

## *catena*-Poly[[[ $\mu$ -pyrazine- $\kappa^2$ N:N'-disilver(I)]-di- $\mu$ -pyrazine- $\kappa^4$ N:N'] bis(trifluoromethanesulfonate) dihydrate]

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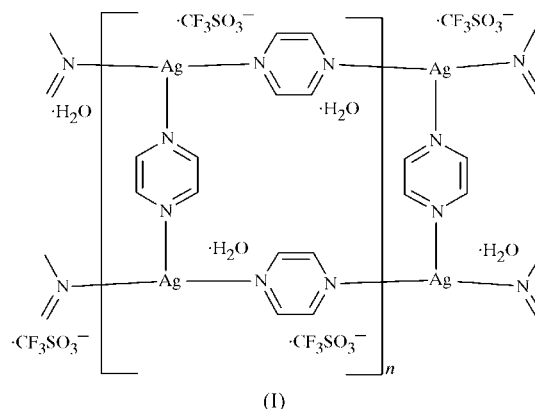
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The title compound,  $\{[\text{Ag}_2(\text{C}_4\text{H}_4\text{N}_2)_3](\text{CF}_3\text{SO}_3)_2 \cdot 2\text{H}_2\text{O}\}_n$ , is a polymeric pyrazine–silver(I) complex. Each  $\text{Ag}^{\text{I}}$  ion is three-coordinated by N atoms of three different pyrazine ligands, forming a T-shaped coordination configuration. In the crystal structure, uncoordinated water molecules are linked to trifluoromethanesulfonate anions through intermolecular  $\text{O} \cdots \text{H} \cdots \text{O}$  hydrogen bonds. There are weaker  $\text{Ag} \cdots \text{O}$  interactions involving the water and sulfonate O atoms.

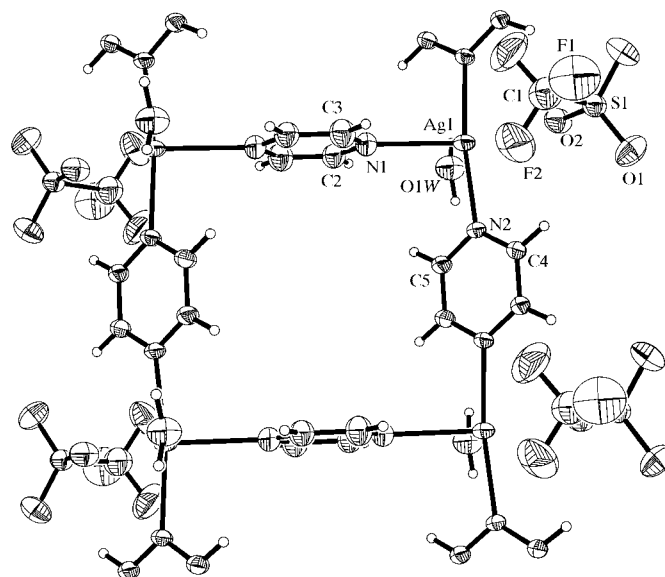
### Comment

Studying the variety of products in the self-assembly processes between labile metal ions and multidentate ligands is an interesting topic in supramolecular chemistry (Zheng *et al.*, 2003; You, Zhu & Liu, 2004; You, Yang *et al.*, 2004). The primary reason for the interest in such compounds is their ability to afford functional solid materials with potentially controllable properties and fascinating molecular structures. Recent developments in supramolecular chemistry have made it possible to select building units for assembly into structures with specific network topologies (Xu *et al.*, 2001). The construction of a wide variety of network topologies has been achieved through ligand design and the use of different transition metal coordination geometries. These include one-dimensional chains, which can be helical, two-dimensional sheets with a variety of connectivities and three-dimensional networks, such as the diamondoid or adamantoid structures (Khlobystov *et al.*, 2001). Crystal engineering of coordination polymeric networks based on multidentate ligands is a growing area of coordination and supramolecular chemistry. We have focused our attention on the assembly of metal ions with flexible ligands, since they can adopt diverse coordination modes according to the different geometric needs of the metal ions (Zhu *et al.*, 2003; Ren *et al.*, 2001). As reported previously, the bidentate ligand 1,2-diaminocyclohexane can give a two-

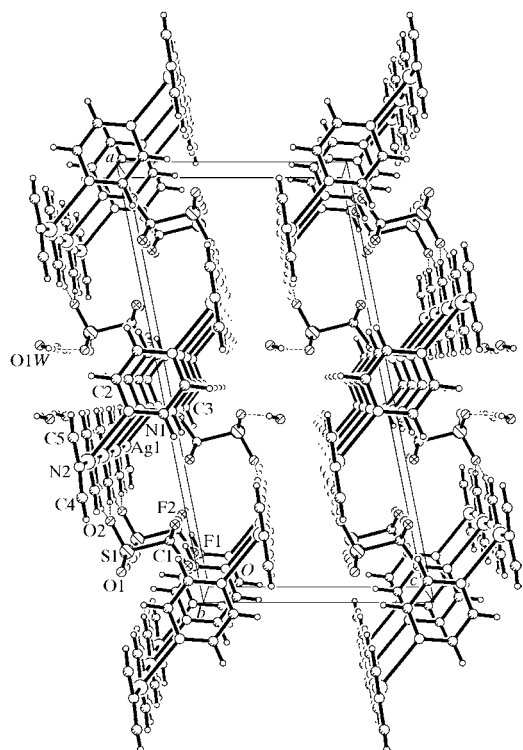
dimensional framework in complexes with metal ions and trifluoromethanesulfonate counter-anions (Usman *et al.*, 2003). We have now extended this work to use pyrazine instead of 1,2-diaminocyclohexane. Surprisingly, reaction of pyrazine with silver(I) trifluoromethanesulfonate gives a one-dimensional chain that is entirely different from that found in the complex formed by 1,2-diaminocyclohexane with silver(I) trifluoromethanesulfonate.



The title compound, (I), is a polymeric pyrazine– $\text{Ag}^{\text{I}}$  complex with an inversion center (Fig. 1). Atoms  $\text{Ag1}$ ,  $\text{N1}$ ,  $\text{C2}$ ,  $\text{C3}$ ,  $\text{Ag1}^{\text{iii}}$ ,  $\text{N1}^{\text{iii}}$ ,  $\text{C2}^{\text{iii}}$  and  $\text{C3}^{\text{iii}}$  lie on a mirror plane and there is a twofold axis through the middle of the  $\text{N1}$ -containing ring [symmetry code: (iii)  $1 - x, -y, 2 - z$ ]. The  $\text{N2}$ -containing ring lies across a mirror plane. Each  $\text{Ag}^{\text{I}}$  ion is three-coordinated by three N atoms of three different pyrazine ligands, forming a T-shaped coordination environment, the  $\text{N2} - \text{Ag1} - \text{N2}^{\text{i}}$  [symmetry code: (i)  $x, -y, z$ ] bond angle being  $171.44(17)^\circ$  (Table 1) and the other two bond angles related to atom  $\text{Ag1}$  being  $94.24(8)^\circ$ . The  $\text{Ag1} - \text{N1}$  bond length [ $2.500(6) \text{ \AA}$ ] is slightly longer than the  $\text{Ag1} - \text{N2}$  bond [ $2.244(4) \text{ \AA}$ ], the difference probably being caused by the



**Figure 1**  
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.



**Figure 2**  
The crystal packing of (I), viewed along the *b* axis. Broken lines show intermolecular hydrogen bonds.

presence of weak static forces related to the interactions of two O atoms with atom Ag1. Atom O2 of the trifluoromethanesulfonate anion and atom O1W of the uncoordinated water molecule are located, respectively, 2.641 (5) and 2.748 (5) Å from atom Ag1.

In the crystal structure, the pyrazine ligands bridge the Ag<sup>I</sup> ions, forming two parallel chains along the *b* axis. The dihedral angle between the two intersecting pyrazine rings is 90.0°. The two chains are then linked by the intersecting bridging pyrazine ligands, forming numerous tetragons with border lengths of 7.768 (2) and 7.250 (2) Å. The tetragons are combined along the *b* axis, forming a one-dimensional ladder-shaped chain. The uncoordinated water molecules and the trifluoromethanesulfonate anions are linked through intermolecular O—H...O hydrogen bonds and are located beside the one-dimensional cationic chains (Table 2 and Fig. 2). There are weaker Ag...O interactions involving the water and sulfonate O atoms.

## Experimental

Pyrazine (0.2 mmol, 16.0 mg) and silver(I) trifluoromethanesulfonate (0.2 mmol, 51.4 mg) were dissolved in a 30% ammonia solution (10 ml). The mixture was stirred at room temperature for 20 min and then filtered. After keeping the colorless filtrate in air for 12 d, colorless block-shaped crystals were formed at the bottom of the vessel on slow evaporation of three-quarters of the solvent. The crystals were isolated, washed three times with distilled water and dried in a vacuum desiccator using anhydrous CaCl<sub>2</sub> (yield 71.2%).

## Crystal data

[Ag<sub>2</sub>(C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>)<sub>3</sub>](CF<sub>3</sub>O<sub>3</sub>S)<sub>2</sub>·2H<sub>2</sub>O  
*M<sub>r</sub>* = 790.18  
 Monoclinic, *C*<sub>2</sub>/*m*  
*a* = 18.630 (4) Å  
*b* = 7.250 (3) Å  
*c* = 9.552 (2) Å  
 β = 101.17 (3)°  
*V* = 1265.7 (7) Å<sup>3</sup>  
*Z* = 2

*D<sub>x</sub>* = 2.073 Mg m<sup>-3</sup>  
 Mo Kα radiation  
 Cell parameters from 987 reflections  
 θ = 2.2–25.8°  
 μ = 1.81 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Block, colorless  
 0.35 × 0.28 × 0.21 mm

## Data collection

Bruker SMART CCD area-detector diffractometer  
 ω scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
*T<sub>min</sub>* = 0.570, *T<sub>max</sub>* = 0.703  
 2918 measured reflections

1393 independent reflections  
 1289 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.037  
 θ<sub>max</sub> = 26.5°  
*h* = -23 → 20  
*k* = -9 → 5  
*l* = -11 → 11

## Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.045  
*wR* (*F*<sup>2</sup>) = 0.113  
*S* = 1.11  
 1393 reflections  
 100 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0594P)^2 + 1.961P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 (Δ/σ)<sub>max</sub> < 0.001  
 Δρ<sub>max</sub> = 0.56 e Å<sup>-3</sup>  
 Δρ<sub>min</sub> = -1.13 e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Ag1—N2	2.244 (4)	Ag1—N1	2.500 (6)
N2 <sup>i</sup> —Ag1—N2	171.44 (17)	N2—Ag1—N1	94.24 (8)

Symmetry code: (i) *x*, -*y*, *z*.

**Table 2**

Hydrogen-bonding geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1W—H1WA...O1 <sup>ii</sup>	0.93	2.03	2.944 (6)	170

Symmetry code: (ii)  $\frac{1}{2} - x, \frac{1}{2} - y, 1 - z$ .

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.96 Å and O—H distances of 0.93 Å. The *U*<sub>iso</sub>(H) value for atom H1WA was fixed at 0.05 Å<sup>2</sup>, and for the remaining H atoms the values were fixed at 0.08 Å<sup>2</sup>.

Data collection: SMART (Bruker, 1998); cell refinement: SMART; data reduction: SAINT (Bruker, 1998); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: SQ1178). Services for accessing these data are described at the back of the journal.

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