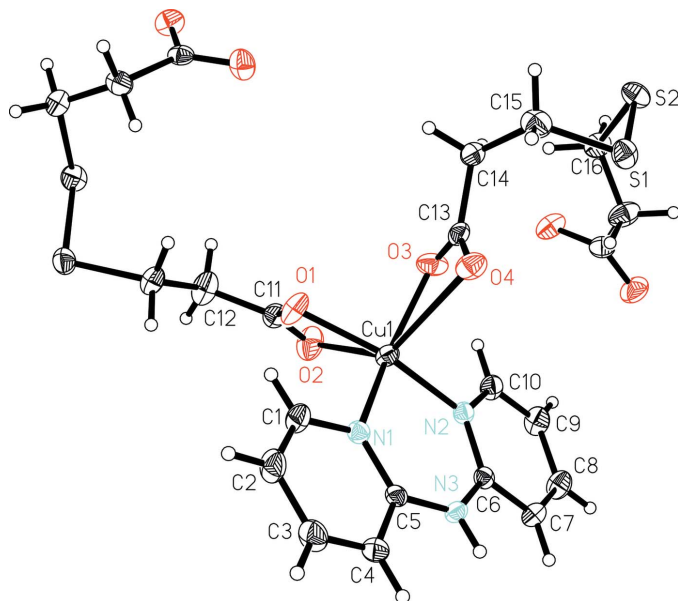


Figure 1

The coordination environment of Cu in (I), showing the atom numbering scheme and displacement ellipsoids drawn at the 50% probability level.

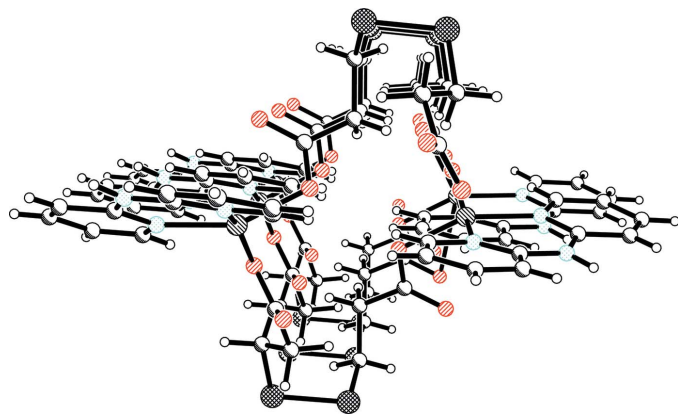


Figure 2

The one-dimensional helical chain of (I).

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