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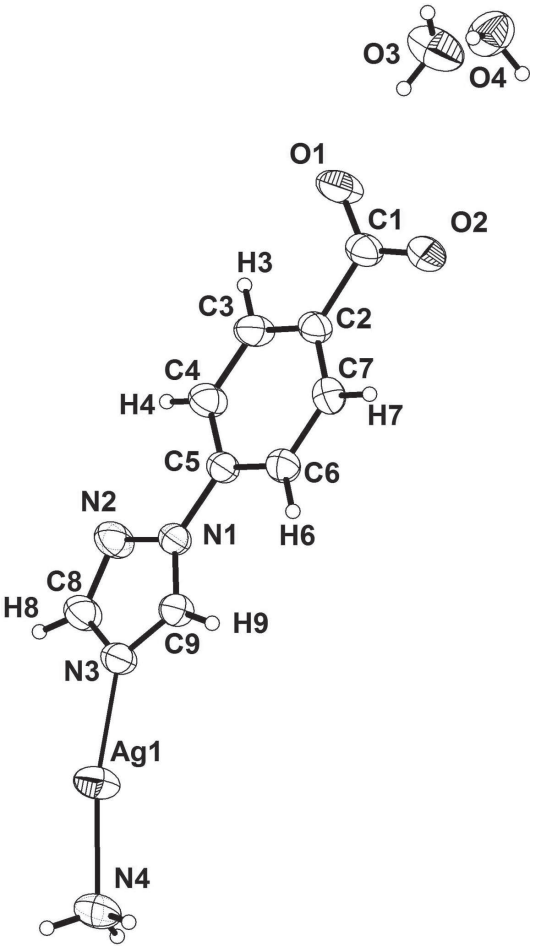
The crystal structure of amine-(4-(1*H*-1,2,4-triazol-1-yl)benzoato-κ*N*)silver(I) dihydrate, $C_9H_{13}AgN_4O_4$



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Abstract

$C_9H_{13}AgN_4O_4$, monoclinic, $C2/c$ (no. 15), $a = 28.123(3)$ Å, $b = 7.0409(7)$ Å, $c = 14.1954(15)$ Å, $\beta = 119.488(2)°$, $V = 2446.8(4)$ Å^3, $Z = 8$, $R_{gt}(F) = 0.0206$, $wR_{ref}(F^2) = 0.0558$, $T = 296(2)$ K.

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

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.45 × 0.44 × 0.44 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	16.6 cm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
$2\theta_{max}$, completeness:	50°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	6809, 2162, 0.022
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2059
$N(param)_{refined}$:	165
Programs:	SHELX [1], Bruker programs [2]

Source of materials

A solution of ammonia (1.0 M) was added dropwise to a mixed solvent (methanol/water = 1:1, 30 mL) solution of 4-(1*H*-1,2,4-triazol-1-yl) benzoic acid (189 mg, 1.0 mmol), and $AgNO_3$ (170 mg, 1.0 mmol), resulting in a transparent solution. After one week, colourless block crystals of the title complex were crystallized, isolated, washed with water (three times), and dried in a desiccator using $CaCl_2$. Yield: 56%.

Experimental details

The carbon H-atoms were placed in calculated positions (C—H_{phenyl} = 0.93 Å), and were included with $U_{iso}(H) = 1.2U_{eq}(C)$. The water H-atoms were placed in calculated positions (O—H = 0.85 Å), and were included with $U_{iso}(H) = 1.2U_{eq}(O)$ [1].

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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	0.678450(7)	0.98414(3)	0.574758(15)	0.04372(11)
N1	0.51628(6)	0.7931(2)	0.46418(12)	0.0275(3)
N2	0.51053(7)	0.8321(3)	0.36477(14)	0.0386(4)
N3	0.59629(6)	0.8859(2)	0.49576(14)	0.0312(4)
N4	0.75492(7)	1.1243(3)	0.66580(16)	0.0442(4)
H4A	0.7502	1.2491	0.6554	0.066*
H4B	0.7780	1.0839	0.6443	0.066*
H4C	0.7685	1.0985	0.7358	0.066*
O1	0.29277(7)	0.4563(2)	0.40628(14)	0.0468(4)
O2	0.33745(7)	0.4960(2)	0.58475(14)	0.0436(4)
O3	0.19373(7)	0.3757(3)	0.39389(18)	0.0646(5)
H3C	0.2250	0.3861	0.3989	0.078*
H3D	0.1881	0.2594	0.4013	0.078*
O4	0.12189(7)	0.6704(3)	0.28560(13)	0.0540(4)
H4D	0.1438	0.5798	0.3185	0.065*
H4E	0.1339	0.7701	0.3240	0.065*
C1	0.33349(9)	0.5063(2)	0.4930(2)	0.0336(5)
C2	0.38212(8)	0.5850(3)	0.48647(16)	0.0299(4)
C3	0.37737(8)	0.6286(3)	0.38699(17)	0.0357(4)
H3	0.3440	0.6113	0.3244	0.043*
C4	0.42139(8)	0.6973(3)	0.37902(16)	0.0349(4)
H4	0.4177	0.7258	0.3118	0.042*
C5	0.47084(7)	0.7229(2)	0.47238(15)	0.0274(4)
C6	0.47678(8)	0.6803(3)	0.57294(16)	0.0316(4)
H6	0.5102	0.6977	0.6355	0.038*
C7	0.43213(8)	0.6114(3)	0.57891(16)	0.0321(4)
H7	0.4358	0.5823	0.6461	0.038*
C8	0.55971(8)	0.8874(3)	0.38858(17)	0.0365(5)
H8	0.5687	0.9244	0.3364	0.044*
C9	0.56764(8)	0.8254(3)	0.54098(16)	0.0296(4)
H9	0.5812	0.8082	0.6148	0.036*

Comment

Coordination compounds of the coinage metals have received considerable attention in the last forty years due to their biological activity. Silver is insufficiently studied because of the poor solubility of silver(I) compounds in common solvents and the sensitivity towards photo decomposition [3–6]. On the other hand, many factors, such as the method of synthesis, the nature of the ligands, solvents, counter-anions, etc., modulate the stereochemistry of silver complexes. We have been interested in the investigation on silver(I) complexes with various organic ligands containing N and/or O atoms.

In the title complex the asymmetric unit consists of one Ag ion, one 4-(1*H*-1,2,4-triazol-1-yl)benzoato ligand, one amine ligand and two water molecules. The Ag(I) shows an almost linear coordination geometry, being coordinated by two nitrogen atoms from the 4-(1*H*-1,2,4-triazol-1-yl)benzoato ligand and the amine ligand. The average bond distances of Ag—N [2.1280 Å] and the N—Ag—N angle [168.93(7)°] are in the normal range. O—H···O hydrogen bonds with the O···O distances ranging from 2.762(3) to 2.824(3) Å connect the title complexes to a two-dimensional framework. Weaker N—H···O hydrogen bonds show N···O distances > 3 Å.

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