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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(C-C) = 0.010$ Å
 R factor = 0.057
 wR factor = 0.122
Data-to-parameter ratio = 13.5

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

Bis(2-aminopyrimidine)silver(I) trifluoromethanesulfonate hemihydrate

In the title compound, $[\text{Ag}(\text{C}_4\text{H}_5\text{N}_3)_2](\text{CF}_3\text{O}_3\text{S})\cdot 0.5\text{H}_2\text{O}$, there are two similar mononuclear Ag^{I} complex cations in the asymmetric unit. Each of the Ag atoms is coordinated by two imine N atoms from two 2-aminopyrimidine ligands and is in a distorted linear geometry. Numerous weak interactions connect the complexes to form a three-dimensional structure.

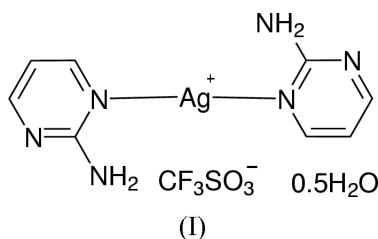
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Comment

The title complex, (I), crystallizes in the triclinic space group $P\bar{1}$ with $Z = 4$, and consists of a 2-aminopyrimidinesilver(I) cation, a trifluoromethylsulfonate anion and water of crystallization. The two crystallographically independent silver(I) complexes have similar structures. Each of the Ag atoms is in a linear configuration and is coordinated by two imine N atoms from different pyrimidine ligands. The average Ag–N bond lengths for Ag1 [2.135 (5) Å] and Ag2 [2.140 (5) Å] are in the normal range for silver(I) complexes with imines. The N–Ag–N angle is 173.68 (18)° for Ag1 and 177.83 (18)° for Ag2, indicating that these two central metal atoms have a similar slightly distorted linear coordination environment. The dihedral angles between the two aromatic rings linked by Ag1 and Ag2 are 16.70 (4) and 6.90 (4)°, respectively. There are a large number of hydrogen bonds (see Fig. 2). These weak interactions connect the complexes to form a three-dimensional network.



Experimental

$\text{CF}_3\text{SO}_3\text{Ag}$ and 2-aminopyrimidine (apd) from a commercial source were used without further purification. $\text{CF}_3\text{SO}_3\text{Ag}$ (0.5 mmol, 128 mg) and apd (1.0 mmol, 95 mg) were dissolved in acetonitrile (6 ml). The mixture was stirred for *ca* 5 min to give a clear solution. After keeping the resulting solution in air for 2 d, large colourless crystals were formed. The crystals were isolated, washed three times with acetonitrile and dried in a vacuum desiccator using anhydrous CaCl_2 (yield 90%). Elemental analysis found: C 23.58, H 2.50, N 18.35%; calculated for $\text{C}_9\text{H}_{11}\text{AgF}_3\text{N}_6\text{O}_{3.5}\text{S}$: C 23.70, H 2.43, N 18.42%.

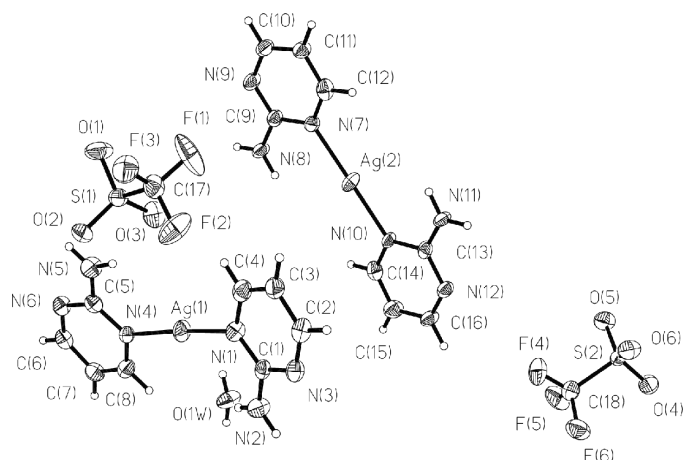


Figure 1
The structure of the asymmetric unit of the title compound, (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

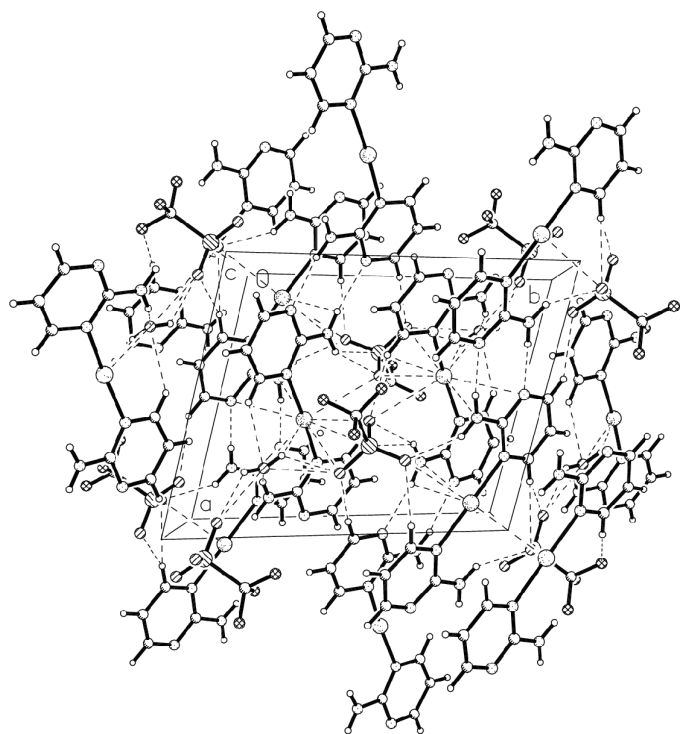


Figure 2
The crystal packing of (I), showing the hydrogen-bonding interactions and the weak interactions around Ag atoms as dashed lines.

Crystal data

[Ag(C₄H₅N₃)₂](CF₃O₃S)·0.5H₂O
M_r = 456.17
 Triclinic, *P* $\bar{1}$
a = 10.194 (2) Å
b = 13.112 (3) Å
c = 13.173 (3) Å
 α = 113.67 (3)°
 β = 105.12 (3)°
 γ = 96.20 (3)°
V = 1511.1 (6) Å³

Z = 4
D_x = 2.005 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 6425 reflections
 θ = 2.5–25.5°
 μ = 1.53 mm⁻¹
T = 293 (2) K
 Prism, colourless
 0.42 × 0.34 × 0.15 mm

Data collection

Siemens SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
*T*_{min} = 0.541, *T*_{max} = 0.795
 6831 measured reflections

5758 independent reflections
 4440 reflections with *I* > 2σ(*I*)
*R*_{int} = 0.025
 θ _{max} = 26.0°
h = −12 → 12
k = −16 → 16
l = −16 → 10

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.057
wR (*F*²) = 0.122
S = 1.04
 5758 reflections
 425 parameters

H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0538P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 2.12 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.62 \text{ e } \text{Å}^{-3}$

Table 1

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>
N2—H2B···N6 ⁱ	0.90	2.14	3.028 (7)	170
N2—H2C···O1W	0.90	2.19	2.999 (7)	149
N5—H5A···O3 ⁱⁱ	0.90	2.24	3.042 (6)	148
N5—H5B···N3 ⁱⁱⁱ	0.90	2.17	3.052 (7)	169
N8—H8B···O2	0.90	2.19	2.990 (6)	148
N8—H8C···N12 ⁱⁱⁱ	0.90	2.15	3.040 (6)	172
N11—H11B···O6 ^{iv}	0.90	2.18	3.002 (6)	151
N11—H11C···N9 ⁱ	0.90	2.10	3.003 (6)	178
O1W—H1WA···O4 ^v	0.71 (9)	2.17 (9)	2.817 (7)	151 (9)
O1W—H1WB···O1	0.88 (10)	1.96 (11)	2.839 (8)	173 (1)

Symmetry codes: (i) 1 + *x*, *y*, *z*; (ii) 1 − *x*, 1 − *y*, 1 − *z*; (iii) *x* − 1, *y*, *z*; (iv) 3 − *x*, 2 − *y*, 2 − *z*; (v) 3 − *x*, 1 − *y*, 2 − *z*.

The H atoms attached to O1W were located in Fourier maps and were refined isotropically. All the other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with N—H and C—H distances of 0.90 and 0.96 Å, respectively. The values for *U*_{iso}(H) were fixed at 0.08 Å². The highest peak is located at (0.4318, 0.3716, 0.8305).

Data collection: SMART (Siemens, 1996); cell refinement: SMART; data reduction: SAINT (Siemens, 1996); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Sheldrick, 1997); software used to prepare material for publication: SHELXTL.

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