Jian-Ge. Wang*

Crystal structure of *catena*-poly[(μ_2 -3-(benzo[d]thiazol-2-yl)-5-carboxybenzoato- $\kappa^2 N:O$)silver(I)], $C_{15}H_8AgNO_4S$

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.25 × 0.24 × 0.23 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.79 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω -scans
$\theta_{\max}$, completeness:	28.5°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	29076, 2942, 0.037
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2696
$N(\text{param})_{\text{refined}}$:	200
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3]

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

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	0.61583(3)	0.42455(2)	0.43263(3)	0.04210(10)
S1	0.50761(8)	0.10441(5)	0.44032(8)	0.02939(18)
O1	0.1158(2)	0.51397(14)	0.3868(2)	0.0372(5)
O2	-0.1337(2)	0.46736(14)	0.2967(2)	0.0305(5)
H2	-0.1557	0.5215	0.3067	0.046*
O3	-0.2334(2)	0.12792(14)	0.1980(2)	0.0319(5)
O4	-0.0182(2)	0.05591(13)	0.1476(2)	0.0304(5)
N1	0.5908(2)	0.27533(15)	0.4474(2)	0.0186(4)
C1	0.0776(3)	0.35716(17)	0.3215(2)	0.0177(5)
C2	-0.0300(3)	0.28860(17)	0.2660(2)	0.0185(5)
H2A	-0.1397	0.3022	0.2389	0.022*
C3	0.0261(3)	0.20007(17)	0.2512(2)	0.0173(5)
C4	0.1900(3)	0.18051(17)	0.2943(2)	0.0181(5)
H4	0.2287	0.1219	0.2817	0.022*
C5	0.2973(3)	0.24720(17)	0.3562(2)	0.0172(5)
C6	0.2398(3)	0.33640(17)	0.3683(3)	0.0189(5)
H6	0.3103	0.3819	0.4078	0.023*
C7	0.0230(3)	0.45392(18)	0.3389(3)	0.0221(5)
C8	-0.0859(3)	0.12231(17)	0.1938(3)	0.0198(5)
C9	0.4663(3)	0.22062(17)	0.4118(2)	0.0170(5)
C10	0.7298(3)	0.22536(18)	0.5020(2)	0.0180(5)
C11	0.7075(3)	0.13031(19)	0.5056(3)	0.0226(6)
C12	0.8349(4)	0.0715(2)	0.5562(3)	0.0339(7)
H12	0.8197	0.0082	0.5582	0.041*
C13	0.9848(4)	0.1104(2)	0.6032(3)	0.0333(7)
H13	1.0721	0.0726	0.6373	0.040*
C14	1.0075(3)	0.2050(2)	0.6007(3)	0.0300(7)
H14	1.1097	0.2294	0.6334	0.036*
C15	0.8822(3)	0.2634(2)	0.5508(3)	0.0234(6)
H15	0.8984	0.3267	0.5496	0.028*

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Abstract

$C_{15}H_8AgNO_4S$, monoclinic, $P2_1/n$ (no. 14), $a = 8.38373(15)$ Å, $b = 14.5293(2)$ Å, $c = 10.5147(2)$ Å, $\beta = 101.0636(18)^\circ$, $V = 1257.00(4)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0340$, $wR_{\text{ref}}(F^2) = 0.0724$, $T = 290(1)$ K.

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A part of the title crystal structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of materials

A mixture of $AgNO_3$ (0.017 g, 0.1 mmol), 5-(benzo[d]thiazol-2-yl)benzene-1,3-dioic acid (0.0299 g, 0.1 mmol), H_2O (10 mL) and ethanol (5 mL) was sealed in a 25 mL Teflon-lined steel vessel and heated at 90 °C for 3 days. The colorless block

*Corresponding author: Jian-Ge. Wang, College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang, Henan 471022, P.R. China, e-mail: miaoshaoxuan@126.com

crystals of the title compound were obtained, which were washed with water and dried in air with a 47% yield.

Experimental details

The hydrogen atoms were assigned with common isotropic displacement factors $U_{\text{iso}}(\text{H}) = 1.2$ times $U_{\text{eq}}(\text{C})$, refined with riding coordinates; $U_{\text{iso}}(\text{H}) = 1.5$ times $U_{\text{eq}}(\text{O})$, refined as rotating group.

Comment

Coordination polymer (CPs) have been extensively investigated in the past few decades because of their vast applications such as gas storage [4], catalysis [5], molecular magnetism [6], luminescence [7], and so on. In particular, luminescent CPs based on d¹⁰ metals represent a rapidly growing field of research [8–12]. It is well known that the properties of CPs mainly depended on the organic ligands and the center metal ions because they are involved in the formation of the final CPs [13]. Herein, we report a Ag(I) CPs based on a bifunctional ligand 5-(benzo[d]thiazol-2-yl)benzene-1,3-dioic acid.

The title compound exhibits one dimensional chain structure. The asymmetric unit of the title structure contains one 3-(benzo[d]thiazol-2-yl)-5-carboxybenzoate anion, and one Ag(I) ion. As shown in the figure, Ag1 is twofold-coordinated by one O atom and one N atom from two different ligands. The Ag–O and the Ag–N bond lengths are 2.1817(19) and 2.187(2) Å, respectively. The 3-(benzo[d]thiazol-2-yl)-5-carboxybenzoate acts as a bidentate chelating ligand, by which adjacent Ag(I) ions are connected into one dimensional chain structure. There exists one intermolecular hydrogen bond (d(O2...O3): 2.591(3) Å), the one dimensional chain are joined to each other by this hydrogen bonds to form a two dimensional supramolecular structure.

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