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Crystal structure of poly[aqua-(μ$_3$-3,5-di(4*H*-1,2,4-triazolyl-4-κ^3*N*,*N*′:*N*″)benzenecarboxylato) silver(I)], $C_{11}H_9AgN_6O_3$

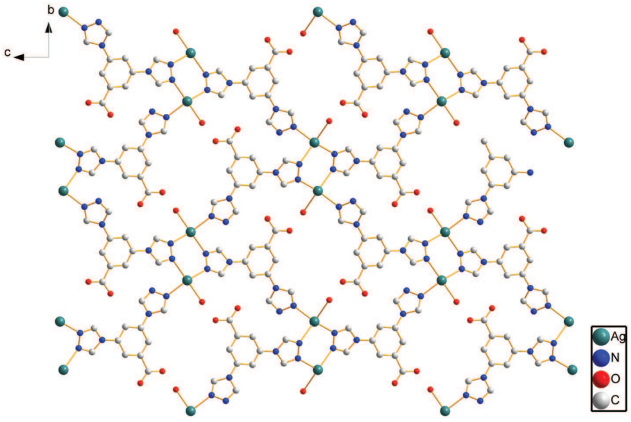

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.38 × 0.21 × 0.14 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	15.8 cm^{-1}
Diffractometer, scan mode:	Bruker SMART, *φ* and *ω*
$2\theta_{max}$, completeness:	51°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	9275, 2414, 0.042
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1895
$N(param)_{refined}$:	190
Programs:	SHELX [1, 2], Bruker programs [3], DIAMOND [4]

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Abstract

$C_{11}H_9AgN_6O_3$, monoclinic, $P2_1/c$ (no. 14), $a = 3.8210(13)$ Å, $b = 15.427(5)$ Å, $c = 21.969(7)$ Å, $\beta = 90.275(4)°$, $V = 1295.0(8)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0457$, $wR_{ref}(F^2) = 0.1096$, $T = 296(2)$ K.

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The packing of 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

The title compound was prepared by a hydrothermal method. A mixture of $AgNO_3$ (0.034 g, 0.2 mmol), 3,5-di(1,2,4-triazole-4)benzenecarboxylic acid (0.0256 g, 0.1 mmol), and H_2O (10 mL) was sealed in a 25 mL Teflon-lined stainless steel vessel and heated at 140 °C for 3 days. The reaction mixture was slowly cooled to room temperature at a rate of 3 °C/h, and the colourless block crystals were collected, washed with water, and dried in air.

Experimental details

All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were assigned with common isotropic displacement factors $U_{iso}(H) = 1.2$ times U_{eq}(C, aromatic ring), and $U_{iso}(H) = 1.5$ times U_{eq}(O, water) and refined as riding on their parent atom.

Discussion

Coordination polymers (CPs) have attracted considerable attention because of their interesting structures and potential application as functional materials [5]. Structural motifs include 1D chains and ladders, 2D grids, 3D networks and interpenetrated structures [6, 7]. The nature of the metal ions and organic ligands strongly influence the structures of CPs [8]; among the latter, aromatic polycarboxyl compounds and 1,2,4-triazole derivatives have been shown to facilitate a large number of coordination modes [9–11]. In this work, we have focussed our attention on 3,5-di(1,2,4-triazole-4)benzenecarboxylic acid.

The asymmetric unit of the title structure consists of one Ag(I) ion, one 3,5-di(1,2,4-triazole-4)benzenecarboxylato ligand, and one coordinated water molecule. Each Ag(I) ion is coordinated to three nitrogen atoms belonging to three

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Ag1	1.06842(17)	0.13495(3)	0.50679(2)	0.0468(2)
N1	0.5765(12)	0.0320(3)	0.34117(18)	0.0216(9)
N2	0.6943(14)	−0.0142(3)	0.4334(2)	0.0303(11)
N3	0.8063(13)	0.0708(3)	0.4281(2)	0.0270(11)
N4	0.1574(12)	0.1781(3)	0.15854(19)	0.0217(10)
N5	−0.0559(14)	0.3077(3)	0.1446(2)	0.0344(12)
N6	0.0560(13)	0.2762(3)	0.0891(2)	0.0312(11)
O1	0.3297(13)	−0.2092(2)	0.19138(18)	0.0412(11)
O2	0.1789(12)	−0.1426(3)	0.10490(17)	0.0392(10)
O3	1.3059(15)	0.2558(4)	0.4491(3)	0.091(2)
H1W	1.4550	0.2500	0.4204	0.137*
H2W	1.1386	0.2864	0.4376	0.137*
C1	0.3143(14)	−0.0552(3)	0.1906(2)	0.0218(11)
C2	0.4366(14)	−0.0505(3)	0.2502(2)	0.0221(11)
H2	0.5015	−0.1007	0.2708	0.026*
C3	0.4615(14)	0.0292(3)	0.2787(2)	0.0206(11)
C4	0.3774(14)	0.1057(3)	0.2494(2)	0.0243(12)
H4	0.3972	0.1590	0.2688	0.029*
C5	0.2613(14)	0.0994(3)	0.1890(2)	0.0199(11)
C6	0.2261(14)	0.0207(3)	0.1597(2)	0.0226(11)
H6	0.1446	0.0184	0.1197	0.027*
C7	0.2731(15)	−0.1435(3)	0.1602(2)	0.0272(12)
C8	0.5592(15)	−0.0347(4)	0.3811(2)	0.0246(12)
H8	0.4626	−0.0886	0.3721	0.030*
C9	0.7313(15)	0.0976(4)	0.3730(2)	0.0264(12)
H9	0.7766	0.1528	0.3579	0.032*
C10	0.0111(15)	0.2494(4)	0.1850(2)	0.0287(13)
H10	−0.0339	0.2551	0.2264	0.034*
C11	0.1783(16)	0.1982(4)	0.0984(2)	0.0292(13)
H11	0.2663	0.1619	0.0683	0.035*

symmetry-equivalent ligands as well as one oxygen atom of a water molecule; this gives rise to a distorted tetrahedral geometry around the metal centre. The carboxylate group does not take part in coordination. The Ag—N bond lengths are in the range of 2.225(4)–2.452(5) Å, and the Ag—O bond length is 2.432(5) Å. Adjacent Ag(I) cations are linked by two-coordinated triazole units of the 3,5-di(1,2,4-triazole-4)benzenecarboxylato ligands into dinuclear secondary building units (SBUs). The SBUs are further connected by the one-coordinated triazole units of the organic ligand to generate a 2D network (*cf.* the figure that extends) along *bc* plane.

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