Supplementary material

Enhanced silver ion binding to a rigid bisarene molecular cleft with formation of nonpolar pleated sheets through nonionic intermolecular forces

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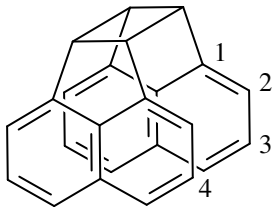
NMR Titration of **1**: 1.76 mg (5.78 μmol) in THF-d_8 solution. Aliquots of a solution of $AgCF_3SO_3$ in THF-d_8 added, monitoring the chemical shifts of protons of **1** (500 MHz, 25°C).



1

[Ag], M	[Ag]/δΔ	$\delta_{CH, aliph}$	Δδ, ppb	δ_{H-2}	$\Delta\delta_{H-2}$, ppb	δ_{H-3}	$\Delta\delta_{H-3}$, ppb	δ_{H-4}	$\Delta\delta_{H-4}$, ppb
0.000	0.0000	4.822	0	7.004	0	7.074	0	7.117	0
0.081	0.0011	4.859	37	7.068	64	7.148	74	7.179	62
0.153	0.0014	4.878	56	7.099	95	7.181	107	7.208	91
0.215	0.0017	4.886	64	7.117	113	7.202	128	7.227	110
0.321	0.0021	4.900	78	7.143	139	7.228	154	7.251	134
0.407	0.0024	4.907	85	7.157	153	7.243	169	7.266	149
0.477	0.0027	4.912	90	7.167	163	7.253	179	7.276	159
0.537	0.0029	4.914	92	7.175	171	7.259	185	7.282	165
0.563	0.0030	4.916	94	7.178	174	7.262	188	7.286	169

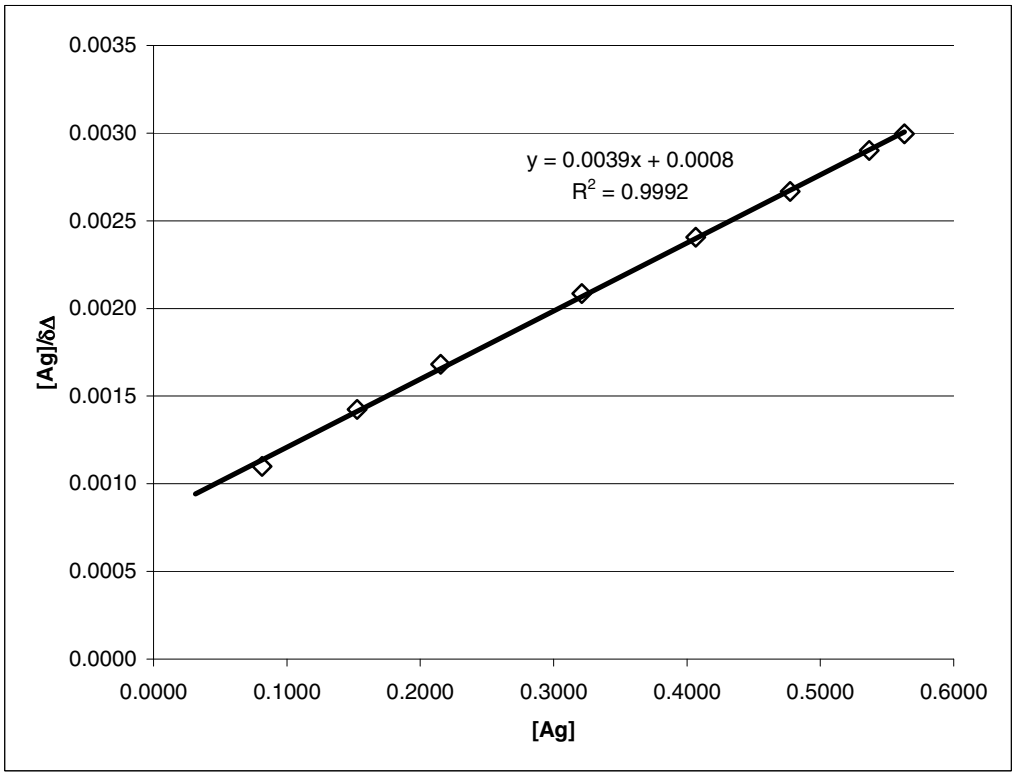


Figure S1: Scott plot for titration of **1** with monitoring of H-3.

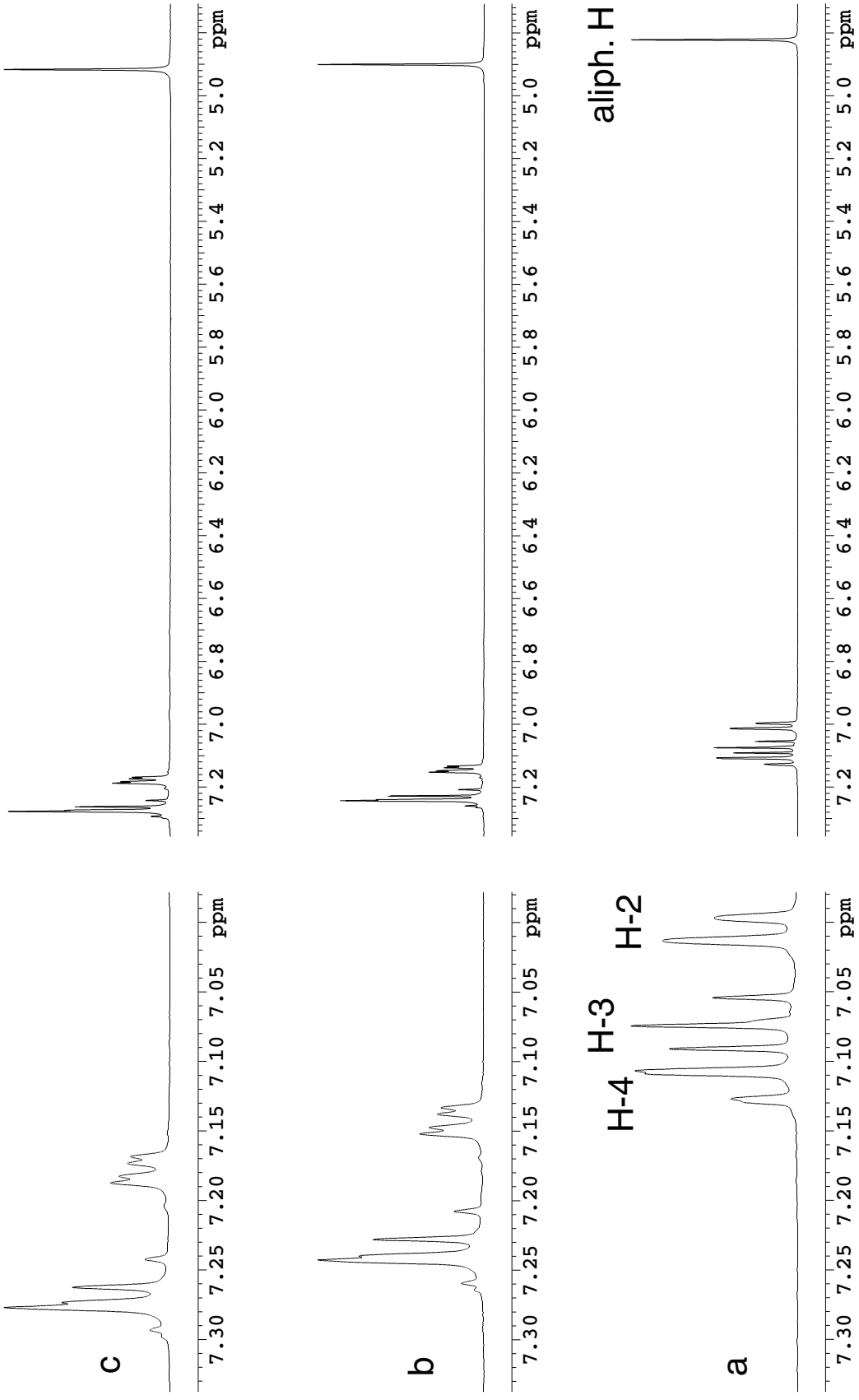


Figure S2: ^{1}H NMR spectra of **1** in the presence of (a) 0 M Ag^{+}, (b) 0.321 M Ag^{+}, (c) 0.563 M Ag^{+} (400 MHz, THF-d_8 solution, 25°C).

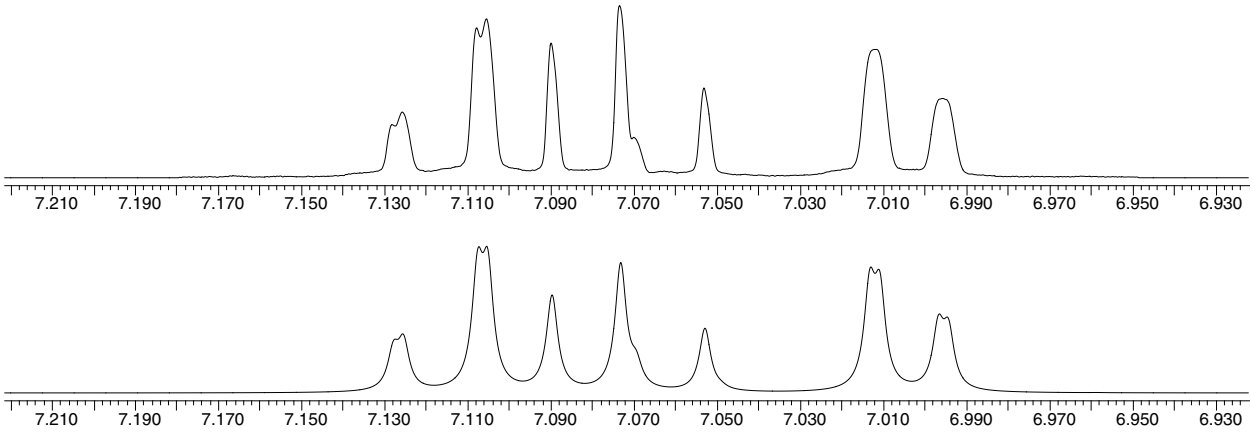


Figure S3: Expansion from the ^{1}H NMR spectrum of **1** in the absence of Ag^+, top: observed (400 MHz, THF-d_8 solution, 25°C), bottom: simulated. Parameters: δ = 7.114 (dd, J = 0.5, 8.2 Hz, 4H, H-4), 7.073 (dd, J = 6.9, 8.2 Hz, 4H, H-3), 7.005 (dd, J = 0.5, 6.9 Hz, 4H, H-2), 4.822 (s, 4H, cyclobutyl, not shown).

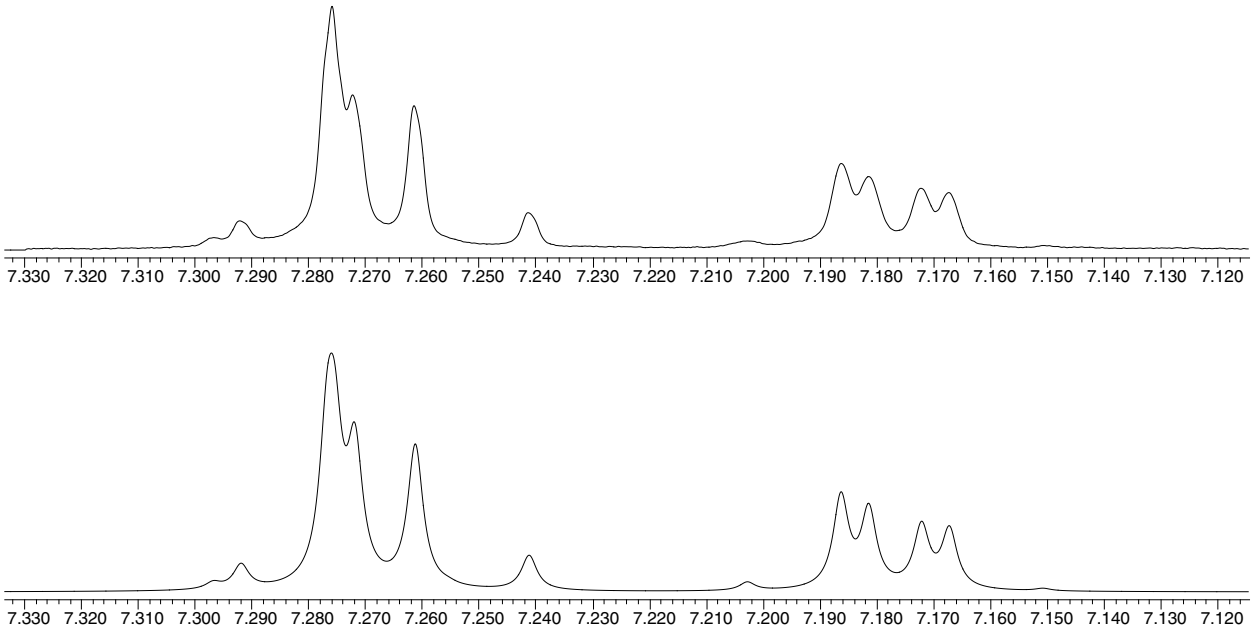


Figure S4: Expansion from the ^{1}H NMR spectrum of **1** in the presence of 0.563 M Ag^+, top: observed (400 MHz, THF-d_8 solution, 25°C), bottom: simulated. Parameters: δ = 7.279 (dd, J = 0.7, 8.1 Hz, 4H, H-4), 7.263 (dd, J = 6.9, 8.1 Hz, 4H, H-3), 7.178 (dd, J = 0.7, 6.9 Hz, 4H, H-2), 4.916 (s, 4H, cyclobutyl, not shown).

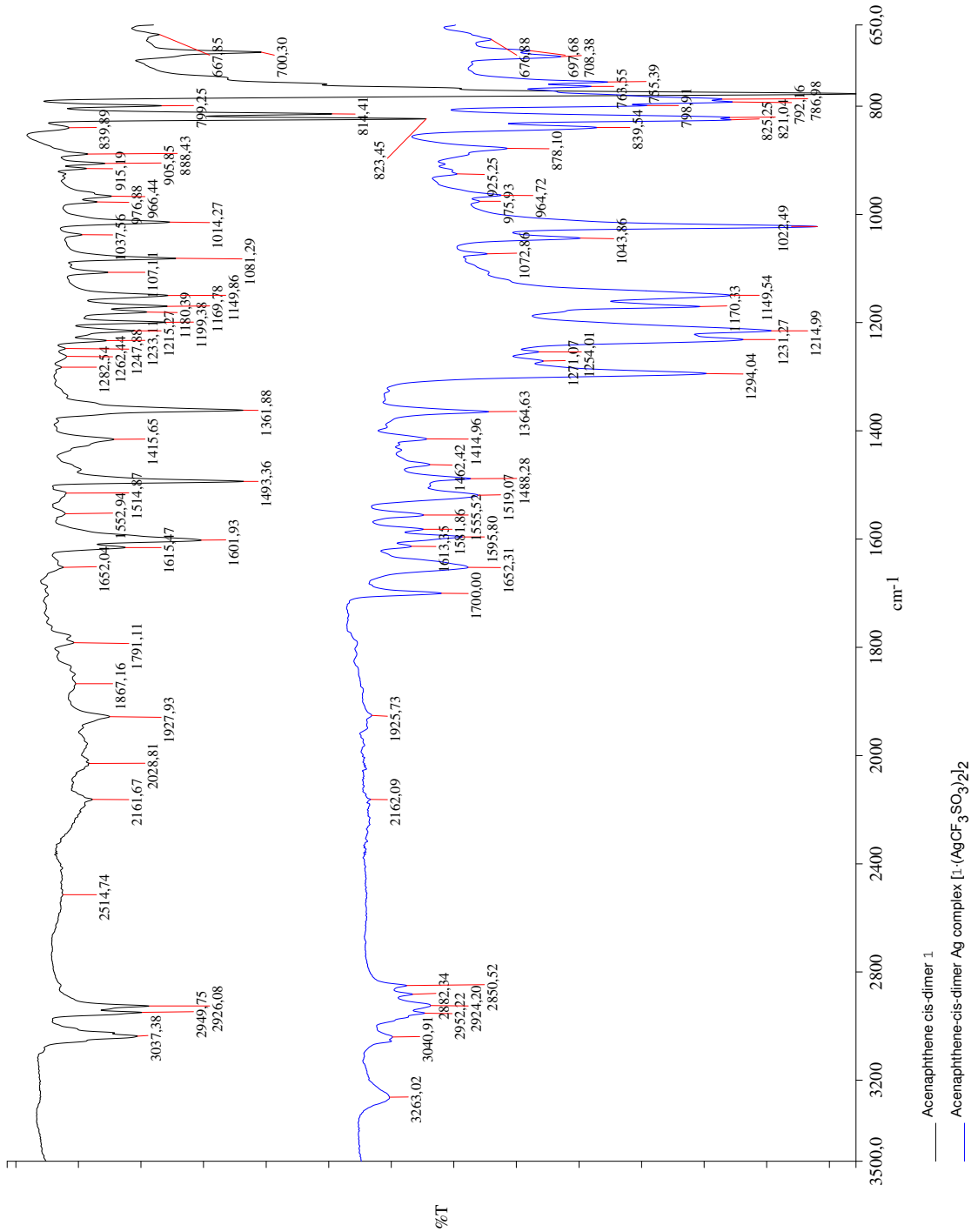


Figure S5: IR spectra of **1** and of $[\mathbf{1}\cdot(AgCF_3SO_3)_2]_2$ (neat, UATR accessory).

Tables of X-ray crystallographic parameters

CRYSTAL STRUCTURE DETERMINATION

Data were collected at room temperature using a Siemens SMART CCD diffractometer with Mo–K_α radiation (λ= 0.71073 Å, graphite monochromator). Full sphere of reciprocal lattices were scanned by 0.3° steps in ω with a crystal–to–detector distance of 3.97 cm, 30 seconds exposure time per frame. Preliminary orientation matrix was obtained from the first frames using SMART [1]. The collected frames were integrated using the preliminary orientation matrix which was updated every 100 frames. Final cell parameters were obtained by refinement on the positions of 8192 reflections with $I > 10\sigma(I)$ after integration of all the frames using SAINT [1]. The data were empirically corrected for absorption and other effects using SADABS [2]. The structures were solved by Patterson technique and refined by full-matrix least squares on all F^2 data using SHELXTL [3]. There is one acenaphthylene cis-dimer (its structure has been described earlier by Welberry [4]) and two crystallografically independent molecules of silver trifluoromethanesulfonate $AgSO_3CF_3$ in the asymmetric unit, forming a complex quadruple (see figures). Hydrogen atoms were constrained to the ideal geometry using an appropriate riding model. The C-H distances were fixed for 0.93Å for aromatic and 0.98Å for tertiary hydrogens. The non-H atoms were refined anisotropically, while the H atoms were refined isotropically. Molecular graphics were obtained using Diamond [5].

RESULTS

The crystallographic and refinement data are summarized in Table 1. Atomic coordinated for non-hydrogen atoms are given in Table 2. Bond lengths and angles are given in Table 3. Anisotropic displacement parameters for non-hydrogen atoms are given in Table 4. Coordinates for hydrogen atoms, together with their isotropic displacement factors are summarized in Table 5. Torsion angles are given in Table 5. The geometry of hydrogen bonds is in Table 7.

The title compound crystallizes in the monoclinic system with space group C2/c. The asymmetric unit contains a complex between one organic acenaphthylene cis-dimer and two crystallographicaly independent silver trifluoromethanesulfonates (see Fig. 1 and 2). The complex quadruple with square-planar configuration is shown on Fig. 3

[1] SMART & SAINT: Area Detector Control and Integration Software, Siemens AXS, Madison, WI, USA, 1995.

[2] G. M. Sheldrick, SADABS, Program for Empirical Absorption Correction of Area Detectors, University of Göttingen, Germany, 1996.

[3] G. M. Sheldrick, *SHELXTL (Version 5.10)*, Structure Determination Programs, Bruker AXS Inc., Madison, Wisconsin, USA, 1997.

[4] T.R.Welberry, *Acta Crystallogr., Sect. B,* **27**, 360 (1971).

[5] K. Brandenburg, *Diamond*: *Visual Crystal Structure Information System* (Version 2.1d), Crystal Impact GbR, Bonn, Germany, 2000.

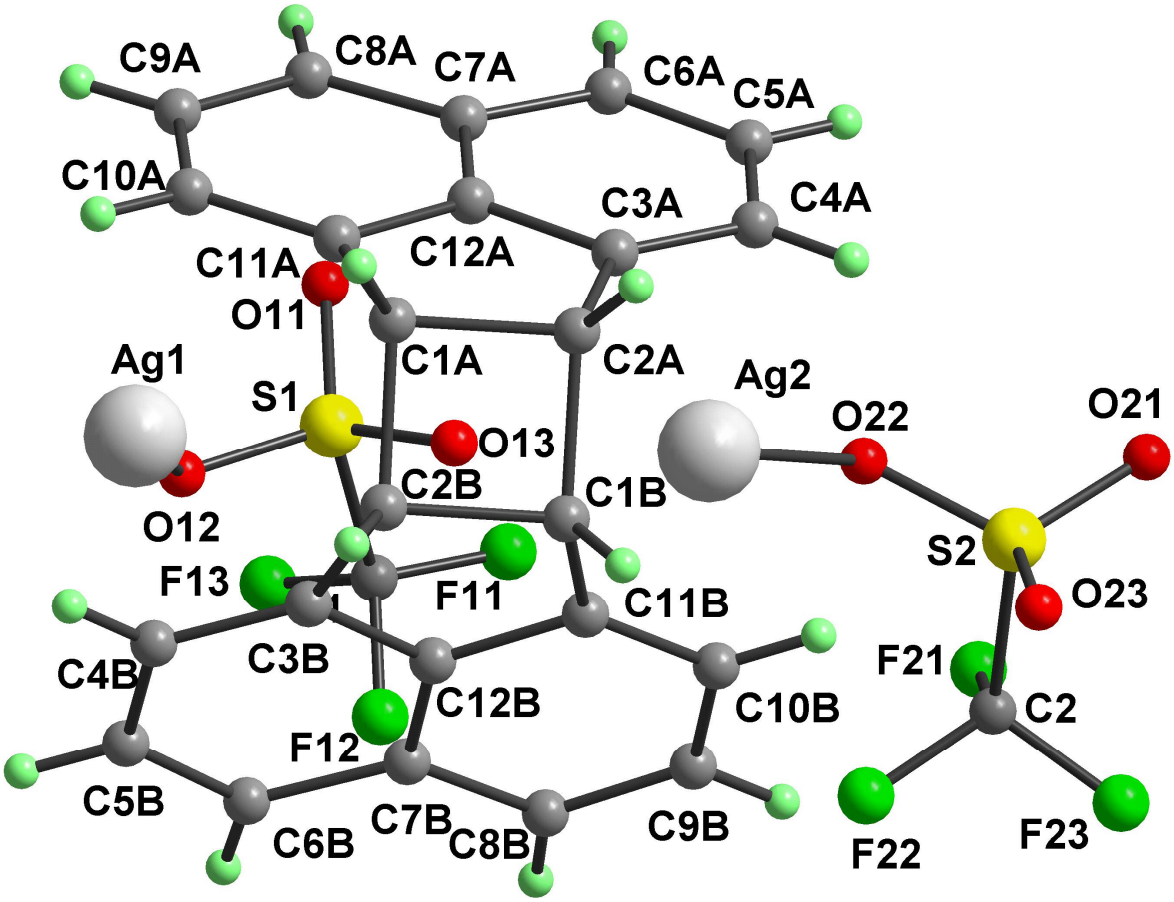


Fig.1. Numbering scheme.

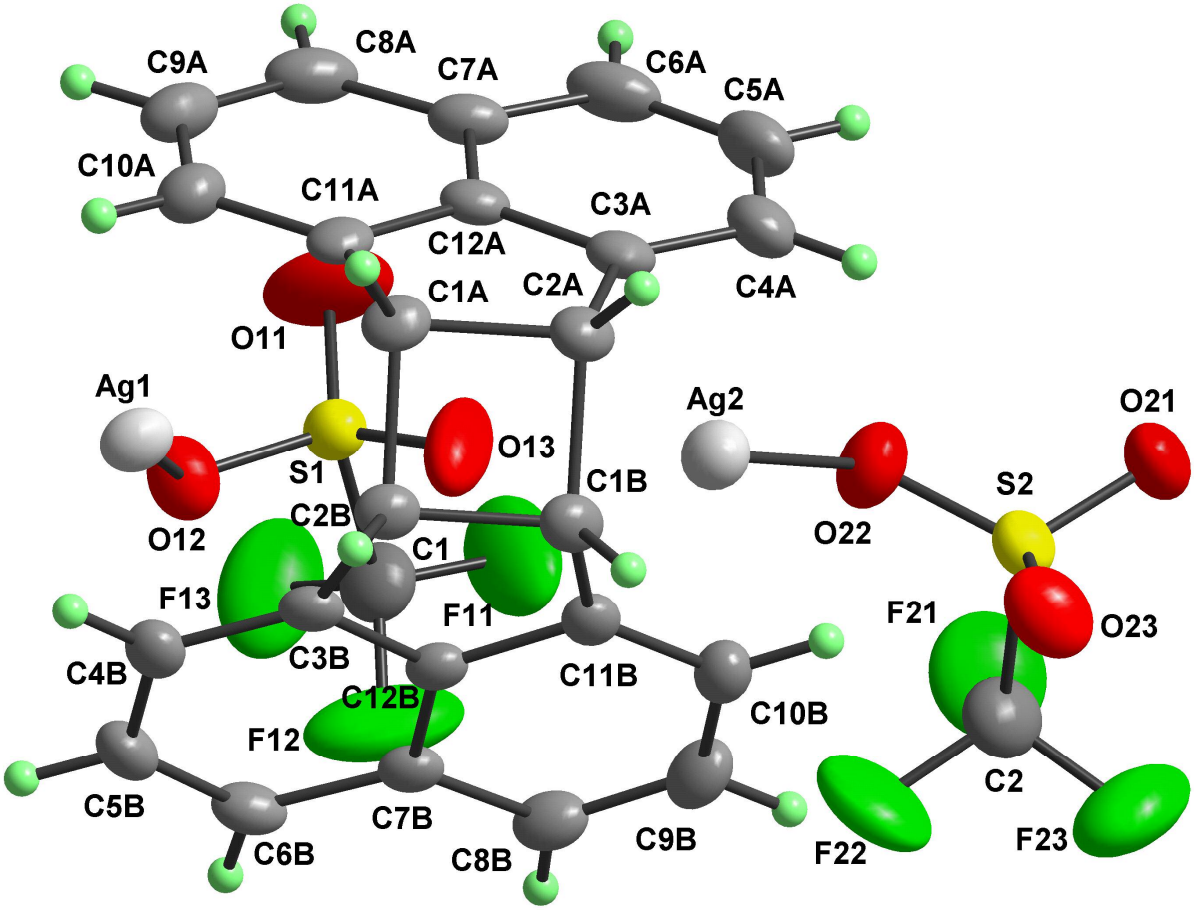


Fig.2. Numbering scheme with thermal ellipsoids at 30% probability level.

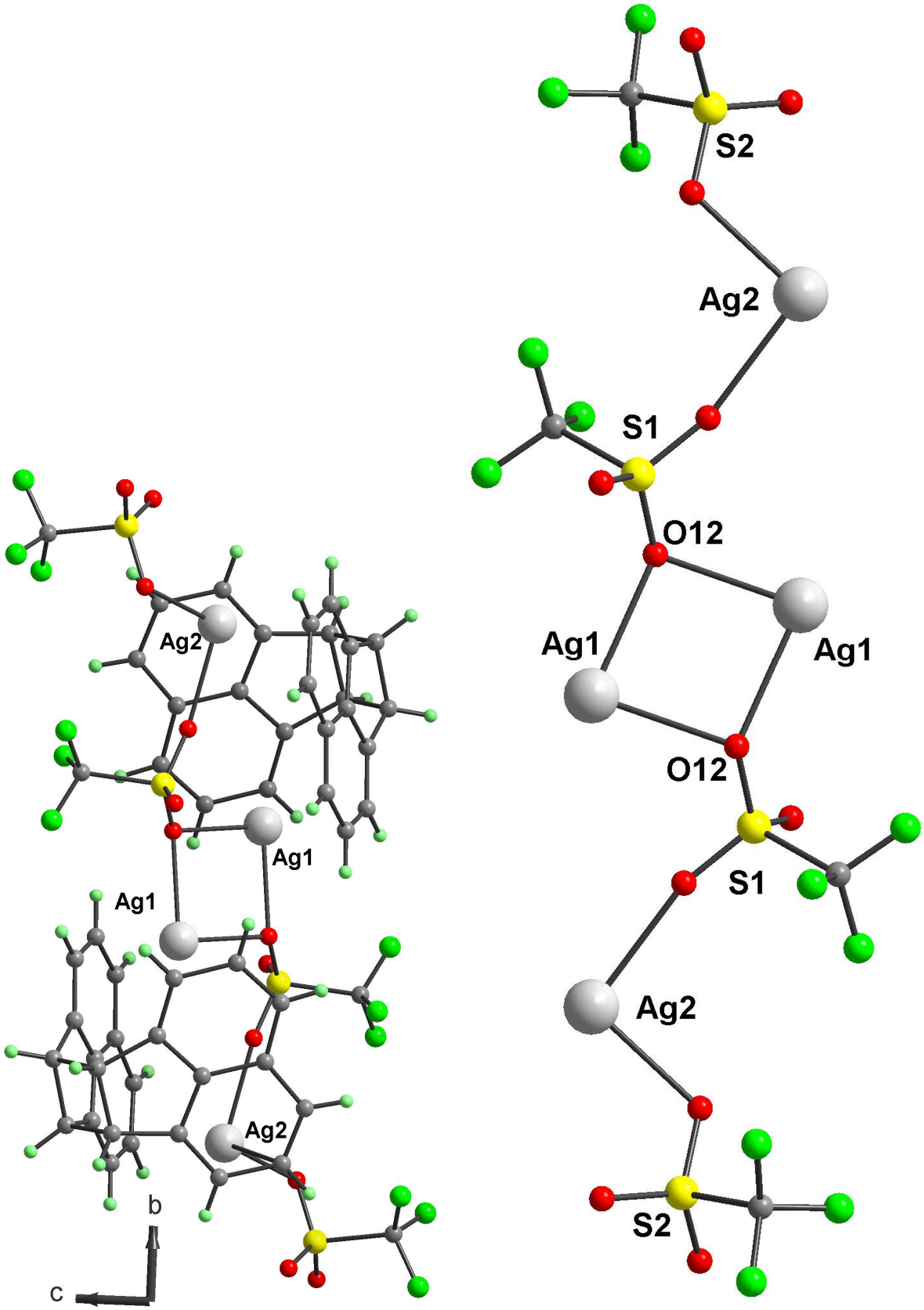


Fig.3a,b. The complex in projection along a-axis.

Table 1. Crystal data and structure refinement for [**1**·$(AgCF_3SO_3)_2$]$_2$.

Empirical formula	$C_{26}H_{16}\ Ag_2F_6\ O_6\ S_2$
Formula weight	818.25
Temperature	297(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 16.6087(2) Å
	b = 17.43310(10) Å β= 102.5420(10)°
	c = 18.4130(2) Å
Volume	5204.10(9) Å^3
Z	8
Density (calculated)	2.089 Mg/m^3
Absorption coefficient	1.752 mm^{-1}
F(000)	3200
Crystal size	0.14 x 0.10 x 0.08 mm^3
Theta range for data collection	1.90 to 25.35°.
Index ranges	-19<=h<=19, -20<=k<=20, -22<=l<=22
Reflections collected	27629
Independent reflections	4767 [R(int) = 0.0603]
Completeness to theta = 25.35°	99.9 %
Absorption correction	multi-scan
Max. and min. transmission	0.8725 and 0.7915
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4767 / 0 / 395
Goodness-of-fit on F^2	0.991
Final R indices [I>2sigma(I)]	R1 = 0.0465, wR2 = 0.1282
R indices (all data)	R1 = 0.0787, wR2 = 0.1504
Largest diff. peak and hole	1.119 and -0.637 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[\mathbf{1}\cdot(AgCF_3SO_3)_2]_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1A)	3649(4)	7306(3)	3040(3)	45(1)
C(2A)	3971(4)	8137(3)	3230(3)	46(1)
C(3A)	4885(4)	8067(4)	3541(3)	47(2)
C(4A)	5493(5)	8594(5)	3794(4)	64(2)
C(5A)	6302(5)	8335(5)	4032(5)	73(2)
C(6A)	6514(4)	7568(5)	4036(4)	69(2)
C(7A)	5910(4)	7017(4)	3788(3)	52(2)
C(8A)	6015(5)	6209(5)	3758(4)	65(2)
C(9A)	5348(5)	5743(4)	3496(4)	62(2)
C(10A)	4548(4)	6030(4)	3253(4)	53(2)
C(11A)	4410(4)	6809(3)	3278(3)	43(1)
C(12A)	5097(3)	7283(4)	3548(3)	43(1)
C(1B)	3387(4)	8217(3)	3795(3)	45(1)
C(2B)	3039(3)	7403(3)	3579(3)	40(1)
C(3B)	3170(3)	6957(3)	4298(3)	39(1)
C(4B)	2968(4)	6226(3)	4475(4)	45(1)
C(5B)	3167(4)	5997(4)	5237(4)	48(2)
C(6B)	3552(4)	6476(4)	5795(3)	48(2)
C(7B)	3772(3)	7230(3)	5633(3)	38(1)
C(8B)	4158(4)	7798(4)	6144(4)	52(2)
C(9B)	4314(4)	8510(4)	5894(4)	58(2)
C(10B)	4109(4)	8717(3)	5130(4)	49(2)
C(11B)	3727(3)	8185(3)	4614(3)	41(1)
C(12B)	3574(3)	7447(3)	4869(3)	37(1)
Ag(1)	4360(1)	5753(1)	4514(1)	55(1)
S(1)	6056(1)	6225(1)	5759(1)	50(1)
O(11)	6805(4)	5995(5)	5609(4)	127(3)
O(12)	5430(3)	5646(3)	5612(3)	70(1)
O(13)	5736(5)	6940(3)	5482(3)	103(2)
C(1)	6267(6)	6336(5)	6765(5)	74(2)
F(11)	6807(6)	6854(5)	6974(4)	169(4)
F(12)	5606(5)	6536(6)	6980(3)	168(4)
F(13)	6522(6)	5717(4)	7104(3)	153(3)
Ag(2)	5571(1)	8280(1)	5177(1)	65(1)

S(2)	6624(1)	9477(1)	6340(1)	53(1)
O(21)	7332(3)	9950(3)	6376(3)	75(2)
O(22)	6698(4)	8712(3)	6081(4)	86(2)
O(23)	5841(3)	9828(3)	6028(3)	84(2)
C(2)	6585(6)	9338(5)	7295(5)	78(2)
F(21)	7287(5)	9058(4)	7676(4)	140(3)
F(22)	5985(5)	8860(4)	7361(4)	141(3)
F(23)	6482(6)	9996(4)	7624(4)	152(3)

Table 3. Bond lengths [Å] and angles [°] for $[\mathbf{1}\cdot(AgCF_3SO_3)_2]_2$.

C(1A)-C(2A)	1.559(9)
C(1A)-C(2B)	1.573(8)
C(1A)-C(11A)	1.518(8)
C(1A)-H(1A)	0.9800
C(2A)-C(3A)	1.506(9)
C(2A)-C(1B)	1.576(8)
C(2A)-H(2A)	0.9800
C(3A)-C(12A)	1.410(9)
C(3A)-C(4A)	1.371(10)
C(4A)-C(5A)	1.395(11)
C(4A)-Ag(2)	2.580(7)
C(4A)-H(4A)	0.9300
C(5A)-C(6A)	1.383(12)
C(5A)-Ag(2)	2.654(8)
C(5A)-H(5A)	0.9300
C(6A)-C(7A)	1.394(10)
C(6A)-H(6A)	0.9300
C(7A)-C(8A)	1.420(10)
C(7A)-C(12A)	1.406(8)
C(8A)-C(9A)	1.375(11)
C(8A)-H(8A)	0.9300
C(9A)-C(10A)	1.399(10)
C(9A)-H(9A)	0.9300
C(10A)-C(11A)	1.379(9)
C(10A)-Ag(1)	2.456(6)
C(10A)-H(10A)	0.9300
C(11A)-C(12A)	1.408(8)
C(1B)-C(11B)	1.492(9)
C(1B)-C(2B)	1.550(8)
C(1B)-H(1B)	0.9800
C(2B)-C(3B)	1.510(8)
C(2B)-H(2B)	0.9800
C(3B)-C(12B)	1.405(8)
C(3B)-C(4B)	1.375(8)
C(4B)-C(5B)	1.427(9)
C(4B)-Ag(1)	2.441(6)
C(4B)-H(4B)	0.9300

C(5B)-C(6B)	1.369(9)
C(5B)-Ag(1)	2.652(6)
C(5B)-H(5B)	0.9300
C(6B)-C(7B)	1.415(8)
C(6B)-H(6B)	0.9300
C(7B)-C(12B)	1.425(8)
C(7B)-C(8B)	1.419(8)
C(8B)-C(9B)	1.367(10)
C(8B)-H(8B)	0.9300
C(9B)-C(10B)	1.420(10)
C(9B)-H(9B)	0.9300
C(10B)-C(11B)	1.380(8)
C(10B)-Ag(2)	2.528(6)
C(10B)-H(10B)	0.9300
C(11B)-C(12B)	1.411(8)
Ag(1)-O(12)	2.393(5)
Ag(1)-O(12)#1	2.481(5)
S(1)-O(13)	1.406(6)
S(1)-O(11)	1.391(6)
S(1)-O(12)	1.431(5)
S(1)-C(1)	1.820(8)
O(12)-Ag(1)#1	2.481(5)
O(13)-Ag(2)	2.405(5)
C(1)-F(11)	1.272(10)
C(1)-F(12)	1.294(11)
C(1)-F(13)	1.271(10)
Ag(2)-O(22)	2.343(6)
S(2)-O(23)	1.438(5)
S(2)-O(22)	1.432(5)
S(2)-O(21)	1.426(5)
S(2)-C(2)	1.791(9)
C(2)-F(23)	1.327(10)
C(2)-F(21)	1.317(10)
C(2)-F(22)	1.325(10)

C(2A)-C(1A)-C(2B)	89.7(4)
C(2A)-C(1A)-C(11A)	104.0(5)
C(2B)-C(1A)-C(11A)	119.3(4)

C(2A)-C(1A)-H(1A)	113.6
C(2B)-C(1A)-H(1A)	113.6
C(11A)-C(1A)-H(1A)	113.6
C(3A)-C(2A)-C(1A)	106.1(5)
C(3A)-C(2A)-C(1B)	118.0(5)
C(1A)-C(2A)-C(1B)	89.9(4)
C(3A)-C(2A)-H(2A)	113.4
C(1A)-C(2A)-H(2A)	113.4
C(1B)-C(2A)-H(2A)	113.4
C(12A)-C(3A)-C(4A)	118.9(6)
C(12A)-C(3A)-C(2A)	108.2(5)
C(4A)-C(3A)-C(2A)	133.0(6)
C(3A)-C(4A)-C(5A)	118.6(7)
C(3A)-C(4A)-Ag(2)	93.9(4)
C(5A)-C(4A)-Ag(2)	77.5(5)
C(3A)-C(4A)-H(4A)	120.7
C(5A)-C(4A)-H(4A)	120.7
Ag(2)-C(4A)-H(4A)	98.3
C(6A)-C(5A)-C(4A)	122.8(7)
C(6A)-C(5A)-Ag(2)	96.9(5)
C(4A)-C(5A)-Ag(2)	71.6(4)
C(6A)-C(5A)-H(5A)	118.6
C(4A)-C(5A)-H(5A)	118.6
Ag(2)-C(5A)-H(5A)	101.7
C(5A)-C(6A)-C(7A)	120.1(7)
C(5A)-C(6A)-H(6A)	120.0
C(7A)-C(6A)-H(6A)	120.0
C(6A)-C(7A)-C(8A)	127.6(7)
C(6A)-C(7A)-C(12A)	116.7(7)
C(8A)-C(7A)-C(12A)	115.7(6)
C(9A)-C(8A)-C(7A)	120.2(6)
C(9A)-C(8A)-H(8A)	119.9
C(7A)-C(8A)-H(8A)	119.9
C(8A)-C(9A)-C(10A)	122.5(7)
C(8A)-C(9A)-H(9A)	118.7
C(10A)-C(9A)-H(9A)	118.7
C(9A)-C(10A)-C(11A)	119.6(7)
C(9A)-C(10A)-Ag(1)	86.2(4)

C(11A)-C(10A)-Ag(1)	96.1(4)
C(9A)-C(10A)-H(10A)	120.2
C(11A)-C(10A)-H(10A)	120.2
Ag(1)-C(10A)-H(10A)	87.7
C(12A)-C(11A)-C(10A)	117.5(6)
C(12A)-C(11A)-C(1A)	109.0(5)
C(10A)-C(11A)-C(1A)	133.4(6)
C(3A)-C(12A)-C(11A)	112.6(5)
C(3A)-C(12A)-C(7A)	122.9(6)
C(11A)-C(12A)-C(7A)	124.4(6)
C(11B)-C(1B)-C(2B)	105.3(5)
C(11B)-C(1B)-C(2A)	120.8(5)
C(2B)-C(1B)-C(2A)	89.9(4)
C(11B)-C(1B)-H(1B)	112.7
C(2B)-C(1B)-H(1B)	112.7
C(2A)-C(1B)-H(1B)	112.7
C(3B)-C(2B)-C(1B)	105.7(5)
C(3B)-C(2B)-C(1A)	120.5(4)
C(1B)-C(2B)-C(1A)	90.3(4)
C(3B)-C(2B)-H(2B)	112.6
C(1B)-C(2B)-H(2B)	112.6
C(1A)-C(2B)-H(2B)	112.6
C(12B)-C(3B)-C(4B)	119.2(5)
C(12B)-C(3B)-C(2B)	107.2(5)
C(4B)-C(3B)-C(2B)	133.6(5)
C(3B)-C(4B)-C(5B)	118.4(6)
C(3B)-C(4B)-Ag(1)	92.4(4)
C(5B)-C(4B)-Ag(1)	82.1(4)
C(3B)-C(4B)-H(4B)	120.8
C(5B)-C(4B)-H(4B)	120.8
Ag(1)-C(4B)-H(4B)	95.4
C(6B)-C(5B)-C(4B)	122.5(6)
C(6B)-C(5B)-Ag(1)	101.3(4)
C(4B)-C(5B)-Ag(1)	65.7(3)
C(6B)-C(5B)-H(5B)	118.7
C(4B)-C(5B)-H(5B)	118.7
Ag(1)-C(5B)-H(5B)	102.9
C(5B)-C(6B)-C(7B)	120.5(5)

C(5B)-C(6B)-H(6B)	119.7
C(7B)-C(6B)-H(6B)	119.7
C(6B)-C(7B)-C(12B)	116.1(5)
C(6B)-C(7B)-C(8B)	127.5(5)
C(12B)-C(7B)-C(8B)	116.4(5)
C(9B)-C(8B)-C(7B)	120.0(6)
C(9B)-C(8B)-H(8B)	120.0
C(7B)-C(8B)-H(8B)	120.0
C(8B)-C(9B)-C(10B)	122.8(6)
C(8B)-C(9B)-H(9B)	118.6
C(10B)-C(9B)-H(9B)	118.6
C(11B)-C(10B)-C(9B)	119.1(6)
C(11B)-C(10B)-Ag(2)	96.6(4)
C(9B)-C(10B)-Ag(2)	82.4(4)
C(11B)-C(10B)-H(10B)	120.5
C(9B)-C(10B)-H(10B)	120.5
Ag(2)-C(10B)-H(10B)	91.0
C(10B)-C(11B)-C(12B)	118.3(6)
C(10B)-C(11B)-C(1B)	133.4(5)
C(12B)-C(11B)-C(1B)	108.3(5)
C(3B)-C(12B)-C(7B)	123.2(5)
C(3B)-C(12B)-C(11B)	113.4(5)
C(7B)-C(12B)-C(11B)	123.3(5)
O(12)-Ag(1)-C(10A)	126.2(2)
O(12)-Ag(1)-C(4B)	125.2(2)
C(10A)-Ag(1)-C(4B)	102.7(2)
O(12)-Ag(1)-O(12)#1	84.75(17)
C(10A)-Ag(1)-O(12)#1	93.2(2)
C(4B)-Ag(1)-O(12)#1	118.74(18)
O(12)-Ag(1)-C(5B)	95.0(2)
C(10A)-Ag(1)-C(5B)	134.9(2)
C(4B)-Ag(1)-C(5B)	32.2(2)
O(12)#1-Ag(1)-C(5B)	109.88(19)
O(13)-S(1)-O(11)	117.8(5)
O(13)-S(1)-O(12)	110.9(4)
O(11)-S(1)-O(12)	113.8(4)
O(13)-S(1)-C(1)	104.4(4)
O(11)-S(1)-C(1)	104.5(4)

O(12)-S(1)-C(1)	103.8(4)
S(1)-O(12)-Ag(1)	118.7(3)
S(1)-O(12)-Ag(1)#1	126.9(3)
Ag(1)-O(12)-Ag(1)#1	95.26(17)
S(1)-O(13)-Ag(2)	164.0(5)
F(11)-C(1)-F(12)	107.8(9)
F(11)-C(1)-F(13)	108.3(9)
F(12)-C(1)-F(13)	107.1(9)
F(11)-C(1)-S(1)	110.6(7)
F(12)-C(1)-S(1)	110.6(6)
F(13)-C(1)-S(1)	112.3(6)
O(22)-Ag(2)-O(13)	96.4(2)
O(22)-Ag(2)-C(10B)	122.7(2)
O(13)-Ag(2)-C(10B)	111.2(2)
O(22)-Ag(2)-C(4A)	119.6(2)
O(13)-Ag(2)-C(4A)	114.5(2)
C(10B)-Ag(2)-C(4A)	93.5(2)
O(22)-Ag(2)-C(5A)	96.9(2)
O(13)-Ag(2)-C(5A)	99.9(3)
C(10B)-Ag(2)-C(5A)	124.3(3)
C(4A)-Ag(2)-C(5A)	30.9(2)
O(23)-S(2)-O(22)	113.5(4)
O(23)-S(2)-O(21)	116.0(3)
O(22)-S(2)-O(21)	115.1(3)
O(23)-S(2)-C(2)	103.2(4)
O(22)-S(2)-C(2)	103.0(4)
O(21)-S(2)-C(2)	103.8(4)
S(2)-O(22)-Ag(2)	115.0(3)
F(23)-C(2)-F(21)	105.3(8)
F(23)-C(2)-F(22)	109.2(9)
F(21)-C(2)-F(22)	108.3(7)
F(23)-C(2)-S(2)	111.5(6)
F(21)-C(2)-S(2)	110.9(7)
F(22)-C(2)-S(2)	111.3(7)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[\mathbf{1}\cdot(AgCF_3SO_3)_2]_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1A)	49(3)	56(4)	27(3)	3(3)	4(2)	8(3)
C(2A)	52(4)	49(3)	40(3)	9(3)	17(3)	3(3)
C(3A)	48(4)	60(4)	39(3)	6(3)	22(3)	0(3)
C(4A)	68(5)	68(5)	61(5)	3(4)	29(4)	-17(4)
C(5A)	62(5)	90(6)	74(5)	-11(4)	28(4)	-28(5)
C(6A)	41(4)	117(7)	50(4)	7(4)	13(3)	-3(4)
C(7A)	41(3)	77(5)	40(4)	7(3)	15(3)	10(3)
C(8A)	57(5)	94(6)	48(4)	16(4)	21(4)	26(4)
C(9A)	79(5)	61(4)	52(4)	5(3)	27(4)	21(4)
C(10A)	65(4)	53(4)	46(4)	-1(3)	18(3)	8(3)
C(11A)	56(4)	52(3)	25(3)	3(2)	17(3)	7(3)
C(12A)	43(3)	60(4)	31(3)	6(3)	17(3)	2(3)
C(1B)	44(3)	44(3)	49(4)	9(3)	13(3)	10(3)
C(2B)	33(3)	49(3)	37(3)	5(2)	4(2)	10(2)
C(3B)	30(3)	52(3)	38(3)	1(3)	13(2)	6(2)
C(4B)	37(3)	47(3)	53(4)	0(3)	13(3)	-2(3)
C(5B)	42(3)	49(3)	56(4)	11(3)	17(3)	-2(3)
C(6B)	45(3)	67(4)	35(3)	13(3)	14(3)	8(3)
C(7B)	29(3)	51(3)	36(3)	1(2)	10(2)	9(2)
C(8B)	45(4)	71(4)	38(4)	-8(3)	4(3)	5(3)
C(9B)	54(4)	57(4)	61(5)	-19(3)	5(3)	0(3)
C(10B)	47(4)	43(3)	59(4)	-6(3)	14(3)	-2(3)
C(11B)	35(3)	41(3)	49(4)	0(3)	15(3)	5(2)
C(12B)	31(3)	47(3)	35(3)	-3(2)	10(2)	5(2)
Ag(1)	54(1)	60(1)	50(1)	-1(1)	9(1)	12(1)
S(1)	46(1)	54(1)	51(1)	-9(1)	11(1)	-6(1)
O(11)	52(4)	217(8)	112(6)	-49(6)	15(4)	17(4)
O(12)	65(3)	74(3)	64(3)	3(2)	-3(3)	-13(2)
O(13)	193(8)	49(3)	68(4)	10(3)	30(4)	-5(4)
C(1)	81(6)	77(5)	57(5)	-9(4)	4(4)	-8(5)
F(11)	227(9)	182(7)	88(4)	-56(4)	17(5)	-115(7)
F(12)	166(7)	285(10)	60(4)	-8(5)	38(4)	79(7)
F(13)	219(8)	125(5)	76(4)	19(3)	-51(5)	13(5)
Ag(2)	69(1)	63(1)	65(1)	-11(1)	17(1)	-7(1)

S(2)	57(1)	50(1)	52(1)	7(1)	12(1)	-4(1)
O(21)	72(3)	58(3)	101(4)	7(3)	32(3)	-10(2)
O(22)	93(4)	65(3)	97(4)	-24(3)	18(3)	-5(3)
O(23)	66(3)	96(4)	81(4)	32(3)	-3(3)	4(3)
C(2)	94(6)	71(5)	70(6)	20(4)	19(5)	7(5)
F(21)	144(6)	157(5)	92(4)	50(4)	-36(4)	24(5)
F(22)	153(6)	178(7)	102(5)	55(4)	52(4)	-37(5)
F(23)	236(8)	141(6)	92(4)	-21(4)	64(5)	40(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for [**1**·($AgCF_3SO_3$)$_2$]$_2$.

	x	y	z	U(eq)
H(1A)	3369	7237	2518	38(15)
H(2A)	3833	8491	2808	90(30)
H(4A)	5369	9113	3808	80(20)
H(5A)	6717	8694	4194	120(40)
H(6A)	7061	7420	4204	100(30)
H(8A)	6537	5996	3917	80(20)
H(9A)	5432	5216	3480	50(17)
H(10A)	4112	5697	3076	53(19)
H(1B)	2972	8620	3654	40(15)
H(2B)	2460	7412	3314	60(19)
H(4B)	2708	5889	4107	80(20)
H(5B)	3029	5504	5360	60(20)
H(6B)	3669	6304	6285	49(17)
H(8B)	4304	7687	6649	49(17)
H(9B)	4565	8874	6239	58(19)
H(10B)	4230	9205	4980	70(20)

Table 6. Torsion angles [°] for [**1**·$(AgCF_3SO_3)_2$]$_2$.

C(2B)-C(1A)-C(2A)-C(3A)	121.6(5)
C(11A)-C(1A)-C(2A)-C(3A)	1.4(6)
C(2B)-C(1A)-C(2A)-C(1B)	2.4(4)
C(11A)-C(1A)-C(2A)-C(1B)	-117.9(5)
C(1A)-C(2A)-C(3A)-C(12A)	-0.5(6)
C(1B)-C(2A)-C(3A)-C(12A)	98.2(6)
C(1A)-C(2A)-C(3A)-C(4A)	179.2(6)
C(1B)-C(2A)-C(3A)-C(4A)	-82.0(8)
C(12A)-C(3A)-C(4A)-C(5A)	1.6(10)
C(2A)-C(3A)-C(4A)-C(5A)	-178.1(6)
C(12A)-C(3A)-C(4A)-Ag(2)	-76.3(5)
C(2A)-C(3A)-C(4A)-Ag(2)	104.0(7)
C(3A)-C(4A)-C(5A)-C(6A)	-1.3(11)
Ag(2)-C(4A)-C(5A)-C(6A)	86.4(7)
C(3A)-C(4A)-C(5A)-Ag(2)	-87.7(6)
C(4A)-C(5A)-C(6A)-C(7A)	0.8(12)
Ag(2)-C(5A)-C(6A)-C(7A)	73.3(7)
C(5A)-C(6A)-C(7A)-C(8A)	-179.5(7)
C(5A)-C(6A)-C(7A)-C(12A)	-0.6(10)
C(6A)-C(7A)-C(8A)-C(9A)	180.0(7)
C(12A)-C(7A)-C(8A)-C(9A)	1.1(9)
C(7A)-C(8A)-C(9A)-C(10A)	-0.3(10)
C(8A)-C(9A)-C(10A)-C(11A)	-0.5(10)
C(8A)-C(9A)-C(10A)-Ag(1)	-95.3(7)
C(9A)-C(10A)-C(11A)-C(12A)	0.4(8)
Ag(1)-C(10A)-C(11A)-C(12A)	89.5(5)
C(9A)-C(10A)-C(11A)-C(1A)	177.5(6)
Ag(1)-C(10A)-C(11A)-C(1A)	-93.4(6)
C(2A)-C(1A)-C(11A)-C(12A)	-1.8(6)
C(2B)-C(1A)-C(11A)-C(12A)	-99.5(6)
C(2A)-C(1A)-C(11A)-C(10A)	-179.0(6)
C(2B)-C(1A)-C(11A)-C(10A)	83.2(8)
C(4A)-C(3A)-C(12A)-C(11A)	179.6(5)
C(2A)-C(3A)-C(12A)-C(11A)	-0.6(7)
C(4A)-C(3A)-C(12A)-C(7A)	-1.6(9)
C(2A)-C(3A)-C(12A)-C(7A)	178.2(5)
C(10A)-C(11A)-C(12A)-C(3A)	179.3(5)

C(1A)-C(11A)-C(12A)-C(3A)	1.6(6)
C(10A)-C(11A)-C(12A)-C(7A)	0.5(8)
C(1A)-C(11A)-C(12A)-C(7A)	-177.3(5)
C(6A)-C(7A)-C(12A)-C(3A)	1.0(9)
C(8A)-C(7A)-C(12A)-C(3A)	-179.9(5)
C(6A)-C(7A)-C(12A)-C(11A)	179.7(5)
C(8A)-C(7A)-C(12A)-C(11A)	-1.2(8)
C(3A)-C(2A)-C(1B)-C(11B)	-2.9(8)
C(1A)-C(2A)-C(1B)-C(11B)	105.4(6)
C(3A)-C(2A)-C(1B)-C(2B)	-110.7(6)
C(1A)-C(2A)-C(1B)-C(2B)	-2.4(4)
C(11B)-C(1B)-C(2B)-C(3B)	2.2(6)
C(2A)-C(1B)-C(2B)-C(3B)	124.3(4)
C(11B)-C(1B)-C(2B)-C(1A)	-119.7(4)
C(2A)-C(1B)-C(2B)-C(1A)	2.4(4)
C(2A)-C(1A)-C(2B)-C(3B)	-110.9(6)
C(11A)-C(1A)-C(2B)-C(3B)	-5.0(8)
C(2A)-C(1A)-C(2B)-C(1B)	-2.4(4)
C(11A)-C(1A)-C(2B)-C(1B)	103.6(6)
C(1B)-C(2B)-C(3B)-C(12B)	-1.7(6)
C(1A)-C(2B)-C(3B)-C(12B)	98.3(6)
C(1B)-C(2B)-C(3B)-C(4B)	177.1(6)
C(1A)-C(2B)-C(3B)-C(4B)	-83.0(8)
C(12B)-C(3B)-C(4B)-C(5B)	0.9(8)
C(2B)-C(3B)-C(4B)-C(5B)	-177.7(6)
C(12B)-C(3B)-C(4B)-Ag(1)	-81.3(5)
C(2B)-C(3B)-C(4B)-Ag(1)	100.1(6)
C(3B)-C(4B)-C(5B)-C(6B)	-0.2(9)
Ag(1)-C(4B)-C(5B)-C(6B)	88.2(6)
C(3B)-C(4B)-C(5B)-Ag(1)	-88.4(5)
C(4B)-C(5B)-C(6B)-C(7B)	-0.1(9)
Ag(1)-C(5B)-C(6B)-C(7B)	68.2(6)
C(5B)-C(6B)-C(7B)-C(12B)	-0.3(8)
C(5B)-C(6B)-C(7B)-C(8B)	178.8(6)
C(6B)-C(7B)-C(8B)-C(9B)	-178.6(6)
C(12B)-C(7B)-C(8B)-C(9B)	0.5(8)
C(7B)-C(8B)-C(9B)-C(10B)	-0.2(10)
C(8B)-C(9B)-C(10B)-C(11B)	0.7(10)

C(8B)-C(9B)-C(10B)-Ag(2)	-92.6(6)
C(9B)-C(10B)-C(11B)-C(12B)	-1.5(8)
Ag(2)-C(10B)-C(11B)-C(12B)	83.5(5)
C(9B)-C(10B)-C(11B)-C(1B)	175.8(6)
Ag(2)-C(10B)-C(11B)-C(1B)	-99.3(6)
C(2B)-C(1B)-C(11B)-C(10B)	-179.5(6)
C(2A)-C(1B)-C(11B)-C(10B)	81.3(8)
C(2B)-C(1B)-C(11B)-C(12B)	-2.0(6)
C(2A)-C(1B)-C(11B)-C(12B)	-101.3(6)
C(4B)-C(3B)-C(12B)-C(7B)	-1.4(8)
C(2B)-C(3B)-C(12B)-C(7B)	177.5(5)
C(4B)-C(3B)-C(12B)-C(11B)	-178.5(5)
C(2B)-C(3B)-C(12B)-C(11B)	0.4(6)
C(6B)-C(7B)-C(12B)-C(3B)	1.1(8)
C(8B)-C(7B)-C(12B)-C(3B)	-178.1(5)
C(6B)-C(7B)-C(12B)-C(11B)	177.9(5)
C(8B)-C(7B)-C(12B)-C(11B)	-1.3(8)
C(10B)-C(11B)-C(12B)-C(3B)	178.9(5)
C(1B)-C(11B)-C(12B)-C(3B)	1.1(6)
C(10B)-C(11B)-C(12B)-C(7B)	1.8(8)
C(1B)-C(11B)-C(12B)-C(7B)	-176.1(5)
C(9A)-C(10A)-Ag(1)-O(12)	23.4(5)
C(11A)-C(10A)-Ag(1)-O(12)	-96.0(4)
C(9A)-C(10A)-Ag(1)-C(4B)	177.1(4)
C(11A)-C(10A)-Ag(1)-C(4B)	57.7(5)
C(9A)-C(10A)-Ag(1)-O(12)#1	-62.5(5)
C(11A)-C(10A)-Ag(1)-O(12)#1	178.1(4)
C(9A)-C(10A)-Ag(1)-C(5B)	175.1(4)
C(11A)-C(10A)-Ag(1)-C(5B)	55.7(6)
C(3B)-C(4B)-Ag(1)-O(12)	95.2(4)
C(5B)-C(4B)-Ag(1)-O(12)	-23.2(4)
C(3B)-C(4B)-Ag(1)-C(10A)	-58.9(4)
C(5B)-C(4B)-Ag(1)-C(10A)	-177.3(4)
C(3B)-C(4B)-Ag(1)-O(12)#1	-159.8(3)
C(5B)-C(4B)-Ag(1)-O(12)#1	81.8(4)
C(3B)-C(4B)-Ag(1)-C(5B)	118.4(6)
C(6B)-C(5B)-Ag(1)-O(12)	40.4(4)
C(4B)-C(5B)-Ag(1)-O(12)	161.1(4)

C(6B)-C(5B)-Ag(1)-C(10A)	-117.0(4)
C(4B)-C(5B)-Ag(1)-C(10A)	3.7(5)
C(6B)-C(5B)-Ag(1)-C(4B)	-120.7(6)
C(6B)-C(5B)-Ag(1)-O(12)#1	126.6(4)
C(4B)-C(5B)-Ag(1)-O(12)#1	-112.7(4)
O(13)-S(1)-O(12)-Ag(1)	31.6(5)
O(11)-S(1)-O(12)-Ag(1)	-104.0(5)
C(1)-S(1)-O(12)-Ag(1)	143.1(4)
O(13)-S(1)-O(12)-Ag(1)#1	154.3(4)
O(11)-S(1)-O(12)-Ag(1)#1	18.7(6)
C(1)-S(1)-O(12)-Ag(1)#1	-94.2(5)
C(10A)-Ag(1)-O(12)-S(1)	47.4(5)
C(4B)-Ag(1)-O(12)-S(1)	-100.8(4)
O(12)#1-Ag(1)-O(12)-S(1)	137.5(5)
C(5B)-Ag(1)-O(12)-S(1)	-113.0(4)
C(10A)-Ag(1)-O(12)-Ag(1)#1	-90.1(3)
C(4B)-Ag(1)-O(12)-Ag(1)#1	121.7(2)
O(12)#1-Ag(1)-O(12)-Ag(1)#1	0.002(1)
C(5B)-Ag(1)-O(12)-Ag(1)#1	109.6(2)
O(11)-S(1)-O(13)-Ag(2)	-51.0(15)
O(12)-S(1)-O(13)-Ag(2)	175.4(14)
C(1)-S(1)-O(13)-Ag(2)	64.2(15)
O(13)-S(1)-C(1)-F(11)	-62.3(9)
O(11)-S(1)-C(1)-F(11)	62.0(9)
O(12)-S(1)-C(1)-F(11)	-178.5(8)
O(13)-S(1)-C(1)-F(12)	56.9(8)
O(11)-S(1)-C(1)-F(12)	-178.7(8)
O(12)-S(1)-C(1)-F(12)	-59.2(8)
O(13)-S(1)-C(1)-F(13)	176.5(8)
O(11)-S(1)-C(1)-F(13)	-59.1(9)
O(12)-S(1)-C(1)-F(13)	60.4(8)
S(1)-O(13)-Ag(2)-O(22)	-18.3(15)
S(1)-O(13)-Ag(2)-C(10B)	-147.2(14)
S(1)-O(13)-Ag(2)-C(4A)	108.5(14)
S(1)-O(13)-Ag(2)-C(5A)	79.9(15)
C(11B)-C(10B)-Ag(2)-O(22)	-168.8(4)
C(9B)-C(10B)-Ag(2)-O(22)	-50.2(5)
C(11B)-C(10B)-Ag(2)-O(13)	-55.7(4)

C(9B)-C(10B)-Ag(2)-O(13)	62.8(4)
C(11B)-C(10B)-Ag(2)-C(4A)	62.3(4)
C(9B)-C(10B)-Ag(2)-C(4A)	-179.1(4)
C(11B)-C(10B)-Ag(2)-C(5A)	63.5(5)
C(9B)-C(10B)-Ag(2)-C(5A)	-178.0(4)
C(3A)-C(4A)-Ag(2)-O(22)	165.4(4)
C(5A)-C(4A)-Ag(2)-O(22)	47.0(5)
C(3A)-C(4A)-Ag(2)-O(13)	51.7(5)
C(5A)-C(4A)-Ag(2)-O(13)	-66.7(5)
C(3A)-C(4A)-Ag(2)-C(10B)	-63.4(5)
C(5A)-C(4A)-Ag(2)-C(10B)	178.1(5)
C(3A)-C(4A)-Ag(2)-C(5A)	118.4(7)
C(6A)-C(5A)-Ag(2)-O(22)	97.5(5)
C(4A)-C(5A)-Ag(2)-O(22)	-140.2(5)
C(6A)-C(5A)-Ag(2)-O(13)	-0.3(6)
C(4A)-C(5A)-Ag(2)-O(13)	122.0(5)
C(6A)-C(5A)-Ag(2)-C(10B)	-124.6(5)
C(4A)-C(5A)-Ag(2)-C(10B)	-2.3(6)
C(6A)-C(5A)-Ag(2)-C(4A)	-122.3(7)
O(23)-S(2)-O(22)-Ag(2)	3.7(5)
O(21)-S(2)-O(22)-Ag(2)	-133.3(3)
C(2)-S(2)-O(22)-Ag(2)	114.5(4)
O(13)-Ag(2)-O(22)-S(2)	-151.9(4)
C(10B)-Ag(2)-O(22)-S(2)	-31.6(5)
C(4A)-Ag(2)-O(22)-S(2)	85.1(4)
C(5A)-Ag(2)-O(22)-S(2)	107.3(4)
O(23)-S(2)-C(2)-F(23)	-59.2(8)
O(22)-S(2)-C(2)-F(23)	-177.5(7)
O(21)-S(2)-C(2)-F(23)	62.1(8)
O(23)-S(2)-C(2)-F(21)	-176.3(6)
O(22)-S(2)-C(2)-F(21)	65.4(7)
O(21)-S(2)-C(2)-F(21)	-54.9(7)
O(23)-S(2)-C(2)-F(22)	63.0(7)
O(22)-S(2)-C(2)-F(22)	-55.3(7)
O(21)-S(2)-C(2)-F(22)	-175.7(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1