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Crystal structure of poly[(μ_2 -2-(1*H*-1,2,4-triazol-1-yl)benzoato- κ^4 O:O':N:N')silver(I)] monohydrate, $C_9H_8AgO_3N_3$

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Abstract

$C_9H_8AgO_3N_3$, monoclinic, $P2_1/n$ (no. 14), $a = 6.5358(3)$ Å, $b = 6.0583(4)$ Å, $c = 24.9951(11)$ Å, $\beta = 92.040(4)^\circ$, $V = 989.08(8)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0297$, $wR_{ref}(F^2) = 0.0552$, $T = 288.74(10)$ 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.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.32 × 0.24 × 0.15 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	2.03 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω
θ_{max} , completeness:	25.5°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	5442, 1806, 0.032
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 1582
$N(param)_{refined}$:	148
Programs:	CrysAlis ^{PRO} [1], SHELX [2], Olex2 [3]

Source of material

The title compound was prepared by hydrothermal method. A mixture of $AgNO_3$ (0.034 g, 0.2 mmol), 2-(1,2,4-triazol-2) benzenecarboxylic acid (0.019 g, 0.1 mmol), and H_2O (15 mL) was sealed in a 25 mL Teflon-lined stainless steel vessel and heated at 160 °C for 3 days. The reaction mixture was slowly cooled to room temperature at a rate of 5 °C/h, and the colorless block crystals were collected, washed with water, and dried in air.

Experimental details

The hydrogen atoms were assigned with common isotropic displacement factors $U_{iso}(H) = 1.2$ times $U_{eq}(C)$, aromatic

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
Ag1	0.60056(3)	0.20502(5)	0.46975(2)	0.03152(12)
O1	0.3103(3)	0.7755(4)	0.43572(9)	0.0283(6)
O2	0.6309(3)	0.8557(4)	0.41562(10)	0.0361(6)
N1	0.1964(4)	0.3556(4)	0.40232(10)	0.0203(6)
N2	0.2703(4)	0.2966(4)	0.45192(10)	0.0220(6)
N3	−0.0734(4)	0.2911(4)	0.44876(11)	0.0242(7)
C1	0.3264(4)	0.4104(5)	0.35913(12)	0.0212(7)
C2	0.4516(4)	0.5952(5)	0.36082(12)	0.0202(7)
C3	0.5654(5)	0.6344(6)	0.31565(13)	0.0292(8)
H3	0.6520	0.7561	0.3153	0.035 [*]
C4	0.5534(5)	0.4978(6)	0.27136(13)	0.0348(9)
H4	0.6291	0.5304	0.2416	0.042 [*]
C5	0.4306(5)	0.3147(6)	0.27120(14)	0.0377(10)
H5	0.4232	0.2221	0.2415	0.045 [*]
C6	0.3178(5)	0.2689(6)	0.31557(14)	0.0319(9)
H6	0.2362	0.1432	0.3162	0.038 [*]
C7	0.4643(5)	0.7539(5)	0.40774(13)	0.0238(8)
C8	−0.0072(4)	0.3512(5)	0.40176(13)	0.0244(8)
H8	−0.0914	0.3859	0.3722	0.029 [*]
C9	0.1023(5)	0.2585(5)	0.47843(14)	0.0235(8)
H9	0.1042	0.2137	0.5140	0.028 [*]
O3	0.9916(4)	0.8653(5)	0.36021(10)	0.0426(7)
H3A	1.0883	0.8483	0.3835	0.064 [*]
H3B	0.8774	0.8591	0.3754	0.064 [*]

ring), and $U_{\text{iso}}(\text{H}) = 1.5$ times $U_{\text{eq}}(\text{O, water})$. The final refinement by using geometrical restraints, with C—H = 0.93 Å (aromatic ring), and O—H = 0.85 Å (water).

Comment

Coordination polymers (CPs) have attracted wide attention owing to their intriguing structures and their promising properties such as gas adsorption, magnetism, luminescence, and so on [4–6]. Benzoic and *N*-containing heterocyclic compounds are the most widely used building ligands in the syntheses of CPs for their rich coordinate sites and diverse coordinate modes [7–9]. Bifunctional ligands with benzoic and *N*-containing heterocyclic fragments present both functionalities in one ligand [10–12].

The asymmetric unit of the title compound consists of one crystallographically independent Ag(I) ions, one 2-(1,2,4-triazol-2)benzenecarboxyl ligand, and one coordinated water molecule (Figure, upper part). The Ag(I) center is four-coordinated with distorted tetrahedral geometry. The geometry is completed by two nitrogen atoms and two oxygen

atoms from four different ligands. The Ag—N bond lengths are 2.257(2) and 2.273(2) Å, and the Ag—O bond lengths are 2.416(2) and 2.523(2) Å, respectively. The 2-(1,2,4-triazol-2)benzenecarboxylato ligand is deprotonated. The carboxyl group connect with two Ag(I) ions, the triazole also coordinate with two Ag(I) ions. By this mode, the organic ligands connect adjacent Ag(I) ions, give a 2D framework, as shown in the lower part of the figure.

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