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Crystal structure of poly-[(μ_2 (carboxylatomethyl)((3-nitrophenyl)sulfonyl)amido- $\kappa^3 N: O: O'$)(μ_2 -4,4'-bipyridine- $\kappa^2 N: N'$)copper(II)], $C_{18}H_{14}CuN_4O_6S$

Table 1: Data collection and handling.

Crystal:	Blue block
Size:	0.26 × 0.22 × 0.21 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.31 mm ⁻¹
Diffractometer, scan mode:	CCD, φ and ω
$\theta_{\max}$, completeness:	28.4°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	18075, 4720, 0.033
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3698
$N(\text{param})_{\text{refined}}$:	271
Programs:	Bruker [1], SHELX [2, 3], Olex2 [4]

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Abstract

$C_{18}H_{14}CuN_4O_6S$, trigonal, $R\bar{3}$ (no. 148), $a = 31.125(7)$ Å, $b = 31.125(3)$ Å, $c = 10.133(2)$ Å, $V = 8501(3)$ Å³, $Z = 18$, $R_{\text{gt}}(F) = 0.0346$, $wR_{\text{ref}}(F^2) = 0.0900$, $T = 296(2)$ K.

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The title crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

Copper(II) acetate monohydrate (99.8 mg, 0.5 mmol), 3-nitrobenzenesulfonylglycine (H_2nbs) (130.1 mg, 0.5 mmol), 4,4'-bipyridine (4,4'-bipy) (78.1 mg, 0.5 mmol) and 15 mL water was added to a 20 mL Teflon-lined reaction vessel. Then the pH of the resulting mixture was adjusted to 7 with 1 mol/L NaOH aqueous solution. After heating at 120 °C for 24 h, it was cooled to room temperature at a rate of 10 °C per hour to give blue block crystals.

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Experimental details

The structure was solved with the ShelXT [2] structure solution program using intrinsic phasing and refined with the ShelXL [3] refinement package using least squares minimisation.

Comment

Metal-organic frameworks (MOFs) are a class of organic-inorganic hybrid materials. In recent years, it has gained great attention due to their diverse structures and rich physical and chemical properties, such as electricity, light, and magnetism *etc.*, and potential applications in gas adsorption/storage and separation [5–8], identification and sensing [9–11], and heterogeneous catalysis [12, 13]. The sulfonlated amino acid compound which has some coordination sites can be used to assemble metal organic frameworks and coordination polymers [14–17].

In this paper, the synthesis and crystal structure of a new copper(II) complex with 3-nitrobenzenesulfonylglycine (H_2nbs) and 4,4'-bipyridine (4,4'-bipy) is reported. The asymmetric unit is composed of one independent Cu(II) ion, one nbs ligand and one 4,4'-bipy ligand. The crystallographically unique Cu²⁺ ion of the title complex is five-coordinated (see the figure) by two N atoms (N3, N4) from 4,4'-bipy group, two O atoms (O1, O2) and one N atom (N1) from nbs group (Cu1–O, 1.9549(15) ~ 2.0309(14) Å, Cu1–N, 2.0150(17) ~ 2.1705(18) Å). A three-dimensional network was formed by Cu–O and Cu–N bonds.

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

Atom	x	y	z	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
Cu1	0.91869(2)	0.61493(2)	0.69823(2)	0.02795(9)
S1	0.81264(2)	0.54406(2)	0.84485(5)	0.02849(13)
O1	0.96602(5)	0.62350(6)	0.83687(16)	0.0390(4)
O2	0.97650(5)	0.59615(6)	1.02793(14)	0.0314(3)
O3	0.79534(6)	0.51970(6)	0.97045(16)	0.0429(4)
O4	0.79736(6)	0.57902(6)	0.80803(19)	0.0448(4)
O5	0.69391(9)	0.50036(9)	0.4349(2)	0.0736(7)
O6	0.65803(7)	0.42132(8)	0.4113(2)	0.0671(6)
N1	0.87009(6)	0.56722(7)	0.83157(17)	0.0304(4)
N2	0.68978(8)	0.46048(9)	0.4591(2)	0.0477(5)
N3	0.70273(7)	0.60979(7)	0.08981(18)	0.0323(4)
N4	0.87125(6)	0.60984(7)	0.55560(17)	0.0290(4)
C1	0.94988(7)	0.59577(7)	0.9350(2)	0.0249(4)
C2	0.89581(8)	0.55827(10)	0.9397(2)	0.0418(6)
H2A	0.891207	0.525165	0.932007	0.050*
H2B	0.882030	0.560559	1.023520	0.050*
C3	0.78311(7)	0.49621(8)	0.7256(2)	0.0283(4)
C4	0.75084(8)	0.49837(8)	0.6359(2)	0.0309(5)
H4	0.746849	0.526017	0.631302	0.037*
C5	0.72479(8)	0.45846(9)	0.5534(2)	0.0357(5)
C6	0.73014(10)	0.41752(10)	0.5557(3)	0.0493(7)
H6	0.711802	0.390965	0.499173	0.059*
C7	0.76320(12)	0.41652(11)	0.6432(3)	0.0606(8)
H7	0.767870	0.389257	0.645065	0.073*
C8	0.78947(10)	0.45543(10)	0.7281(3)	0.0469(6)
H8	0.811648	0.454278	0.787455	0.056*
C9	0.70693(9)	0.62805(9)	0.2118(2)	0.0414(6)
H9	0.686819	0.641029	0.235410	0.050*
C10	0.73959(9)	0.62848(9)	0.3036(2)	0.0414(6)
H10	0.741259	0.641502	0.387320	0.050*
C11	0.77000(8)	0.60947(8)	0.2712(2)	0.0290(4)
C12	0.76639(9)	0.59151(10)	0.1445(2)	0.0409(6)
H12	0.786451	0.578839	0.117742	0.049*
C13	0.73267(9)	0.59261(10)	0.0584(2)	0.0417(6)
H13	0.730846	0.580599	−0.026714	0.050*
C14	0.80483(8)	0.60855(8)	0.3679(2)	0.0293(4)
C15	0.82601(9)	0.64540(9)	0.4625(2)	0.0357(5)
H15	0.818141	0.670546	0.465005	0.043*
C16	0.85852(9)	0.64486(9)	0.5522(2)	0.0348(5)
H16	0.872513	0.670269	0.614122	0.042*
C17	0.85045(8)	0.57388(8)	0.4650(2)	0.0340(5)
H17	0.858334	0.548737	0.466386	0.041*
C18	0.81814(8)	0.57204(8)	0.3702(2)	0.0351(5)
H18	0.805266	0.546653	0.307999	0.042*

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