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Crystal structure of *catena*-poly[(μ_2 -3,3'-thiodipropionato- $\kappa^2 O:O'$)-(bipyridine- $\kappa^2 N,N'$)copper(II)] $C_{16}H_{16}CuN_2O_4S$

Table 1: Data collection and handling.

Crystal:	Block, blue
Size:	2.9 × 2.6 × 2.2 mm
Wavelength:	Mo K α radiation ($\lambda = 0.71073$ Å)
μ :	1.479 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX II, Φ and ω -scans
$2\theta_{\max}$, completeness:	27.5°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	10083, 3738, 0.0429
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2\sigma(I_{\text{obs}})$, 2609
$N(\text{param})_{\text{refined}}$:	217
Programs:	Bruker programs [1], SHELX [2]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.35467(3)	0.07738(2)	0.27169(3)	0.03618(10)
N1	0.45341(18)	-0.02601(11)	0.23193(17)	0.0353(5)
N2	0.25102(18)	0.04832(11)	0.10036(18)	0.0343(5)
O1	0.22703(16)	0.16156(10)	0.31474(15)	0.0432(4)
O2	0.18393(18)	0.05126(11)	0.43105(19)	0.0631(6)
O3	-0.50493(16)	0.11366(11)	0.40913(15)	0.0447(4)
O4	-0.44737(17)	0.16790(11)	0.22878(16)	0.0507(5)
S1	-0.11241(7)	0.20563(5)	0.64109(6)	0.0521(2)
C1	0.1644(2)	0.12512(16)	0.3984(2)	0.0375(6)
C2	0.0651(2)	0.17951(15)	0.4577(2)	0.0433(6)
H2A	-0.006650	0.194416	0.390317	0.052
H2B	0.109276	0.231401	0.488502	0.052
C3	0.0045(2)	0.13926(16)	0.5691(2)	0.0467(7)
H3A	0.076214	0.123524	0.635982	0.056
H3B	-0.041126	0.087878	0.538015	0.056
C4	-0.2719(2)	0.16730(17)	0.5617(2)	0.0455(6)
H4A	-0.278686	0.107374	0.578846	0.055
H4B	-0.343382	0.195515	0.599222	0.055
C5	-0.2912(2)	0.18118(17)	0.4170(2)	0.0478(7)
H5A	-0.220366	0.151752	0.380100	0.057
H5B	-0.280706	0.240943	0.400693	0.057
C6	-0.4233(2)	0.15293(15)	0.3464(2)	0.0387(6)
C7	0.5534(2)	-0.06223(15)	0.3096(2)	0.0427(6)
H7	0.579534	-0.039051	0.391180	0.051
C8	0.6187(3)	-0.13261(16)	0.2724(3)	0.0480(7)
H8	0.686382	-0.157381	0.329131	0.058
C9	0.5832(3)	-0.16609(15)	0.1509(3)	0.0482(7)
H9	0.627852	-0.212855	0.123339	0.058
C10	0.4799(2)	-0.12892(14)	0.0704(2)	0.0429(6)
H10	0.454805	-0.150124	-0.012651	0.051
C11	0.4147(2)	-0.06063(13)	0.1138(2)	0.0333(5)

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Abstract

$C_{16}H_{16}CuN_2O_4S$, monoclinic, $P2_1/c$ (no. 14), $a = 10.0742(14)$ Å, $b = 15.843(2)$ Å, $c = 10.3745(15)$ Å, $V = 1643.0(4)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0335$, $wR_{\text{ref}}(F^2) = 0.0666$, $T = 273(2)$ K.

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Source of materials

The reaction was carried out by the solvothermal method. 3,3'-Thiodipropionic acid thiodiacetic acid (0.395 g, 1 mmol), copper(II) acetate (0.199 g, 1 mmol) and 2,2'-bipyridine (0.156 g, 1 mmol) were added to the airtight vessel with the ratio of ethanol and water 1:2 reacting in 393 K for 3 days. The resulting blue solution was filtered. The filtrate was placed for several days yielding blue block-shaped crystals.

Yield: 78% (based on Cu element), and **elemental analysis**: calc. for $C_{16}H_{16}CuN_2O_4S$: C 48.54, H 4.07, N 7.08; found: C 48.31, H 4.29, N 7.13. The elemental analyses were performed with PERKIN ELMER MODEL 2400 SERIES II.

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Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
C12	0.2994(2)	−0.01777(14)	0.0395(2)	0.0339(5)
C13	0.2420(2)	−0.04298(16)	−0.0833(2)	0.0438(6)
H13	0.275030	−0.089275	−0.124299	0.053
C14	0.1348(3)	0.00269(17)	−0.1425(2)	0.0513(7)
H14	0.094867	−0.012712	−0.224834	0.062
C15	0.0870(2)	0.07010(17)	−0.0813(2)	0.0477(7)
H15	0.015425	0.101494	−0.121318	0.057
C16	0.1470(2)	0.09075(15)	0.0411(2)	0.0411(6)
H16	0.113588	0.136112	0.083928	0.049

Experimental details

All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were assigned with common isotropic displacement factors $U_{\text{iso}}(\text{H}) = 1.2$ times U_{eq} (C, methylene and pyridine groups), and refined as riding on their parent atom.

Comment

The syntheses of coordination polymers have received great interest owing to their magnetic, luminescence, gas storage/separation, catalytic properties [3–5]. The general strategy for the design of coordination polymers relies on the utilization of multidentate ligands which can act as bridging ligands. It is well known that the most widely used multidentate ligands are polycarboxylates due to their diverse coordination modes in the construction of coordination polymers [6, 7]. In this study, 3,3'-thiodipropionic acid, as a flexible aliphatic dicarboxylic acid, has been used as a versatile educt. Moreover, the N-donor ligand was also used to obtain coordination polymers [8].

In this structure, the asymmetric unit of this title complex consist of a Cu(II) ion, one 2,2-bipy ligand and a 3,3'-thiodipropionato ligand, exhibiting a four-coordinated geometry. The environment of Cu atom, growing by the symmetry operation, exhibits a four-coordinated with two N atoms from 2,2'-bipyridine and two O atoms from the

3,3'-thiodipropionato ligand. The first coordination sphere gives a slightly distorted square-planar geometry (*cf.* the figure). The distances of Cu–O bonds are 1.948(2) Å and 1.966(2) Å and Cu–N bonds are 1.991(2) Å and 2.001(3) Å, showing the different coordination modes of two Cu–O and Cu–N bonds. The 1D coordinated polymer was formed by the coordination bonds along the *a* axis.

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