

μ -2-Methylpyrazine- μ -trifluoroacetato-silver(I)Hai-Liang Zhu^a and
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Key indicators

Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.012$ Å
Disorder in main residue
 R factor = 0.055
 wR factor = 0.180
Data-to-parameter ratio = 12.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The 1/1 adduct of silver(I) trifluoroacetate and 2-methylpyrazine, $[\text{Ag}(\text{CF}_3\text{O}_2)(\text{C}_5\text{H}_6\text{N}_2)]_n$, adopts a layer structure in which the Ag atom is linked to two trifluoroacetate anions and two 2-methylpyrazine heterocycles. The two independent Ag atoms exist in tetrahedral environments.

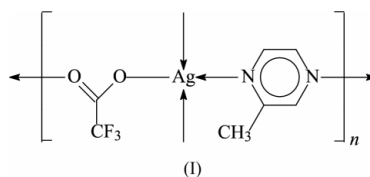
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Comment

Silver(I) trifluoroacetate affords a number of adducts with *N*-heterocycles; with some, such as chalcogenobis-3,3'-bipyridine (Kim *et al.*, 2002) and 4-aminopyridine (Zhu *et al.*, 2003), the trifluoroacetate unit engages in coordination, whereas in the phenanthroline complex, the anion does not participate as the silver atom is already chelated by two heterocycles (Paramonov *et al.*, 2003). The complexes of silver trifluoroacetate now include the 2-methylpyrazine complex, (I). The heterocyclic ligand uses both N donor sites to bind to Ag atoms, as does the carboxylate anion, so that the two independent Ag atoms are coordinated by four atoms in a tetrahedral environment. The μ_2 bridging modes of the heterocycle and anion lead to the formation of a three-dimensional network structure. For the adduct with 4-aminopyridine, the Ag atom is coordinated by two pyridyl N atoms but the trifluoroacetate anion is only unidentate to the Ag atom (Zhu *et al.*, 2003).



Experimental

The reagents were commercial products. Silver trifluoroacetate (1 mmol, 0.22 g) and 2-aminopyrazine (1 mmol, 94 mg) were dissolved in dilute aqueous ammonia (10 ml); stirring the mixture briefly gave a clear solution. The solution was set aside for a day to allow the ammonia gas to escape. Large colorless crystals separated from the solution; these were collected and washed three times with water. The compound was isolated in about 80% yield.

Crystal data

$[\text{Ag}(\text{CF}_3\text{O}_2)(\text{C}_5\text{H}_6\text{N}_2)]$
 $M_r = 315.01$
Monoclinic, $P2_1/n$
 $a = 12.479$ (2) Å
 $b = 12.611$ (2) Å
 $c = 12.597$ (2) Å
 $\beta = 95.963$ (2)°
 $V = 1971.7$ (5) Å³
 $Z = 8$

$D_x = 2.122$ Mg m⁻³
Mo $K\alpha$ radiation
Cell parameters from 2633 reflections
 $\theta = 2.3$ – 24.2 °
 $\mu = 2.07$ mm⁻¹
 $T = 298$ (2) K
Block, colorless
0.21 × 0.15 × 0.15 mm

Data collection

Bruker SMART APEX area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2002)
 $T_{\min} = 0.398$, $T_{\max} = 0.732$
 10949 measured reflections

4234 independent reflections
 3041 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.041$
 $\theta_{\text{max}} = 27.1^\circ$
 $h = -15 \rightarrow 13$
 $k = -13 \rightarrow 16$
 $l = -11 \rightarrow 15$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.055$
 $wR(F^2) = 0.180$
 $S = 1.07$
 4234 reflections
 330 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0899P)^2 + 2.7689P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 1.50 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.71 \text{ e } \text{\AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

Ag1—N1	2.283 (6)	Ag2—N3	2.278 (6)
Ag1—N2 ⁱ	2.318 (6)	Ag2—N4 ⁱⁱ	2.288 (6)
Ag1—O1	2.387 (7)	Ag2—O2 ⁱⁱⁱ	2.392 (7)
Ag1—O4	2.407 (6)	Ag2—O3	2.398 (6)
N1—Ag1—N2 ⁱ	120.6 (3)	N3—Ag2—N4 ⁱⁱ	120.9 (2)
N1—Ag1—O1	121.1 (2)	N3—Ag2—O2 ⁱⁱⁱ	104.5 (3)
N1—Ag1—O4	111.5 (2)	N3—Ag2—O3	120.3 (2)
N2 ⁱ —Ag1—O1	107.3 (3)	N4 ⁱⁱ —Ag2—O2 ⁱⁱⁱ	106.7 (2)
N2 ⁱ —Ag1—O4	99.2 (2)	N4 ⁱⁱ —Ag2—O3	107.6 (2)
O1—Ag1—O4	90.9 (2)	O2 ⁱⁱⁱ —Ag2—O3	91.6 (2)

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

The structure is twinned, and it was refined with the twin matrix (001,0 $\bar{1}$ 0,100) to give a second twin component of 0.181 (3). The two trifluoromethyl groups are disordered; the occupancies were refined. The C—F bond lengths were restrained to 1.33 (1) \AA and the F...F distances to 2.17 (2) \AA ; the displacement parameters of the disordered F atoms were restrained to be approximately isotropic. The occupancy of the major F1, F2 and F3 set refined to 0.76 (3) and that of the major F4, F5 and F6 set to 0.56 (3).

H atoms were positioned geometrically (C—H 0.93 \AA for the aromatic H atoms and C—H 0.96 \AA for the methyl H atoms; N—H 0.86 \AA), and were refined as riding, with $U(\text{H}) = 1.2U_{\text{eq}}(\text{C}_{\text{aromatic}}, \text{N})$ or $1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$.

The final difference Fourier map had large peaks at about 1 \AA from both Ag atoms.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve

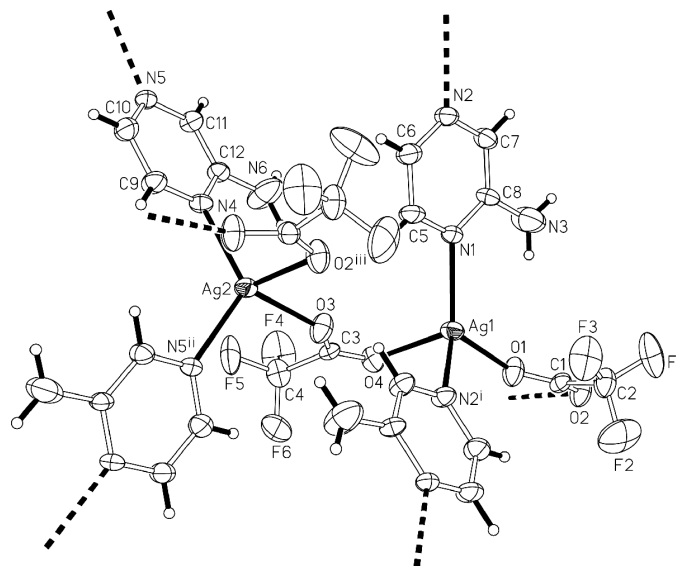


Figure 1 ORTEP (Johnson, 1976) plot of a portion of the layer structure of (I), with displacement ellipsoids drawn at the 30% probability level. H atoms are shown as spheres of arbitrary radii. Symmetry codes as in Table 1.

structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPII (Johnson, 1976); software used to prepare material for publication: SHELXL97.

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