Zhongyu Zhang*, Xiaoxia Men, Bing Han and Chunyan Sun

Crystal structure of (1,10-phenanthroline- κ^2 *N,N'*)-bis(3-thiophenecarboxylato- κ^2 *O,O'*) copper(II), $C_{22}H_{14}N_2O_4S_2Cu$

Table 1: Data collection and handling.

Crystal:	Blue block
Size:	0.30 × 0.30 × 0.20 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.530 mm ⁻¹
Diffractometer, scan mode:	Bruker Smart APEX-II, φ and ω
$\theta_{\max}$, completeness:	26.0°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	12,036, 2003, 0.023
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1737
$N(\text{param})_{\text{refined}}$:	148
Programs:	Bruker [1], Olex2 [2]

Source of material

3-Thiophenecarboxylic acid (2.0 mmol) was dissolved in 20 mL of anhydrous methanol. $Cu(CH_3COO)_2 \cdot H_2O$ (1.0 mmol) dissolved in 15 mL of anhydrous methanol was added dropwise to the above 3-thiophenecarboxylic acid solution and stirred for 4 h at 55 °C. Then 1,10-phenanthroline (1.0 mmol) was dissolved in 10 mL of anhydrous methanol and added dropwise to the above solution and stirred for 4 h at 55 °C cooled and filtered. The filtrate was left for slow evaporation at room temperature. The blue block crystals were formed 20 days later. Yield: 41.6%. **Anal. Calcd.** for $C_{22}H_{14}N_2O_4S_2Cu$: C, 53.06; H, 2.83; N, 5.62; S, 12.88; found: C, 53.10; H, 2.85; N, 5.58; S, 12.84.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms. There is a disorder at the thiophenyl moiety (Figure, Table 2).

Comment

Heterocyclic compounds are widely distributed in nature and essential to many biochemical processes [3–5]. Thiophene carboxylates and its metal complex has attracted extensive attention. Some of these metal complexes have excellent biological activities and chemical properties [6, 7]. As a part of our current research on the

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Abstract

$C_{22}H_{14}N_2O_4S_2Cu$, orthorhombic, *Pbcn* (no. 60), $a = 20.171(7)$ Å, $b = 9.684(3)$ Å, $c = 10.372(4)$ Å, $V = 2025.9(12)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0334$, $wR_{\text{ref}}(F^2) = 0.0908$, $T = 273.15$ K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

***Corresponding author: Zhongyu Zhang**, Shandong Provincial Engineering Laboratory of Novel Pharmaceutical Excipients, Sustained and Controlled Release Preparations, College of Medicine and Nursing, Dezhou University, Dezhou, 253000, Shandong, China, E-mail: dzzhangzhongyu@163.com. <https://orcid.org/0000-0003-0901-1016>

Xiaoxia Men, Bing Han and Chunyan Sun, Shandong Provincial Engineering Laboratory of Novel Pharmaceutical Excipients, Sustained and Controlled Release Preparations, College of Medicine and Nursing, Dezhou University, Dezhou, 253000, Shandong, China

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

Atom	x	y	z	U _{iso} ^a /U _{eq}
Cu1	0.5000	0.32688 (3)	0.7500	0.02922 (15)
S1 ^a	0.74295 (7)	0.74380 (13)	0.69779 (9)	0.0536 (4)
S1A ^b	0.7661 (6)	0.6985 (17)	0.8438 (9)	0.057 (2)
O1	0.56695 (9)	0.46185 (16)	0.70243 (17)	0.0407 (3)
O2	0.60449 (8)	0.37895 (16)	0.88747 (17)	0.0407 (3)
N1	0.54449 (9)	0.17100 (17)	0.6566 (2)	0.0317 (4)
C1	0.60899 (11)	0.4592 (2)	0.7950 (2)	0.0288 (5)
C2	0.66458 (11)	0.5595 (2)	0.7859 (2)	0.0294 (5)
C3	0.67754 (11)	0.6359 (2)	0.6781 (2)	0.0364 (5)
H3	0.6518	0.6341	0.5936	0.044*
C4 ^a	0.7539 (4)	0.6895 (10)	0.8584 (5)	0.0462 (11)
H4 ^a	0.7854	0.7243	0.9153	0.055*
C5	0.70914 (12)	0.5887 (3)	0.8867 (2)	0.0428 (6)
H5	0.7058	0.5540	0.9697	0.051*
C6	0.58804 (12)	0.1758 (3)	0.5610 (3)	0.0410 (6)
H6	0.6034	0.2613	0.5333	0.049*
C7	0.61158 (13)	0.0567 (3)	0.5005 (3)	0.0481 (6)
H7	0.6417	0.0634	0.4328	0.058*
C8	0.59013 (13)	−0.0698 (3)	0.5413 (3)	0.0470 (6)
H8	0.6050	−0.1494	0.5004	0.056*
C9	0.54548 (11)	−0.0797 (2)	0.6452 (3)	0.0389 (6)
C10	0.52351 (11)	0.0453 (2)	0.6989 (2)	0.0317 (5)
C11	0.52084 (13)	−0.2066 (3)	0.6993 (3)	0.0488 (7)
H11	0.5340	−0.2903	0.6635	0.059*
C4A ^b	0.7379 (13)	0.712 (4)	0.6900 (15)	0.0462 (11)
H4A ^b	0.7585	0.7605	0.6240	0.055*

^aOccupancy: 0.853 (3), ^bOccupancy: 0.147 (3).

biological activity of heterocyclic transition metal complexes, we report herein a new copper complex.

Single crystal X-ray diffraction analysis demonstrates that the asymmetric unit of the title structure contains one half of a copper(II) cation, one 3-thiophenecarboxylate ligand and one half of a 1, 10-phenanthroline ligand. The bond distances of Cu–N are 2.0058(19) Å, bond lengths of Cu–O are 1.9430(17) Å, respectively, which are similar with the reference [8, 9]. In the title complex, the bond angles of O(1)–Cu(1)–N(1a), O(1a)–Cu(1)–N(1) and O(2)–Cu(1)–O(2a), are 160.04 (7), 160.04 (7) and 157.583 (5)° respectively. The copper(II) is 4+2 coordinated by four oxygen and two nitrogen atoms with Cu1–O2 distances that are significantly longer than the others [10].

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