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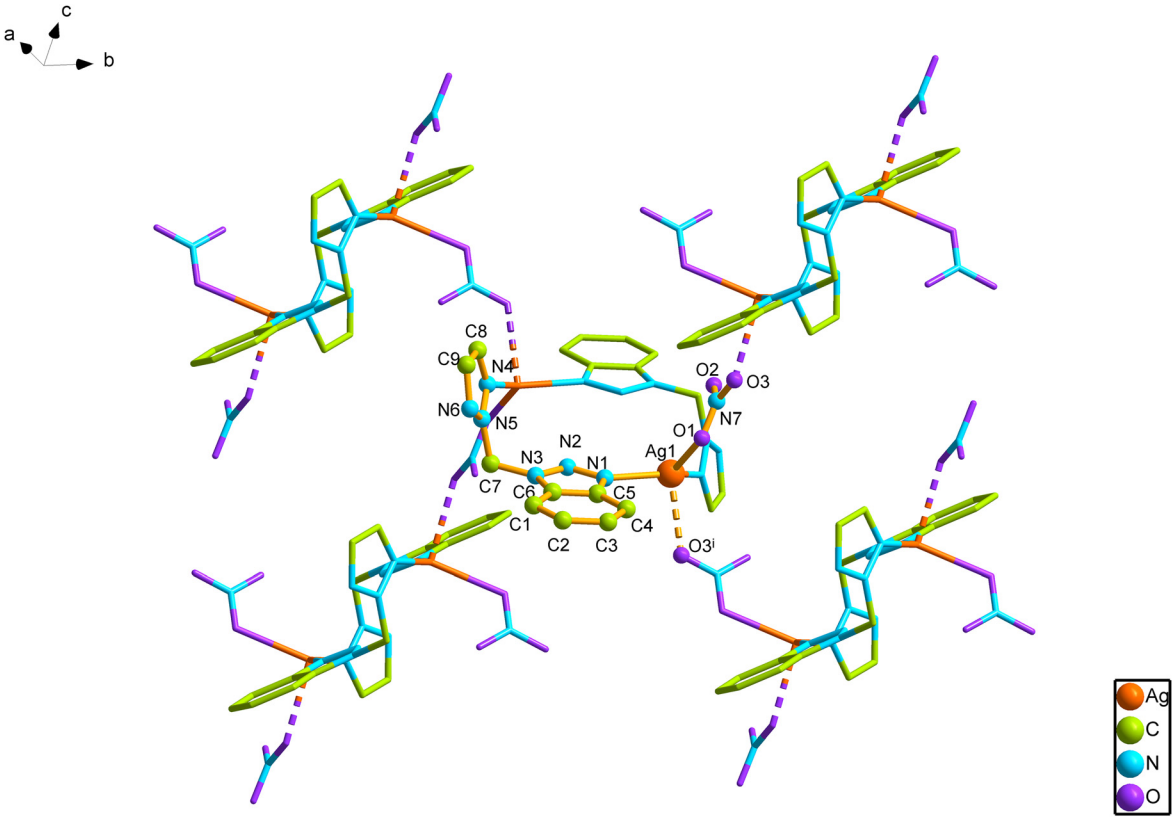
Crystal structure of (poly[μ2-(1*H*-pyrazol-1-yl) methyl]-1*H*-benzotriazole-κ^2N:*N*)-(nitrato-κ^2O:*O*′) silver(I), $C_9H_8AgN_7O_3$



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Abstract

$C_9H_8AgN_7O_3$, monoclinic, $P2_1/c$ (no. 14), a = 8.3179(3) Å, b = 16.6800(5) Å, c = 9.0138(3) Å, β = 103.839(4)°, Z = 4, V = 1214.30(7) Å^3, $R_{gt}(F)$ = 0.0423, w$R_{ref}(F^2)$ = 0.1065, T = 293(2) K.

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The molecular 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.

Table 1: Data collection and handling.

Crystal:	Colourless prism
Size:	0.26 × 0.19 × 0.07 mm
Wavelength:	Cu *K*α radiation (1.54184 Å)
μ:	13.6 mm^{-1}
Diffractometer, scan mode:	Xcalibur, ω
θ_{max}, completeness:	67.1°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	4477, 2169, 0.031
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 1866
$N(param)_{refined}$:	181
Programs:	CrysAlis^{PRO} [1], SHELX [2]

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

Atom	x	y	z	U_{iso}*/U_{eq}
Ag1	−0.15282 (5)	0.64058 (3)	0.87488 (5)	0.05015 (17)
C1	0.2778 (6)	0.5166 (3)	0.5312 (5)	0.0326 (10)
H1	0.3358	0.4719	0.5108	0.039*
C2	0.2819 (7)	0.5891 (3)	0.4579 (6)	0.0408 (12)
H2	0.3446	0.5933	0.3856	0.049*
C3	0.1946 (7)	0.6564 (3)	0.4891 (6)	0.0408 (12)
H3	0.2019	0.7039	0.4370	0.049*
C4	0.0992 (7)	0.6548 (3)	0.5932 (6)	0.0356 (11)
H4	0.0414	0.6996	0.6131	0.043*
C5	0.0937 (6)	0.5815 (3)	0.6682 (5)	0.0275 (9)
C6	0.1811 (5)	0.5152 (3)	0.6373 (5)	0.0271 (9)
C7	0.2117 (6)	0.3766 (3)	0.7560 (5)	0.0299 (10)
H7A	0.2319	0.3559	0.6616	0.036*
H7B	0.1316	0.3419	0.7864	0.036*
C8	0.5294 (7)	0.3717 (4)	1.0902 (6)	0.0455 (13)
H8	0.5748	0.3669	1.1947	0.055*
C9	0.6155 (7)	0.3869 (4)	0.9812 (7)	0.0511 (15)
H9	0.7296	0.3933	0.9998	0.061*
N1	0.0123 (5)	0.5599 (2)	0.7792 (5)	0.0305 (8)
N2	0.0447 (5)	0.4847 (2)	0.8161 (4)	0.0302 (8)
N3	0.1452 (5)	0.4569 (2)	0.7309 (4)	0.0271 (8)
N4	0.3704 (5)	0.3650 (3)	1.0212 (5)	0.0324 (9)
N5	0.3654 (5)	0.3762 (2)	0.8741 (4)	0.0283 (8)
N6	0.5101 (6)	0.3909 (3)	0.8442 (5)	0.0459 (11)
N7	0.1071 (5)	0.7690 (2)	1.0497 (5)	0.0342 (9)
O1	0.0595 (6)	0.7488 (3)	0.9147 (5)	0.0603 (12)
O2	0.0546 (7)	0.7350 (4)	1.1468 (6)	0.0819 (17)
O3	0.2094 (6)	0.8242 (3)	1.0856 (5)	0.0585 (12)

Source of material

All starting materials are commercially available without further purification. The 1-[(1*H*-pyrazol-1-yl)methyl]-1*H*-benzotriazole (pmb) was prepared according to the literature method [3]. The ligand pmb (0.02 mmol, 0.0040 g) was dissolved in a 2 mL methanol solution, slowly added dropwise to the methanol solution of $AgNO_3$ (0.02 mmol, 0.0034 g). The resulting solution was placed at room temperature. After 2 weeks colourless crystals were obtained.

Experimental details

H atoms were generated geometrically and refined as riding atoms with C–H = 0.93 Å and the U_{iso}(H) = 1.2 times U_{eq}(C) for aromatic H atoms, and with C–H = 0.97 Å and U_{iso}(H) = 1.2 times U_{eq}(C) for methylene H atoms.

Comment

Metal complexes have many biological activities, such as antifungal, antimalarial, antioxidant, anticancer and other activities; for example: [4]. Nitrogen- containing heterocyclic organic compounds such as benzotriazole have been widely used as ligands in the construction of metal complexes [5], and they usually have biological activities, which can provide more ideas for the design and synthesis of new drug candidate [6, 7]. In addition, metal ions such as silver have antibacterial properties, and have been applied to reduce the occurrence of urinary tract infections and the occurrence of local infections in burn patients [8]. Therefore, Ag(I)-containing coordination polymers have attracted considerable recent interest owing to its various coordination modes and special properties [9].

In this study, a Ag(I) complex is synthesized by 1-[(1*H*-pyrazol-1-yl)methyl]-1*H*-benzotriazole (pmb) ligand with $AgNO_3$ at room temperature. The title compound contains a binuclear complex. As shown in the Figure, the Ag(I) atom is four-coordinated by two N atoms from two crystallographically dependent pmb ligands, two O atoms from two nitrate ions (with the Ag–N1 bond lengths of 2.238(4) Å; the Ag–N4i bond lengths of 2.230(4) Å; the Ag–O1 bond lengths of 2.490(5) Å, and the Ag–O3i bond lengths of 2.651 Å; Symmetry code: (i) $-x$, $-y+1$, $-z+2$). The Ag–O3i bond length is longer than Ag–O1 bond lengths, and the Ag–O3i bond length is longer than that of the directly related complexes [10], indicating that the acting force between Ag ion and O3 atom is weaker. The bond angles of Ag range from 90.65(15)° to 140.46(15)°. The neighboring two Ag(I) ions are connected to each other by two ligands pmb to form a binuclear unit, and all of the binuclear units are joined together through the nitrato ligands (see the figure), which leads to the 2D polymer. In addition, the benzimidazol rings in adjacent molecules are parallel, with an average interplanar distance of 4.186 Å, so that the π–π interaction can be ruled out.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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