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Chain structure of $\{[Ag(bpy)]NO_3\}_n$ (bpy = 4,4′-bipyridine)

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Crystallographic analysis shows that *catena*-poly[[silver(I)-μ-4,4′-bipyridine] nitrate], $\{[Ag(C_{10}H_8N_2)]NO_3\}_n$, is a new Ag–4,4′-bipyridine coordination polymer with a chain structure. A weak interaction between Ag and a nitrate O atom results in a two-dimensional supermolecular structure. X-ray diffraction shows the crystal to be orthorhombic, in space group *Pnma*. The nitrate ion and Ag atom lie in a mirror plane that relates the two bipyridine rings.

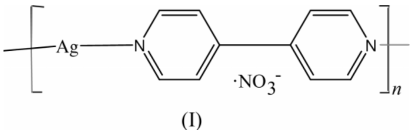
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.038
wR factor = 0.081
Data-to-parameter ratio = 11.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Recently, the design and syntheses of novel coordination polymers have attracted the attention of inorganic chemists. The reason is that these polymers possess not only intriguing structures, but some important functions, such as luminescent, electric and magnetic properties (Yaghi *et al.*, 1996). According to the theory of Hoskins (Hoskins & Robson, 1990) and Robson (Robson *et al.*, 1992), 4,4′-bipyridine is an excellent ditopic bridging ligand and can form 'scaffolding-like materials' using proper metal centers (Robinson & Zaworotko, 1995). It is well known that silver(I) has several coordination environments, especially linear and tetrahedral (Cotton & Wilkinson, 1988). To the best of our knowledge, several T-shaped (Yaghi *et al.*, 1996) and interpenetrating diamondoid (Carlucci *et al.*, 1994) frameworks have been studied and some linear (Blake *et al.*, 2000) and rectangular structures (Tong *et al.*, 2000) have also been reported.



(I)

In this paper, we report a new one-dimensional coordination polymer, $[Ag(bpy)(NO_3)]_n$, in which a weak interaction between Ag and a nitrate O atom results in a two-dimensional supermolecular structure. X-ray crystallography shows each silver(I) ion to be coordinated by the two N atoms of 4,4′-bipyridine, which leads to a linear structure, the Ag—N bond length being 2.211 (4) Å. The distances between Ag and the nitrate O atoms are Ag$\cdots$O1 = 2.794 (6), Ag$\cdots$O2 = 2.835 (6), Ag$\cdots$O2^{iii} = 2.787 (5) and Ag$\cdots$O3^{iii} = 2.747 (6) Å [symmetry code: (iii) $x-1/2$, y, $1/2-z$], which are typical of ionic interactions in metal nitrates (Lancashire, 1987). A terminal two-dimensional framework was obtained as a result of a weak interaction between the nitrate O atoms and all the line of silver(I) and 4,4′-bipyridine.

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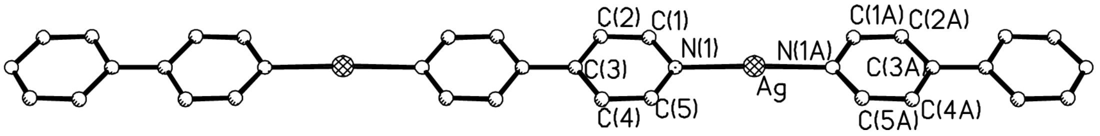

Figure 1
The coordination environment of the Ag^I atom in (I).

Experimental

4,4′-Bipyridine (0.031 g, 0.2 mmol) was dissolved in 10 ml of a mixture of DMSO (DMSO is dimethyl sulfoxide) and CH_2Cl_2 ($DMSO:CH_2Cl_2 = 1:1$), and the solution was placed in the bottom of a tube. A solution of $AgNO_3$ (0.034 g, 0.2 mmol) in 10 ml methanol was then carefully layered on top and the tube was kept in the dark. After about a week, colorless crystals were obtained in 68% yield.

Crystal data

$[Ag(C_{10}H_8N_2)]NO_3$
$M_r = 326.06$
Orthorhombic, *Pnma*
$a = 10.5315$ (16) Å
$b = 11.5313$ (17) Å
$c = 9.0821$ (13) Å
$V = 1102.9$ (3) $Å^3$
$Z = 8$
$D_x = 1.964$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 63 reflections
$\theta = 2.9–25.1°$
$\mu = 1.83$ mm^{-1}
$T = 293$ (2) K
Prism, colorless
0.40 × 0.16 × 0.10 mm

Data collection

Siemens SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.524$, $T_{max} = 0.835$
3206 measured reflections
1010 independent reflections
749 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 25.1°$
$h = -12 \rightarrow 11$
$k = -13 \rightarrow 7$
$l = -9 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.081$
$S = 1.18$
1010 reflections
85 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0257P)^2 + 1.3172P]$ $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.68$ e $Å^{-3}$
$\Delta\rho_{min} = -0.42$ e $Å^{-3}$

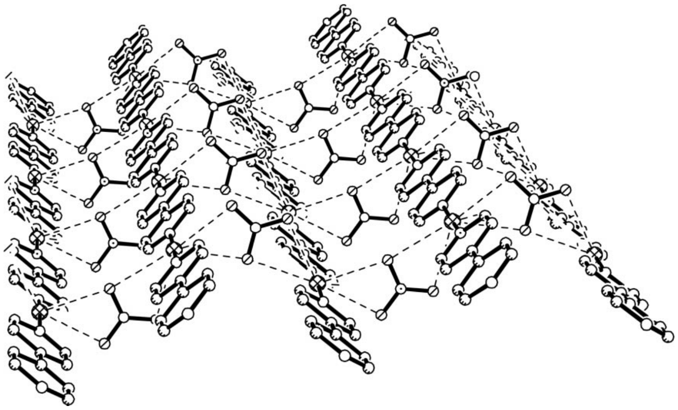

Figure 2
The two-dimensional packing structure of the title complex.

Table 1
Selected geometric parameters (Å, °).

Ag—N1	2.211 (4)	N2—O1	1.249 (8)
N1—C5	1.329 (6)	C2—C3	1.380 (7)
N1—C1	1.335 (6)	C3—C4	1.387 (7)
C1—C2	1.375 (7)	$C3—C3^i$	1.499 (8)
N2—O2	1.237 (8)	C4—C5	1.375 (7)
N2—O3	1.246 (8)		
$N1^{ii}—Ag—N1$	174.2 (2)	C2—C3—C4	116.6 (4)
C5—N1—C1	115.9 (4)	$C2—C3—C3^i$	122.0 (3)
O2—N2—O3	119.6 (8)	$C4—C3—C3^i$	121.4 (3)
O2—N2—O1	120.4 (7)	C5—C4—C3	119.4 (5)
O3—N2—O1	120.0 (7)	N1—C5—C4	124.3 (5)
C1—C2—C3	119.9 (5)		

Symmetry codes: (i) $x, \frac{1}{2} - y, z$; (ii) $x, \frac{3}{2} - y, z$.

The positions of all the H atoms were generated geometrically (C—H bond fixed at 0.96 Å), assigned isotropic displacement parameters, and allowed to ride on their respective parent C atoms before the final cycle of least-squares refinement.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1994); program(s) used to solve structure: *SHELXTL* (Siemens, 1994); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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