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Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.007\text{ \AA}$
 R factor = 0.044
 wR factor = 0.076
Data-to-parameter ratio = 17.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**catena-Poly[[silver(I)- μ -1,2-bis(4-pyridyl)ethane- $\kappa^2\text{N}:\text{N}'$] trifluoromethanesulfonate]**

The title compound, $\{[\text{Ag}(\text{bpe})](\text{OTf})\}_n$ (OTf = trifluoromethanesulfonate) or $\{[\text{Ag}(\text{C}_{12}\text{H}_{12}\text{N}_2)](\text{CF}_3\text{O}_3\text{S})\}_n$, has been prepared from the reaction of 1,2-bis(4-pyridyl)ethane (bpe) and $\text{Ag}(\text{CF}_3\text{SO}_3)$ in $\text{MeCN}/\text{H}_2\text{O}$. The Ag^{I} atom is two-coordinate in a slightly distorted linear arrangement, and the bpe ligands link the Ag^{I} atoms, in an *anti* fashion, into a one-dimensional linear chain of alternating Ag^{I} and bpe.

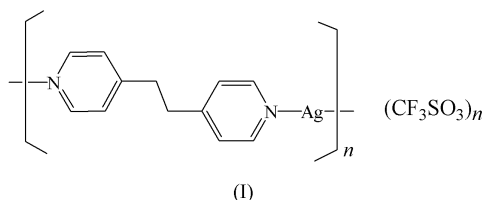
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Comment

The design and synthesis of supramolecular frameworks has made rapid progress in recent years owing to their intriguing structural diversities and their potential application as functional materials (Eddaoudi *et al.*, 2001; Hagrman *et al.*, 1999; Moulton & Zaworotko, 2001). Metal–pyridine coordination is an important tool in the construction of these frameworks. A number of pyridine-donor bis-monodentate ligands bearing rigid (Fujita *et al.*, 1995; MacGillivray *et al.*, 1994) or flexible (Carlucci *et al.*, 1997; Hennigar *et al.*, 1997) alkyl and aryl spacers have been extensively employed to develop supramolecular complexes with various structures and functions. 1,2-Bis(4-pyridyl)ethane (bpe) can adopt the *gauche* and *anti* conformations, which may lead to supramolecular isomerism in coordination polymers (Fu *et al.*, 2002; Hennigar *et al.*, 1997). Silver(I) is an extremely soft acid and has a good affinity for most coordinating atoms in a ligand. The self-assembly of silver(I) with organic ligands can give rise to a variety of supramolecular complexes, in which silver(I) exhibits labile coordination modes, such as linear, trigonal, tetrahedral, square-planar, pentagonal, square-pyramidal and even octahedral (LaDuca *et al.*, 2000*a*; Khlobystov *et al.*, 2001; Munakata *et al.*, 1997; Su *et al.*, 2002; Tong *et al.*, 2000). The combination of Ag^{I} and bpe ligands can result in some interesting structural topologies (LaDuca *et al.*, 2000*a*). Moreover, the assembly process may be influenced by the solvent system, the ratio of metal to ligand, and the presence of template and counter-ions. Sometimes, an alteration in any of these factors can result in new complexes with different structures and different functions. Here, we report a one-dimensional silver(I) compound $\{[\text{Ag}(\text{bpe})](\text{OTf})\}_n$ (OTf = trifluoromethanesulfonate), (I).



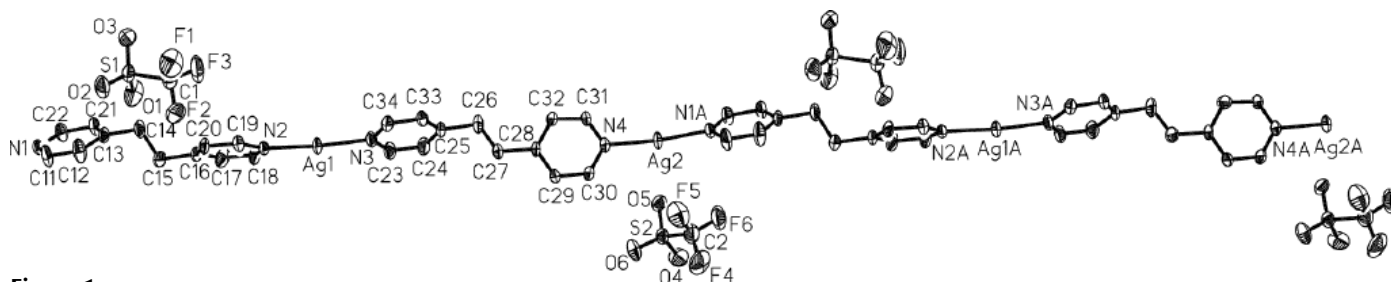


Figure 1

View of the structure of (I), with H atoms omitted for clarity. Displacement ellipsoids are drawn at the 30% probability level.

Single-crystal X-ray diffraction analysis of (I) reveals that the title compound crystallizes in monoclinic space group $P2_1/c$ and consists of slightly distorted linear $[Ag(bpe)]_n$ chains and counter anions OTf. As shown in Fig. 1, each Ag^I center is coordinated by two N atoms from different bpe ligands, in a slightly distorted linear fashion, to form a linear chain of alternating Ag^I and bpe. $Ag-N$ bond distances are in the range 2.149 (5) to 2.168 (5) Å, typical values for Ag^I-N_{py} coordination distances (LaDuca *et al.*, 2000b; Khlobystov *et al.*, 2001; Munakata *et al.*, 1997). The bond angles $N3-Ag1-N2$ and $N4-Ag2-N1A$ are 170.0 (2) and 161.8 (2)°, respectively, indicative of the presence of a distortion from linearity in the compound. Bpe acts as an *exo*-bidentate ligand in an *anti* conformation, linking two-coordinate Ag^I atoms into a one-dimensional linear chain. The dihedral angles between the two pyridyl rings are 37.8 and 62.8° in the bpe ligands. The short bond distances of C14–C15 [1.446 (6) Å] and C26–C27 [1.372 (6) Å] suggest conformational disorder in the bridging ethane groups of bpe. $Ag \cdots Ag$ separations across bpe are 13.605 and 13.619 Å. The closest $Ag \cdots Ag$ distance in adjacent chains is 3.55 Å, which is longer than the summed van der Waals radii of two silver atoms (3.44 Å). It is noteworthy that there are two types of distinctly different OTf, *i.e.* one acts only as a counter-anion while the other not only serves as a counter-anion but also acts as a bridge to link adjacent chains into a two-dimensional layer structure through weak $Ag \cdots O$ interactions (Fig. 2) [$Ag1 \cdots O4^i = 2.758$ (4) Å and $Ag2 \cdots O5 = 2.717$ (3) Å; symmetry code: (i) $-x, y + \frac{1}{2}, -z - \frac{1}{2}$].

Experimental

A solution of $Ag(CF_3SO_3)$ (0.13 g, 0.5 mmol) in H_2O (10 ml) was added slowly to a stirred solution of bpe (0.10 g, 0.50 mmol) in methanol (20 ml). The reaction mixture was stirred for 3 h at room temperature and gave a colorless solution which was filtered. Colorless crystals of the title compound were obtained by standing the resulting solution in air for one week.

Crystal data

$[Ag(C_{12}H_{12}N_2)](CF_3O_3S)$	$D_x = 1.878 \text{ Mg m}^{-3}$
$M_r = 441.18$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 5201 reflections
$a = 9.8575$ (15) Å	$\theta = 2.8\text{--}27.6^\circ$
$b = 15.195$ (2) Å	$\mu = 1.47 \text{ mm}^{-1}$
$c = 20.974$ (3) Å	$T = 293$ (2) K
$\beta = 96.654$ (4)°	Block, colorless
$V = 3120.4$ (8) Å ³	$0.46 \times 0.32 \times 0.25 \text{ mm}$
$Z = 8$	

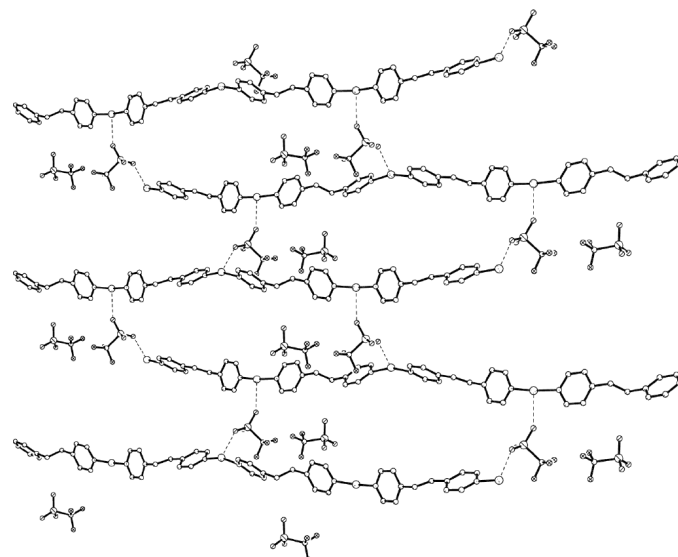


Figure 2

View of the two-dimensional layer, formed through weak $Ag \cdots O$ interactions, along the a axis.

Data collection

Siemens SMART CCD diffractometer	7176 independent reflections
ω scans	2940 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{int} = 0.067$
$T_{min} = 0.574, T_{max} = 0.692$	$\theta_{max} = 27.6^\circ$
21114 measured reflections	$h = -12 \rightarrow 12$
	$k = -18 \rightarrow 19$
	$l = -27 \rightarrow 18$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.044$	$w = 1/[\sigma^2(F_o^2) + (0.0132P)^2]$
$wR(F^2) = 0.076$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.95$	$(\Delta/\sigma)_{max} = 0.004$
7176 reflections	$\Delta\rho_{max} = 0.53 \text{ e \AA}^{-3}$
415 parameters	$\Delta\rho_{min} = -0.55 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Ag1–N3	2.143 (3)	Ag2–N1 ⁱⁱ	2.167 (4)
Ag1–N2	2.155 (3)	Ag2–O5	2.717 (3)
Ag1–O4 ⁱ	2.758 (4)		
Ag2–N4	2.166 (3)		
N3–Ag1–N2	170.27 (15)	N4–Ag2–O5	89.71 (13)
N3–Ag1–O4 ⁱ	97.37 (15)	N1 ⁱⁱ –Ag2–O5	101.90 (12)
N2–Ag1–O4 ⁱ	88.59 (14)		
N4–Ag2–N1 ⁱⁱ	161.97 (15)		

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

All H atoms were positioned geometrically (C–H bond fixed at 0.96 Å), assigned isotropic displacement parameters and allowed to ride on their respective parent C atoms.

Data collection: *SMART* (Siemens, 1994); cell refinement: *SMART*; data reduction: *SAINTE* (Siemens, 1994); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXL97*.

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