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Poly[silver(I)-μ_2-2-methylpyrazine-μ_2-trifluoroacetato], a reinvestigation

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.040
wR factor = 0.096
Data-to-parameter ratio = 12.8

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

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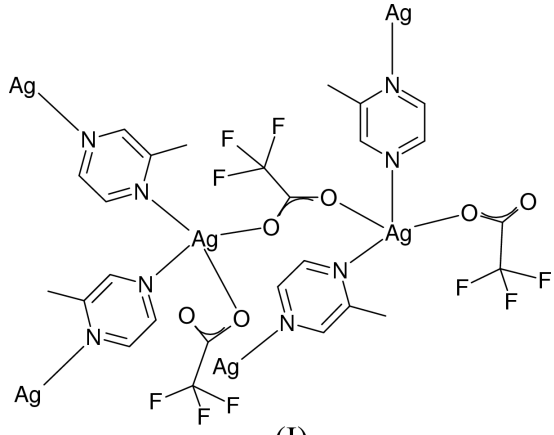
This work is a reinvestigation of a previously reported structure [Zhu & Ng (2004). *Acta Cryst.* E**60**, m939–m940], where the crystal measured was twinned. The title compound, $[Ag(C_2F_3O_2)(C_5H_6N_2)]_n$, is a polymeric silver(I) complex. Each Ag^I atom is in a tetrahedral configuration and is four-coordinated by two O atoms of two 3-fluoroacetate anions and two N atoms of two 2-methylpyrazine ligands. The 3-fluoroacetate anion and the 2-methylpyrazine ligand both act as bidentate bridging ligands and coordinate to the Ag^I atoms through the carboxylate O atoms and the pyridine N atoms, respectively, forming a three-dimensional network.

Comment

This work is a reinvestigation of the structure of the title complex (Zhu & Ng, 2004) in which the crystal measured was twinned. We report here results from an untwinned crystal.



(I)

The title compound, (I), is a polymeric silver(I) complex (Fig. 1). Each Ag^I atom is four-coordinated by two O atoms of two 3-fluoroacetate anions and two N atoms of two 2-methylpyrazine ligands. This AgO_2N_2 framework forms a distorted tetrahedral configuration, with angles subtended at atom Ag1 in the range 90.90 (10)–120.81 (11)°, and angles subtended at atom Ag2 in the range 91.47 (10)–121.10 (11)°. The 3-fluoroacetate anion and the 2-methylpyrazine ligand both act as bidentate bridging ligands and coordinate to the Ag^I atoms through the carboxylate O atoms and the pyridine N atoms, respectively, forming a three-dimensional network (Fig. 2). All the Ag—O and Ag—N bond lengths are comparable to the values observed in another silver(I) complex (Zhu *et al.*, 2003). All the other bond lengths in the complex are within normal ranges (Allen *et al.*, 1987).

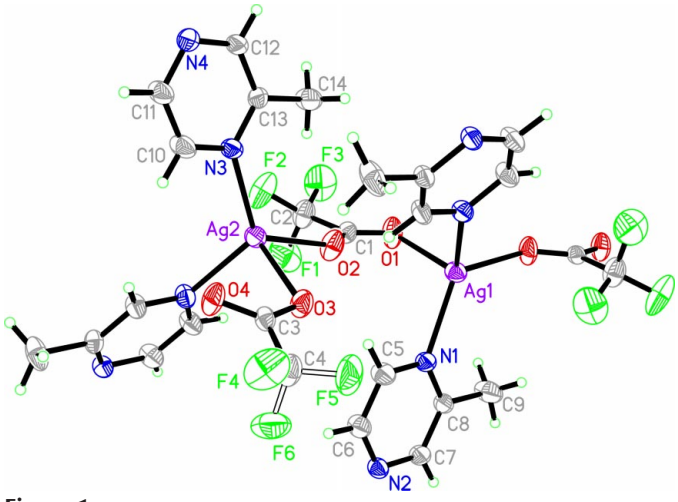


Figure 1
Part of the polymeric structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Only half of the disordered F atoms are shown.

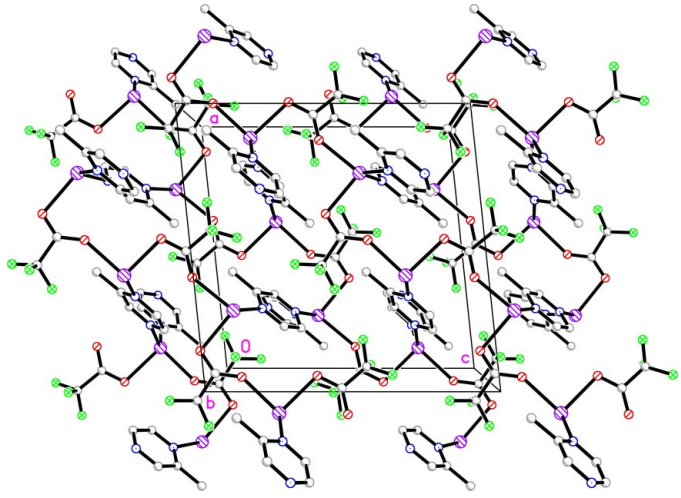


Figure 2
The crystal packing of (I), viewed along the *b* axis. H atoms have been omitted

Experimental

Silver 3-fluoroacetate (0.1 mmol, 21.8 mg) and 2-methylpyrazine (0.1 mmol, 9.4 mg) were dissolved in an aqueous ammonia solution (10 ml, 30%). The mixture was stirred for about 10 min at room temperature to obtain a clear colorless solution. The resulting solution was kept in the dark and, after slow evaporation of the solvent over a period of 3 d, crystals of (I) were isolated, washed three times with water and dried in a vacuum desiccator using anhydrous $CaCl_2$ (yield 59%). Analysis calculated: C 26.7, H 1.9, N 8.9%; found: C 26.6, H 1.9, N 8.8%.

Crystal data

$[Ag(C_2F_3N_2)(C_5H_6N_2)]$
M_r = 315.01
Monoclinic, $P2_1/n$
a = 12.452 (2) Å
b = 12.619 (2) Å
c = 12.654 (2) Å
β = 96.002 (1)°
V = 1977.5 (5) Å^3
Z = 8
D_x = 2.116 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3292 reflections
θ = 2.3–27.4°
μ = 2.06 mm^{-1}
T = 293 (2) K
Block, colorless
0.28 × 0.21 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.596, T_{max} = 0.790
9751 measured reflections
4191 independent reflections
3127 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 27.0°
$h = -15 \rightarrow 11$
$k = -14 \rightarrow 16$
$l = -16 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.096
S = 1.01
4191 reflections
327 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0429P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.314
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}

The F atoms of each trifluoroacetate anion were disordered over two distinct sites. For the F atoms attached to atom C2, the occupancies of the disordered positions F1 and F1′, F2 and F2′, and F3 and F3′ were 0.52 (2) and 0.48 (2), respectively. For the F atoms attached to C4, the occupancies of the disordered positions F4 and F4′, F5 and F5′, and F6 and F6′ were 0.53 (2) and 0.47 (2), respectively. All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances of 0.93–0.96 Å, and with U_{iso}(H) = 1.2 or 1.5U_{eq}(C).

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

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