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NOTE

Hydrothermal Synthesis and Crystal Structure of [4,4']Bipyridinyl Silver Nitrate Ion

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One new silver compound $Ag(NO_3)$, thiophene-2,5-dicarboxylic acid and [4,4']bipyridinyl (bpp) has been successfully synthesized. The compound has been characterized by X-ray single-crystal diffraction, compound shows a one-dimensional framework. The 3D supramolecular structure is formed *via* hydrogen bonding connection.

Keywords: Coordination polymer, Crystal structure, Silver.

Metal organic frameworks (MOFs) have received much attention in the field of crystal engineering and supramolecular chemistry because of their diverse structures and promising applications in functional materials such as luminescent materials, gas adsorption and magnetism. Hydrogen bonds are well suited for the design of polymeric arrangement and crystal engineering because of their important directional interactions and because they can interlink 1-D, or 3-D structures into higher-dimensionality systems.

All reagent and solvents employed were commercially available and used as received without further purification.

General procedure: A mixture of $AgNO_3$ (0.30 mmol), thiophene-2,5-dicarboxylic acid (0.15 mmol) and bpp ([4,4']bipyridinyl) (0.15 mmol) and distilled water (15 mL) was heated in a 25 mL stainless steel reactor with a Teflon liner 413 K for 48 h, followed by slow cooling to room temperature. Colourless crystals of the compound formed.

Diffraction intensity data of the single crystal of the five compounds were collected on a Bruker SMART APEXII CCD diffractometer equipped with a graphite monochromated MoK_α radiation (λ = 0.71073 Å) by using a ω-scan mode. All the structures were solved by direct methods and refined by full-matrix least-squares methods on F^2 using the program SHEXL 97[1]. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were located by geometrically calculations and their positions and thermal parameters were fixed during the structure refinement. The crystallographic data and experimental details of structural analyses for coordination polymers are summarized in Table-1. Selected bond and angle parameters are listed in Table-2. CCDC: 984017.

X-ray diffraction analysis revealed that the fundamental building unit consists of metal silver ion and bpp ([4,4']bipyridinyl) as bridging ligands to construct a new coordination polymer. It is well known that pyridines are important building blocks of many important compounds widely used in industry, medicine, agriculture and coordination chemistry[2,3]. The versatility of organic ligands has also been accepted as the major advantage of coordination polymers. Judicious selection/design of organic ligands is the key approach for desired structures and functions[4,5]. On the pyridine ring, the hydrogen atoms were assigned with Uiso(H) = 1.2 Ueq(C) and included in the final refinement by using geometrical restraints, with d(C---H) = 0.93 Å, In the molecular structure of the title compound (Fig. 1), one nitrogen atom N1 from bpp ligand. The Ag-N bond lengths are 2.162(4) Å. The N-O bonds within the nitrate ion are significant, The Ag-N bond lengths are 1.251(7) Å, 1.297(8) Å and 1.090(8) Å, respectively. The chains are further

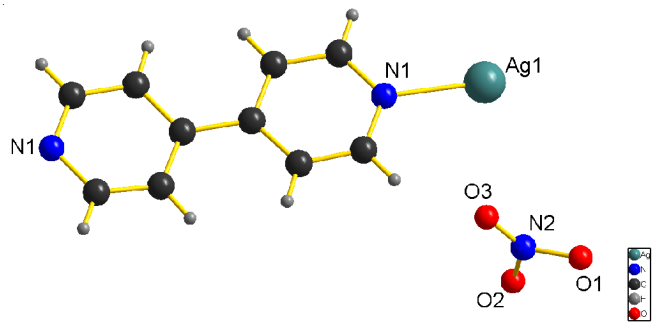

Fig. 1. Molecular structure of the title compound at 30 % probability displacement ellipsoids

TABLE-1
CRYSTALLOGRAPHIC DATA AND STRUCTURE REFINEMENT SUMMARY FOR SILVER COMPLEX

Empirical formula	$C_{10}H_8N_3O_3Ag$	Z, Calculated density (mg/m^3)	16, 1.945
Formula weight	326.06	Absorption coefficient (mm^{-1})	1.809
Crystal system space group	Orthorhombic, Fddd	F(000)	2560
Unit cell dimensions	a = 9.922(5) Å	Limiting indices	$-12 \le h \le 11$
	b = 12.987(7) Å		$-15 \le k \le 15$
	c = 34.569(20) Å		$-41 \le l \le 41$
Volume ($Å^3$)	4454(4)	Largest diff. peak and hole ($e/Å^3$)	0.672 and -1.165
θ range for data collection	2.65-25.49	Goodness-of-fit on F^2	1.056
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0377$; $wR_2 = 0.0945$	R indices (all data)	$R_1 = 0.0396$; $wR_2 = 0.0970$

TABLE-2
SELECTED BOND LENGTHS (Å) AND ANGLES (°) FOR SILVER COMPLEX

Ag(1)-N(1)	2.162(4)	N(2)-O(1)	1.251(7)
N(2)-O(3)	1.090(8)	N(2)-O(2)	1.297(8)
N(1)#1-Ag(1)-N(1)	173.8(2)	O(1)-N(2)-O(2)	108.1(5)
C(1)-N(1)-Ag(1)	121.6(3)	O(3)-N(2)-O(2)	122.6(6)
C(5)-N(1)-Ag(1)	120.8(3)	O(3)-N(2)-O(1)	129.2(7)

Symmetry codes: #1 –x + 5/4, y, -z + 1/4

assembled by the intermolecular hydrogen bonding interaction leading to the formation of a 3D framework (Fig. 2).

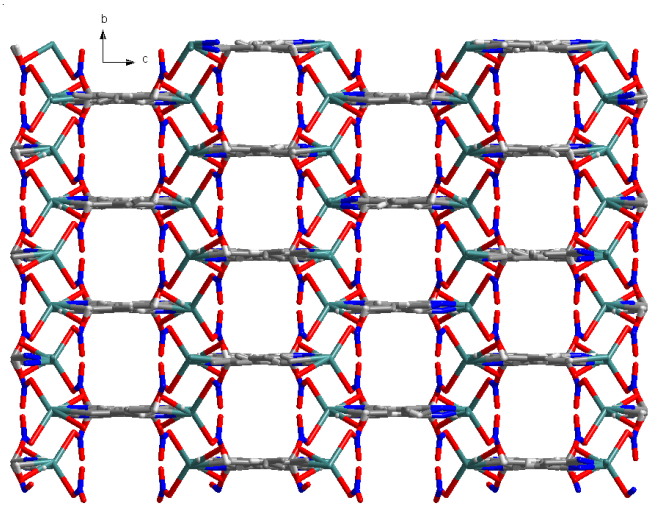

Fig. 2. 3D structure formed *via* hydrogen bonding interactions

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