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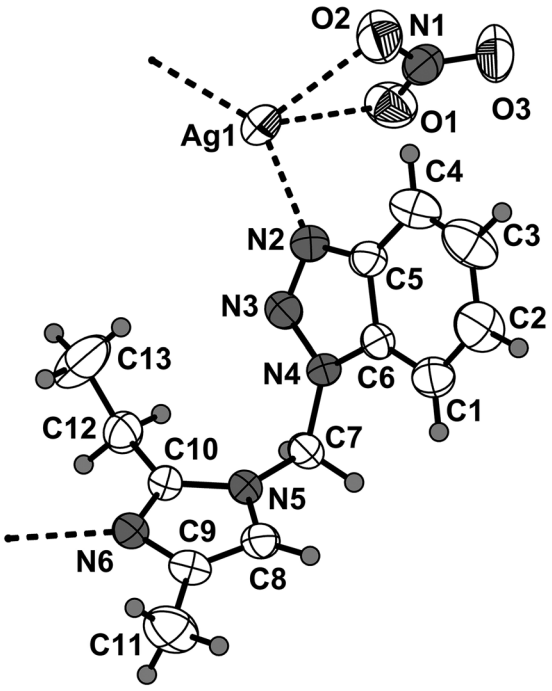
Crystal structure of *catena*-poly[(μ_2-1-((2-ethyl-4-methyl-1*H*-imidazol-1-yl)methyl)-1*H*-benzotriazole-κ^2N:N′)-(nitrato-κ^2O,O′)silver (I)], $C_{13}H_{15}Ag_1N_6O_3$



https://doi.org/10.1515/ncrs-2021-0316
Received August 4, 2021; accepted August 29, 2021; published online September 16, 2021

Abstract

$C_{13}H_{15}Ag_1N_6O_3$, monoclinic, $P2_1/c$ (no. 14), a = 9.0684(6) Å, b = 21.5490(10) Å, c = 9.1728(7) Å, β = 118.101(10)°, Z = 4, V = 1581.2(2) Å^3, $R_{gt}(F)$ = 0.0425, $wR_{ref}(F^2)$ = 0.0877, T = 293(2) K.

CCDC no.: 2106204

A part of the polymeric title 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.

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Table 1: Data collection and handling.

Crystal:	Colorless prism
Size:	0.14 × 0.12 × 0.10 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	1.30 mm^{-1}
Diffractometer, scan mode:	Xcalibur, ω
θ_{max}, completeness:	26.4°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	6782, 3229, 0.030
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2235
$N(param)_{refined}$:	210
Programs:	CrysAlis^{PRO} [1], SHELX [2], Diamond [3]

Source of material

All starting materials are commercially available and used without further purification. The 1-((2-ethyl-4-methyl-1*H*-imidazol-1-yl)methyl)-1*H*-benzotriazole (emimb) was prepared according to the literature method [4]. The ligand emimb (0.04 mmol, 0.0096 g) in methanol (6 mL) was added dropwise to an aqueous solution (6 mL) of $Ag(NO_3)_2$ (0.04 mmol, 0.0093 g). The resulting solution was allowed to stand at room temperature. After two weeks colorless crystals were obtained from the dried in air.

Experimental details

H atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

In recent years, the study of metal complexes has been mainly tractive because of their potential applications [5–8]. Imidazole derivatives play an important role in the synthesis of metal complexes since these compounds have special coordination abilities to different metal ions, such as silver [9], zinc [10] and copper [11]. Although a great deal of studies has been carried out on imidazole, only a little attention has been paid to

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.84632 (4)	0.18090 (2)	0.57332 (4)	0.06680 (17)
C1	0.3201 (5)	0.03459 (19)	0.5719 (5)	0.0515 (10)
H1	0.2108	0.0211	0.5076	0.062*
C2	0.4127 (5)	0.0177 (2)	0.7332 (5)	0.0683 (13)
H2	0.3658	−0.0091	0.7795	0.082*
C3	0.5760 (6)	0.0393 (2)	0.8321 (5)	0.0721 (14)
H3	0.6326	0.0271	0.9422	0.087*
C4	0.6541 (5)	0.0772 (2)	0.7726 (5)	0.0589 (12)
H4	0.7628	0.0910	0.8386	0.071*
C5	0.5629 (4)	0.09452 (17)	0.6066 (4)	0.0419 (9)
C6	0.3999 (4)	0.07325 (16)	0.5102 (4)	0.0383 (8)
C7	0.1992 (4)	0.09230 (17)	0.2038 (4)	0.0440 (10)
H7A	0.2238	0.0955	0.1120	0.053*
H7B	0.1514	0.0516	0.1992	0.053*
C8	−0.0584 (4)	0.12915 (18)	0.2122 (4)	0.0464 (10)
H8	−0.0813	0.0933	0.2542	0.056*
C9	−0.1509 (4)	0.18085 (18)	0.1657 (4)	0.0442 (10)
C10	0.0627 (4)	0.19748 (16)	0.1238 (4)	0.0380 (9)
C11	−0.3156 (5)	0.1947 (2)	0.1596 (6)	0.0734 (14)
H11A	−0.3997	0.1996	0.0466	0.110*
H11B	−0.3069	0.2323	0.2193	0.110*
H11C	−0.3459	0.1611	0.2089	0.110*
C12	0.1818 (5)	0.22721 (18)	0.0764 (5)	0.0508 (10)
H12A	0.1191	0.2454	−0.0326	0.061*
H12B	0.2541	0.1955	0.0694	0.061*
C13	0.2885 (6)	0.2767 (2)	0.1947 (7)	0.0923 (18)
H13A	0.3582	0.2953	0.1539	0.138*
H13B	0.3574	0.2585	0.3010	0.138*
H13C	0.2180	0.3079	0.2045	0.138*
N1	1.0328 (4)	0.06958 (17)	0.7405 (5)	0.0542 (9)
N2	0.6040 (4)	0.13066 (15)	0.5084 (4)	0.0533 (9)
N3	0.4783 (4)	0.13236 (15)	0.3589 (4)	0.0528 (9)
N4	0.3540 (3)	0.09815 (13)	0.3582 (3)	0.0404 (8)
N5	0.0776 (3)	0.13929 (13)	0.1859 (3)	0.0386 (7)
N6	−0.0740 (3)	0.22366 (14)	0.1120 (3)	0.0412 (8)
O1	0.9710 (4)	0.07624 (14)	0.5877 (4)	0.0709 (9)
O2	1.0432 (4)	0.11612 (14)	0.8237 (3)	0.0773 (10)
O3	1.0796 (4)	0.01895 (15)	0.8064 (4)	0.0891 (11)

compounds of benzotriazole systems containing an imidazole moiety.

X-ray crystallographic analysis reveals that the compound is a one-dimensional chain structure. As shown in the Figure, each Ag(I) ion is four coordinated by two nitrogen donors arising from two emimb ligands, and two oxygen atoms from one coordinated nitrate ion in a distorted tetrahedral coordination geometry (with the Ag1–N2 bond lengths of 2.263(3) Å, the Ag1–N6 bond lengths of 2.153(3) Å, and the Ag1–O1 bond lengths of 2.498(3) Å, the Ag1–O2 bond lengths of 2.559(3) Å.). The bond angles around Ag(I) ion range from 49.69(9) to 138.18(11)°. In each emimb ligand, the dihedral angle between benzotriazole and imidazole is 61.3°. The distance between two Ag ions bridged by the emimb ligand is 8.541 Å. In addition, the benzotriazole rings in adjacent chain are parallel, with an average interplanar distance of 3.728 Å. The geometric parameters are all in the expected ranges for coordinated benzotriazole ligands [12, 13].

Author contributions: The author has accepted responsibility for the entire content of this submitted manuscript and approved submission.

Research funding: None declared.

Conflict of interest statement: The author declares no conflicts of interest regarding this article.

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