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Key indicators

Single-crystal X-ray study
 $T = 150$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.025
 wR factor = 0.047
Data-to-parameter ratio = 13.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**catena-Poly[[bis(μ_4 -hexafluoroglutarato)-
bis(tetrahydrofuran)tetrasilver(I)]- μ_2 -4,4'-
biphenyldicarbonitrile]**

The title complex, $[\text{Ag}_4(\text{C}_5\text{F}_6\text{O}_4)_2(\text{C}_{14}\text{H}_8\text{N}_2)(\text{C}_4\text{H}_8\text{O})_2]_n$, exhibits a one-dimensional chain structure propagated through inversion centres, with two crystallographically independent Ag^{I} atoms in the asymmetric unit. One of the Ag atoms has a distorted trigonal-pyramidal coordination, defined by two carboxyl O atoms from two hexafluoroglutarate (HFG^{2-}) anions, one N atom from 4,4'-biphenyldicarbonitrile and one apical O atom of tetrahydrofuran. The other Ag atom is coordinated by two O atoms from two HFG^{2-} anions.

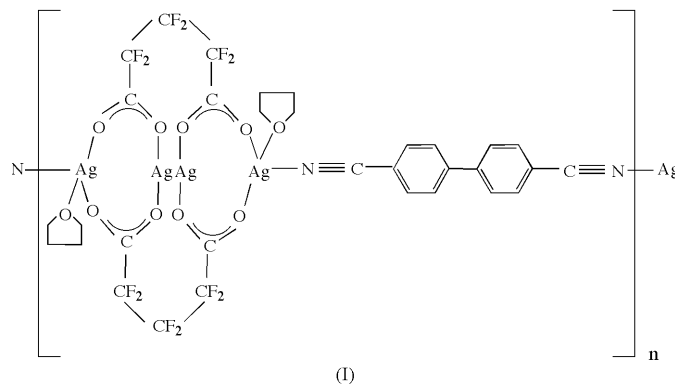
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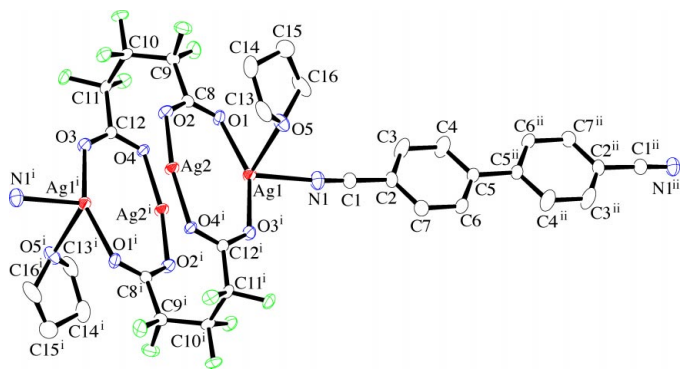
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Comment

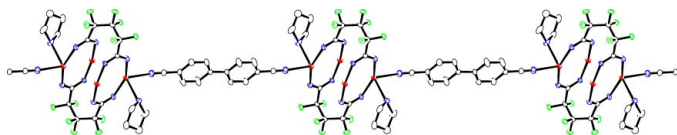
In recent years, significant research effort has been focused on coordination polymers, because of their potential application in catalysis, ion exchange and gas separation (Eddaoudi *et al.*, 2002; Moulton & Zaworotko, 2001). Popular bridging ligands in this field are the bidentate 4,4'-bipyridine and its derivatives (Eddaoudi *et al.*, 2001). Numerous complexes with these ligands have been extensively investigated, while new complexes are constantly being synthesized. Other bidentate ligands, such as 4,4'-biphenyldicarbonitrile (BPCN), however, have received much less attention (Hirsch *et al.*, 1995). We selected BPCN as ligand to react with the silver salt of the dicarboxylate HFG^{2-} (hexafluoroglutarate), generated *in situ*, and isolated a new Ag^{I} complex, $[\text{Ag}_4(\text{BPCN})(\text{THF})_2(\text{HFG})_2]$, (I). Its crystal structure is reported here.



In complex (I), there are two independent Ag^{I} atoms. Atom $\text{Ag}1$ is four-coordinate and adopts a distorted trigonal-pyramidal geometry (Fig. 1), involving one N atom of BPCN, two O atoms from two HFG^{2-} anions and one apical O atom of THF. The coordination geometry of atom $\text{Ag}2$ is approximately linear but slightly distorted, with an $\text{O}2-\text{Ag}2-\text{O}4^{\text{I}}$ [symmetry code: (i) $-x, 1-y, 1-z$] bond angle of $167.13(6)^\circ$, involving two O atoms from two HFG^{2-} anions. Two HFG^{2-} anions are linked through $\text{O}-\text{Ag}-\text{O}$ bonds to


Figure 1

Part of the structure of (I), with the atom-numbering scheme, showing displacement ellipsoids at the 50% probability level. All H atoms and the F-atom numbers have been omitted for clarity. [Symmetry codes: (i) $-x, 1 - y, 1 - z$; (ii) $2 - x, -y, 1 - z$.]


Figure 2

One-dimensional chain structure of (I) along the $[1\bar{1}0]$ direction. All H atoms have been omitted for clarity.

form a ring with composition $\text{Ag}_4(\text{HFG})_2$, and BPCN molecules act as bridging ligands to link these rings to afford a one-dimensional chain with THF molecules as terminal ligands (Fig. 2). The distance between atoms Ag1 and Ag2 [2.9852 (6) Å] is shorter than the sum of the van der Waals radii of two Ag atoms (3.44 Å), indicating the existence of $\text{Ag} \cdots \text{Ag}$ interactions.

The Ag–N bond length in (I) [2.385 (2) Å] is longer than those in trifluoromethanesulfonatesilver(I)- μ_2 -4,4'-biphenyldicarbonitrile [2.133 (3) and 2.138 (3) Å; Hirsch *et al.*, 1995], difluorophosphatesilver(I)- μ_2 -4,4'-dicyanodiphenylacetylene [2.186 (3) Å; Hirsch *et al.*, 1996] and silver(I)- μ_2 -1,4-dicyanobenzene [2.211 (2) and 2.284 (2) Å; Venkataraman *et al.*, 1996], while the Ag–O bond lengths in (I) [2.141 (2)–2.284 (2) Å] are shorter because the coordination ability of dicarboxylate anions is stronger than that of monoanions, resulting in the weaker Ag–N bond interactions. The Ag1–O5 bond [2.516 (2) Å] is substantially longer than the others. The O1–Ag1–O3ⁱ bond angle [153.64 (6)°] is larger than the other two about atom Ag1 in the basal plane, *viz.* O1–Ag1–N1 [105.78 (7)°] and O3ⁱ–Ag1–N1 [100.23 (7)°], apparently as a result of the $\text{Ag} \cdots \text{Ag}$ interactions. The HFG^{2-} anion adopts a *cis* configuration and coordinates to four Ag atoms belonging to one repeat unit.

Experimental

Hexafluoroglutaric acid (0.4 mmol, 96.0 mg) and silver(I) trifluoroacetate (0.1 mmol, 22.1 mg) were dissolved in THF with stirring for 20 min, then 4,4'-biphenyldicarbonitrile (0.025 mmol, 5.1 mg) was added to the above solution. The mixture was stirred for another 20 min. The resulting solution was introduced into a glass tube and

layered with tetradecane. The glass tube was sealed under argon. After standing at room temperature for 6 d, colourless needle-shaped crystals of (I) were isolated (yield 63%). Analysis calculated for $\text{C}_{32}\text{H}_{24}\text{Ag}_4\text{F}_{12}\text{N}_2\text{O}_{10}$: C 30.60, H 1.93, N 2.23%; found: C 30.36, H 1.91, N 2.18%.

Crystal data

$[\text{Ag}_4(\text{C}_5\text{F}_6\text{O}_4)_2(\text{C}_{14}\text{H}_8\text{N}_2)(\text{C}_4\text{H}_8\text{O})_2]$
 $M_r = 1256.00$
 Monoclinic, $P2_1/c$
 $a = 5.737$ (2) Å
 $b = 18.801$ (6) Å
 $c = 16.518$ (6) Å
 $\beta = 93.368$ (4)°
 $V = 1778.6$ (11) Å³
 $Z = 2$

$D_x = 2.345$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 5730 reflections
 $\theta = 3.2$ – 27.5°
 $\mu = 2.29$ mm⁻¹
 $T = 150.2$ K
 Needle, colourless
 $0.25 \times 0.15 \times 0.10$ mm

Data collection

Rigaku/MSC Mercury CCD diffractometer
 ω scans
 Absorption correction: multi-scan (Jacobson, 1998)
 $T_{\min} = 0.659$, $T_{\max} = 0.795$
 13 771 measured reflections

4068 independent reflections
 3744 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$
 $\theta_{\max} = 27.5^\circ$
 $h = -5 \rightarrow 7$
 $k = -18 \rightarrow 24$
 $l = -21 \rightarrow 21$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.025$
 $wR(F^2) = 0.047$
 $S = 1.11$
 3744 reflections
 271 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0156P)^2 + 1.6769P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 0.40$ e Å⁻³
 $\Delta\rho_{\min} = -0.41$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Ag1–O1	2.284 (2)	O1–C8	1.240 (3)
Ag1–O3 ⁱ	2.257 (2)	O2–C8	1.245 (3)
Ag1–O5	2.516 (2)	O3–C12	1.224 (3)
Ag1–N1	2.385 (2)	O4–C12	1.268 (3)
Ag2–O2	2.141 (2)	N1–C1	1.122 (3)
Ag2–O4 ⁱ	2.173 (2)		
O1–Ag1–O3 ⁱ	153.64 (6)	O3 ⁱ –Ag1–N1	100.23 (7)
O1–Ag1–O5	85.03 (6)	O5–Ag1–N1	86.88 (7)
O1–Ag1–N1	105.78 (7)	O2–Ag2–O4 ⁱ	167.13 (6)
O3 ⁱ –Ag1–O5	100.80 (6)		

Symmetry code: (i) $-x, -y + 1, -z + 1$.

All H atoms were placed in calculated positions and refined as riding, with C–H = 0.95 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{parent atom})$.

Data collection: *CrystalClear* (Rigaku Corporation, 2001); cell refinement: *CrystalClear*; data reduction: *TEXSAN* (Molecular Structure Corporation, 2000); program(s) used to solve 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: *TEXSAN*.

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