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Key indicators

Single-crystal X-ray study
 T = 200 K
 Mean $\sigma(\text{C}-\text{C}) = 0.011 \text{ \AA}$
 R factor = 0.045
 wR factor = 0.117
 Data-to-parameter ratio = 12.1

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

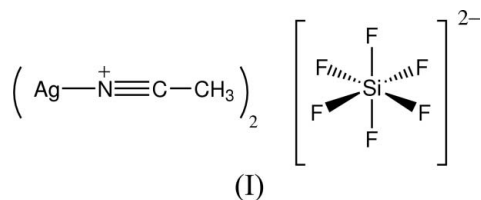
Bis[acetonitrilesilver(I)] hexafluorosilicate

In the title compound, poly[μ_4 -hexafluorosilicato-bis[acetonitrilesilver(I)]], $[\text{Ag}_2(\text{SiF}_6)(\text{CH}_3\text{CN})_2]_n$, the Ag atom is bonded to acetonitrile and four F atoms of three different SiF_6^{2-} ions. The cations are linked *via* the SiF_6^{2-} counter-ion by secondary $\text{Ag} \cdots \text{F}$ interactions, leading to a five-coordinated Ag atom.

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Comment

Silver cations coordinated by acetonitrile and a hexafluoro anion, *e.g.* $[\text{Ag}(\text{NCCH}_3)_2][\text{WF}_6]$, are described in the literature, but no structural investigation has been carried out so far (Prescott *et al.* 1973, 1975; Iqbal *et al.*, 1989). As part of our present research, the title compound, $[\text{Ag}(\text{NCCH}_3)_2]\text{SiF}_6$, (I), was obtained unintentionally.



The formation of hexafluorosilicate resulted from the reaction of SeF_4 with glass in the presence of silver cations and did not yield the desired selenium-containing material. According to the Cambridge Structural Database (Version 5.27, November 2005; Allen, 2002) and the Inorganic Crystal Structure Database (Release 2006-1, June 2006; ICSD, 2006), the only known X-ray crystal structure involving acetonitrile coordinated to Ag is $[\text{Ag}(\text{NCCH}_3)][\text{N}(\text{NO}_2)_2]$ (Ang *et al.* 2002). In $[\text{Ag}(\text{NCCH}_3)][\text{N}(\text{NO}_2)_2]$, which exists in the solid state as $[\text{Ag}(\text{NCCH}_3)]_4[\text{Ag}_3\{\text{N}(\text{NO}_2)_2\}_4]$, the $[\text{Ag}(\text{NCCH}_3)]_4^+$ cation contains an Ag atom tetrahedrally bonded to four acetonitrile molecules. In salt (I), the Ag atom is bonded to one acetonitrile molecule and coordinated by four F atoms of hexafluorosilicate anions. The Ag–N distance [2.178 (5) Å] is shorter than that in $[\text{Ag}(\text{NCCH}_3)]_4^+$ [2.259 (3) Å] and the distances within the acetonitrile molecule are normal [N1–C1 = 1.119 (9), C1–C2 = 1.445 (11) Å] and comparable to the distances in the tetrahedrally coordinated cation [1.123 (4), 1.449 (4) Å]. The $\text{Ag} \cdots \text{F}$ contacts are in the range 2.402 (3)–2.706 (3) Å and significantly shorter than the sum of the silver–fluorine van der Waals radii (3.19 Å; Bondi, 1964). These contacts lead to a slightly distorted square-pyramidal coordination around the Ag atom with contacts $\text{Ag} \cdots \text{F1}$ and $\text{Ag} \cdots \text{F2}$ and their symmetry equivalents but no contacts $\text{Ag} \cdots \text{F3}$.

Experimental

A suspension of AgF (1.77 mmol) in CH₃CN (6 ml) was stirred for 1 h with SeF₄ (1.77 mmol) in a glass vessel at ambient temperature. After addition of [Ph₄P]Cl (1.77 mmol) a grey precipitate was obtained and separated. The remaining solution was stored for 2 d at 277 K to form colourless crystals of (I). The crystals decompose upon contact with air at room temperature when taken out of solution. Thus, the crystal was mounted on the goniometer head under an inert atmosphere at 253 K and immediately transferred into the cold stream of the diffractometer. The presence of Si in the structure results from the reaction of SeF₄ with glass.

Crystal data

[Ag ₂ (SiF ₆)(C ₂ H ₃ N) ₂]	Z = 2
<i>M_r</i> = 439.94	<i>D_x</i> = 2.863 (1) Mg m ⁻³
Monoclinic, <i>P</i> 2 ₁ / <i>c</i>	Mo <i>K</i> α radiation
<i>a</i> = 8.8952 (14) Å	<i>μ</i> = 4.01 mm ⁻¹
<i>b</i> = 5.6792 (9) Å	<i>T</i> = 200 (2) K
<i>c</i> = 10.1049 (18) Å	Block, colourless
<i>β</i> = 91.378 (14)°	0.19 × 0.15 × 0.08 mm
<i>V</i> = 510.33 (15) Å ³	

Data collection

Oxford Xcalibur3 CCD area-detector diffractometer	4849 measured reflections
<i>ω</i> scans	991 independent reflections
Absorption correction: multi-scan (ABSPACK; Oxford Diffraction, 2005)	919 reflections with <i>I</i> > 2σ(<i>I</i>)
<i>T</i> _{min} = 0.458, <i>T</i> _{max} = 0.723	<i>R</i> _{int} = 0.099
	<i>θ</i> _{max} = 26.0°

Refinement

Refinement on <i>F</i> ²	All H-atom parameters refined
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)] = 0.045	<i>w</i> = 1/[σ ² (<i>F</i> _o ²) + (0.0776 <i>P</i>) ²]
<i>wR</i> (<i>F</i> ²) = 0.117	where <i>P</i> = (<i>F</i> _o ² + 2 <i>F</i> _c ²)/3
<i>S</i> = 1.12	(Δ/ <i>σ</i>) _{max} = 0.024
991 reflections	Δ <i>ρ</i> _{max} = 1.83 e Å ⁻³
82 parameters	Δ <i>ρ</i> _{min} = -1.23 e Å ⁻³

The highest peak and deepest hole in the final difference map were located 1.05 and 0.83 Å, respectively, from atom Ag1.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2005); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2005); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1996); software used to prepare material for publication: *SHELXL97*.

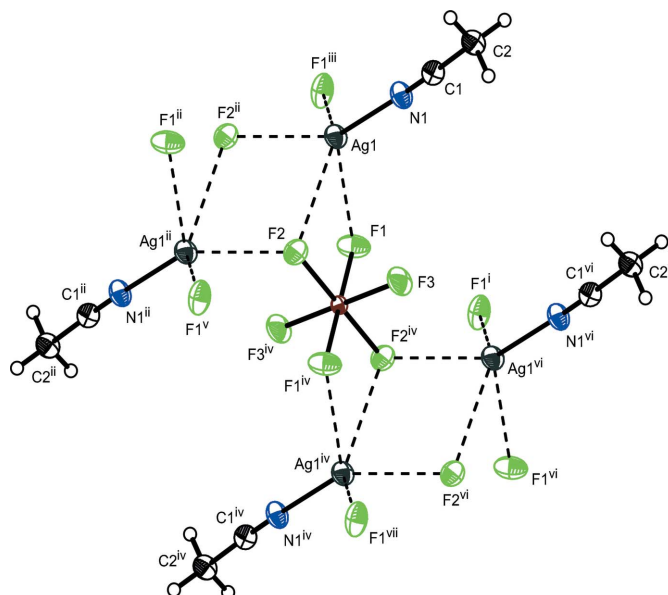


Figure 1

Part of the polymeric structure of [Ag(NCCH₃)₂SiF₆] generated by Ag...F interactions, with displacement ellipsoids drawn at the 50% probability level. [Symmetry codes: (i) 1 - *x*, ½ + *y*, ¾ - *z*; (ii) 1 - *x*, -1 - *y*, 2 - *z*; (iii) 1 - *x*, *y* - ½, ¾ - *z*; (iv) 1 - *x*, -*y*, 2 - *z*; (v) *x*, -½ - *y*, ½ + *z*; (vi) *x*, 1 + *y*, *z*; (vii) *x*, ½ - *y*, ½ + *z*.]

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