Supporting Information for

Terthiophene Radical Cations End-Capped by Bicyclo[2.2.2]octene Units: Formation of Bent π-Dimers Mutually Attracted at the Central Position

Daisuke Yamazaki, Nobuhide Tanino, Tohru Nishinaga, and Koichi Komatsu*

Institute for Chemical Research, Kyoto University, Uji, Kyoto 611-0011, Japan, and Department of Chemistry, Graduate School of Science, Tokyo Metropolitan University, Hachioji, Tokyo 192-0397, Japan

Contents

General

^{1}H (300 MHz) and ^{13}C (75.4 MHz) NMR spectra were recorded on a Varian Mercury-300 spectrometer. Chemical shifts are reported in δ ppm from TMS using the signals of the solvent ($CDCl_3$; δ 7.26 in ^{1}H ($CHCl_3$) and δ 77.0 in ^{13}C NMR, respectively) as internal references. Mass spectra (EI) were recorded on a JEOL JMS-HX110 or JMS700 spectrometer. ESR spectra were taken on a Bruker EMX spectrometer. Separation by gel-permeation chromatography (GPC) was performed with a JAI LC-908 chromatograph equipped with JAIGEL 1H and 2H columns. Cyclic voltammetry was performed on a BAS-50W electrochemical analyzer. The CV cell consisted of a glassy carbon working electrode, a Pt wire counter electrode, and an $Ag/AgNO_3$ reference electrode. The measurements were carried out with 1.0 mM solutions of substrate using tetrabutylammonium perchlorate as a supporting electrolyte (0.1 M), and the values of oxidation potential were calibrated using ferrocene as an internal standard.

All reactions were conducted under a dry argon atmosphere unless otherwise stated. THF was distilled from sodium benzophenone ketyl. Dichloromethane, hexane, carbon tetrachloride, and carbon disulfide were distilled over CaH_2. The reagents were of the reagent grade obtained commercially unless otherwise stated.

4,5:4”,5”-Bis(bicyclo[2.2.2]octeno)-2,2’:5’,2”-terthiophene (2). In a 50 mL flask, a mixture of 2-(trimethylstannyl)-4,5-bicyclo[2.2.2]octenothiophene[1] (0.640 g, 1.96 mmol), 2,5-dibromothiophene (0.215 g, 0.887 mmol), $Pd(PPh_3)_4$ (0.114 g, 0.0982 mmol) and CuO (0.156 g, 1.96 mmol) in 20 mL of dry DMF was degassed with a vacuum pump for 1 minute and the reaction vessel was refilled with argon. The mixture was stirred at 100 °C for 5 h and then cooled to room temperature. To the mixture was added 50 mL of CH_2Cl_2 and the precipitates were filtered off. Removal of the volatiles of the filtrate under reduced pressure and GPC

separation of the residue gave 0.350 g of **2** (96%) as a yellow solid: mp 263.2-264.1 °C; UV-vis(CH_2Cl_2) λ_{max}(log ε) 379(4.42) 252(3.96)nm; ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.98 (s, 2H), 6.96 (s, 2H), 3.25 (s, 2H), 3.18 (s, 2H), 1.85-1.72 (m, 8H), 1.45-1.37 (m, 8H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 144.8, 139.8, 136.2, 132.4, 123.0, 120.7, 31.4, 31.3, 27.4, 26.9; HRMS calcd for $C_{24}H_{24}S_3$ 408.1040, found 408.1032. Anal. Calcd for $C_{24}H_{24}S_3$: C, 70.54; H, 5.92. Found: C, 70.27; H, 5.82.

Hexafluoroantimonate Salt of Radical Cation of Terthiophene 2 ($2^{\bullet+}SbF_6^-$). Terthiophene **2** (20.6 mg, 0.050 mmol) and $NO^+SbF_6^-$ (13.4 mg, 0.050 mmol) were placed in a Pyrex tube connectable to a vacuum line under an argon atmosphere and the tube was evacuated. On the other hand, 2 mL of CH_2Cl_2 was dried over CaH_2, degassed by three freeze-pump-thaw cycles, and vapor-transferred directly into the cooled tube containing **2** and $NO^+SbF_6^-$. Then the connection to a vacuum line was closed, and the Pyrex tube was warmed to room temperature. When **2** and $NO^+SbF_6^-$ were completely dissolved in dry CH_2Cl_2 by mixing, the color of the solution turned to dark blue. After 5-minute mixing, the tube was connected to the vacuum line again, and 10 mL of hexane, which had been dried and degassed, was vapor-transferred onto the blue solution at −78°C. Slow diffusion of hexane under an argon atmosphere at room temperature for two weeks gave 28.5 mg of $\mathbf{2}^{\bullet+}SbF_6^-$ salts (88%) as a dark blue solid: mp(dec) 219.4-220.2 °C; UV-vis-NIR(CH_2Cl_2) λ_{max}(log ε) 618(4.73) 931(4.51)nm. Anal. Calcd for $C_{24}H_{24}F_6S_3Sb$: C, 44.73; H, 3.75. Found: C, 44.33; H, 3.76.

Reference

1. Wakamiya, A.; Yamazaki, D.; Nishinaga, T.; Kitagawa, T.; Komatsu, K. *J. Org. Chem.* **2003**, *68*, 8305-8314.

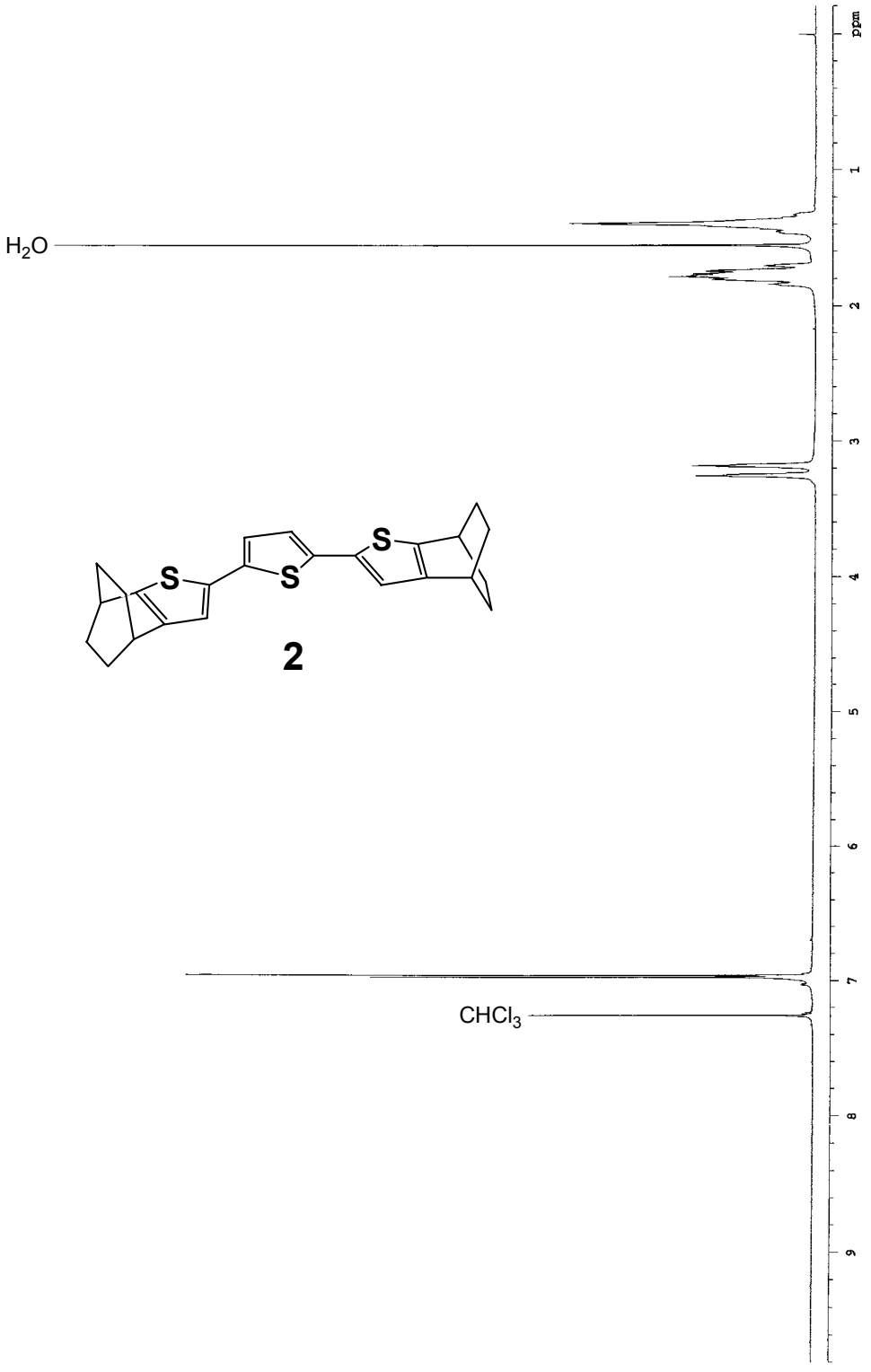


Figure S1. ^{1}H NMR (300 MHz) spectrum of 2

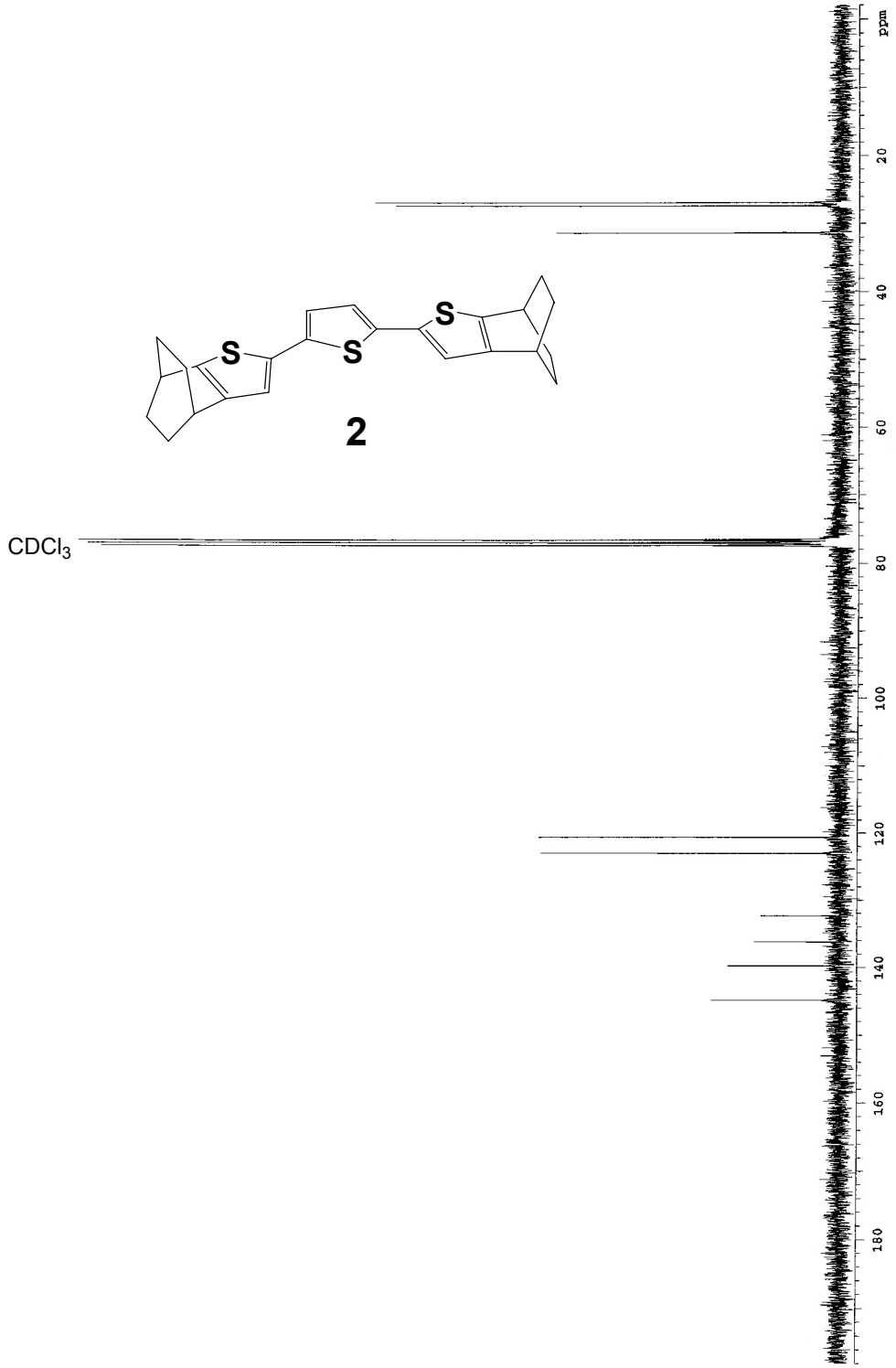


Figure S2. ^{13}C NMR (75.4 MHz) spectrum of 2

X-Ray Structural Determination. The intensity data were collected on a Bruker SMART APEX equipped with a CCD area detector with graphite monochromated MoKα radiation. Frames corresponding to an arbitrary hemispher of data were collected at –150 °C using ω scans of 0.3° counted for a total of 10 s per frame. The structures were solved using Bruker SHELXTL program package. Crystallographic data for terthiophene **2**, $\mathbf{2}^{\cdot+}SbF_6^{-}\cdot(CH_2Cl_2)_2$ are given in the CIF files.

X-Ray Crystallography of 2.

Table 1. Crystal data and structure refinement for **2**.

Identification code	2	
Empirical formula	C24 H24 S3	
Formula weight	408.61	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 40.384(4) Å	α= 90°.
	b = 6.3078(6) Å	β= 124.144(2)°.
	c = 27.942(3) Å	γ = 90°.
Volume	5890.9(10) $Å^3$	
Z	12	
Density (calculated)	1.382 Mg/m^3	
Absorption coefficient	0.384 mm^{-1}	
F(000)	2592	
Crystal size	0.30 x 0.30 x 0.10 mm^3	
Theta range for data collection	2.06 to 25.00°.	
Index ranges	-48<=h<=47, -7<=k<=7, -33<=l<=26	
Reflections collected	14701	
Independent reflections	5186 [R(int) = 0.0370]	
Completeness to theta = 25.00°	99.8 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9626 and 0.8934	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5186 / 2 / 423	
Goodness-of-fit on F^2	1.001	
Final R indices [I>2sigma(I)]	R1 = 0.0375, wR2 = 0.0754	
R indices (all data)	R1 = 0.0544, wR2 = 0.0792	
Largest diff. peak and hole	0.735 and -0.251 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(2)	7247(1)	8767(1)	1532(1)	23(1)
S(1)	6655(1)	11851(2)	2259(1)	27(1)
C(3)	6599(2)	8157(9)	1862(4)	33(2)
C(1)	6325(1)	10079(4)	2234(1)	27(1)
C(2)	6321(1)	8166(3)	2017(1)	24(1)
C(103)	6626(9)	11120(30)	2183(12)	107(17)
S(101)	6616(3)	7489(13)	1795(4)	27(2)
S(3)	7812(1)	12033(2)	836(1)	23(1)
C(10)	7928(2)	8234(8)	1215(3)	26(2)
C(11)	8107(1)	8318(3)	898(1)	24(1)
C(12)	8063(1)	10287(4)	678(1)	24(1)
C(110)	7845(9)	11240(30)	885(12)	125(18)
S(103)	7959(3)	7541(12)	1324(4)	23(2)
S(4)	5318(1)	6016(2)	9095(1)	23(1)
C(27)	5460(2)	2279(9)	8899(3)	29(2)
C(127)	5345(6)	5160(40)	9050(11)	78(11)
S(104)	5481(2)	1587(11)	8831(3)	23(1)
S(5)	5000	2869(1)	7500	25(1)
C(7)	7522(1)	12531(3)	1697(1)	27(1)
C(4)	6805(1)	9989(3)	1961(1)	20(1)
C(6)	7267(1)	12503(3)	1892(1)	26(1)
C(19)	8334(1)	6840(3)	758(1)	26(1)
C(25)	5536(1)	4204(3)	9636(1)	25(1)
C(8)	7545(1)	10622(3)	1489(1)	22(1)
C(29)	5143(1)	4764(3)	8030(1)	22(1)
C(5)	7095(1)	10587(3)	1835(1)	20(1)
C(28)	5302(1)	4148(4)	8619(1)	20(1)
C(24)	8066(1)	9028(3)	-145(1)	25(1)
C(9)	7761(1)	10080(4)	1231(1)	22(1)
C(14)	6122(1)	8621(3)	2838(1)	31(1)
C(34)	5816(1)	779(3)	9993(1)	29(1)

C(22)	8249(1)	10651(3)	352(1)	25(1)
C(30)	5081(1)	6728(3)	7797(1)	32(1)
C(31)	5686(1)	4487(4)	10259(1)	34(1)
C(17)	6096(1)	6428(3)	2576(1)	32(1)
C(23)	8696(1)	10119(4)	768(1)	30(1)
C(35)	6218(1)	1854(4)	10445(1)	38(1)
C(16)	6014(1)	6681(4)	1972(1)	32(1)
C(26)	5598(1)	2277(3)	9494(1)	23(1)
C(20)	8748(1)	7842(4)	1006(1)	32(1)
C(15)	5616(1)	9940(4)	1851(1)	47(1)
C(21)	8111(1)	6763(3)	98(1)	27(1)
C(36)	5575(1)	556(4)	10262(1)	38(1)
C(13)	6034(1)	10370(4)	2399(1)	33(1)
C(18)	5607(1)	7777(4)	1589(1)	45(1)
C(32)	6140(1)	4017(4)	10617(1)	40(1)
C(33)	5485(1)	2766(4)	10401(1)	43(1)

Table 3. Bond lengths [Å] and angles [°] for **2**.

S(2)-C(8)	1.731(2)
S(2)-C(5)	1.733(2)
S(1)-C(1)	1.712(2)
S(1)-C(4)	1.733(2)
C(3)-C(4)	1.357(7)
C(3)-C(2)	1.416(7)
C(1)-C(2)	1.345(3)
C(1)-C(103)	1.46(3)
C(1)-C(13)	1.494(3)
C(2)-C(16)	1.501(3)
C(2)-S(101)	1.680(7)
C(103)-C(4)	1.39(2)
S(101)-C(4)	1.698(8)
S(3)-C(12)	1.717(2)
S(3)-C(9)	1.738(2)
C(10)-C(9)	1.359(6)
C(10)-C(11)	1.422(7)
C(11)-C(12)	1.353(3)
C(11)-C(19)	1.505(3)
C(11)-S(103)	1.678(7)
C(12)-C(110)	1.43(3)
C(12)-C(22)	1.488(3)
C(110)-C(9)	1.39(2)
S(103)-C(9)	1.743(7)
S(4)-C(25)	1.695(2)
S(4)-C(28)	1.750(2)
C(27)-C(28)	1.359(7)
C(27)-C(26)	1.427(8)
C(127)-C(28)	1.28(3)
C(127)-C(25)	1.49(2)
S(104)-C(26)	1.692(7)
S(104)-C(28)	1.732(6)
S(5)-C(29)	1.730(2)
S(5)-C(29)#1	1.730(2)

C(7)-C(8)	1.363(3)
C(7)-C(6)	1.410(3)
C(4)-C(5)	1.450(3)
C(6)-C(5)	1.359(3)
C(19)-C(21)	1.535(3)
C(19)-C(20)	1.540(3)
C(25)-C(26)	1.346(3)
C(25)-C(31)	1.497(3)
C(8)-C(9)	1.451(3)
C(29)-C(30)	1.355(3)
C(29)-C(28)	1.446(3)
C(24)-C(22)	1.539(3)
C(24)-C(21)	1.548(3)
C(14)-C(13)	1.537(3)
C(14)-C(17)	1.541(3)
C(34)-C(26)	1.494(3)
C(34)-C(36)	1.536(3)
C(34)-C(35)	1.544(3)
C(22)-C(23)	1.540(3)
C(30)-C(30)#1	1.404(4)
C(31)-C(33)	1.534(3)
C(31)-C(32)	1.547(3)
C(17)-C(16)	1.533(3)
C(23)-C(20)	1.546(3)
C(35)-C(32)	1.536(3)
C(16)-C(18)	1.534(3)
C(15)-C(18)	1.538(3)
C(15)-C(13)	1.539(3)
C(36)-C(33)	1.543(3)

C(8)-S(2)-C(5)	92.18(10)
C(1)-S(1)-C(4)	90.62(12)
C(4)-C(3)-C(2)	115.7(4)
C(2)-C(1)-C(103)	99.3(6)
C(2)-C(1)-C(13)	115.8(2)
C(103)-C(1)-C(13)	144.9(6)

C(2)-C(1)-S(1)	114.62(17)
C(103)-C(1)-S(1)	15.4(6)
C(13)-C(1)-S(1)	129.53(18)
C(1)-C(2)-C(3)	109.3(3)
C(1)-C(2)-C(16)	113.46(19)
C(3)-C(2)-C(16)	137.1(3)
C(1)-C(2)-S(101)	124.2(3)
C(3)-C(2)-S(101)	14.9(4)
C(16)-C(2)-S(101)	122.3(3)
C(4)-C(103)-C(1)	119.0(11)
C(2)-S(101)-C(4)	88.0(4)
C(12)-S(3)-C(9)	90.32(12)
C(9)-C(10)-C(11)	115.0(3)
C(12)-C(11)-C(10)	109.6(3)
C(12)-C(11)-C(19)	113.17(19)
C(10)-C(11)-C(19)	137.3(3)
C(12)-C(11)-S(103)	125.7(3)
C(10)-C(11)-S(103)	16.3(4)
C(19)-C(11)-S(103)	121.0(3)
C(11)-C(12)-C(110)	98.8(6)
C(11)-C(12)-C(22)	116.0(2)
C(110)-C(12)-C(22)	145.2(6)
C(11)-C(12)-S(3)	114.61(18)
C(110)-C(12)-S(3)	15.8(6)
C(22)-C(12)-S(3)	129.37(17)
C(9)-C(110)-C(12)	120.4(12)
C(11)-S(103)-C(9)	86.6(3)
C(25)-S(4)-C(28)	90.21(12)
C(28)-C(27)-C(26)	114.9(4)
C(28)-C(127)-C(25)	123.1(16)
C(26)-S(104)-C(28)	86.6(3)
C(29)-S(5)-C(29)#1	92.60(15)
C(8)-C(7)-C(6)	113.2(2)
C(3)-C(4)-C(103)	96.8(10)
C(3)-C(4)-C(5)	131.0(3)
C(103)-C(4)-C(5)	132.1(10)

C(3)-C(4)-S(101)	12.8(4)
C(103)-C(4)-S(101)	109.5(10)
C(5)-C(4)-S(101)	118.3(3)
C(3)-C(4)-S(1)	109.8(3)
C(103)-C(4)-S(1)	13.0(10)
C(5)-C(4)-S(1)	119.15(16)
S(101)-C(4)-S(1)	122.5(3)
C(5)-C(6)-C(7)	113.8(2)
C(11)-C(19)-C(21)	107.50(17)
C(11)-C(19)-C(20)	107.13(17)
C(21)-C(19)-C(20)	108.01(18)
C(26)-C(25)-C(127)	96.1(11)
C(26)-C(25)-C(31)	115.5(2)
C(127)-C(25)-C(31)	148.4(11)
C(26)-C(25)-S(4)	115.74(18)
C(127)-C(25)-S(4)	19.7(10)
C(31)-C(25)-S(4)	128.71(18)
C(7)-C(8)-C(9)	128.7(2)
C(7)-C(8)-S(2)	110.52(16)
C(9)-C(8)-S(2)	120.71(16)
C(30)-C(29)-C(28)	129.5(2)
C(30)-C(29)-S(5)	109.81(16)
C(28)-C(29)-S(5)	120.72(17)
C(6)-C(5)-C(4)	129.3(2)
C(6)-C(5)-S(2)	110.31(16)
C(4)-C(5)-S(2)	120.29(16)
C(127)-C(28)-C(27)	96.7(9)
C(127)-C(28)-C(29)	132.5(9)
C(27)-C(28)-C(29)	130.8(3)
C(127)-C(28)-S(104)	109.3(9)
C(27)-C(28)-S(104)	12.5(4)
C(29)-C(28)-S(104)	118.2(3)
C(127)-C(28)-S(4)	13.3(9)
C(27)-C(28)-S(4)	110.0(3)
C(29)-C(28)-S(4)	119.22(17)
S(104)-C(28)-S(4)	122.5(2)

C(22)-C(24)-C(21)	109.87(17)
C(10)-C(9)-C(110)	96.2(11)
C(10)-C(9)-C(8)	131.8(3)
C(110)-C(9)-C(8)	131.9(11)
C(10)-C(9)-S(3)	110.5(3)
C(110)-C(9)-S(3)	14.3(11)
C(8)-C(9)-S(3)	117.67(17)
C(10)-C(9)-S(103)	12.4(4)
C(110)-C(9)-S(103)	108.4(11)
C(8)-C(9)-S(103)	119.6(3)
S(3)-C(9)-S(103)	122.7(3)
C(13)-C(14)-C(17)	109.91(18)
C(26)-C(34)-C(36)	108.13(18)
C(26)-C(34)-C(35)	106.50(18)
C(36)-C(34)-C(35)	107.65(19)
C(12)-C(22)-C(24)	107.26(17)
C(12)-C(22)-C(23)	106.50(17)
C(24)-C(22)-C(23)	107.69(17)
C(29)-C(30)-C(30)#1	113.89(13)
C(25)-C(31)-C(33)	106.74(18)
C(25)-C(31)-C(32)	106.78(18)
C(33)-C(31)-C(32)	107.7(2)
C(16)-C(17)-C(14)	110.17(18)
C(22)-C(23)-C(20)	110.19(17)
C(32)-C(35)-C(34)	109.94(19)
C(2)-C(16)-C(17)	108.29(18)
C(2)-C(16)-C(18)	106.74(19)
C(17)-C(16)-C(18)	107.53(19)
C(25)-C(26)-C(27)	109.1(3)
C(25)-C(26)-C(34)	113.9(2)
C(27)-C(26)-C(34)	136.7(3)
C(25)-C(26)-S(104)	124.9(3)
C(27)-C(26)-S(104)	15.8(4)
C(34)-C(26)-S(104)	121.0(3)
C(19)-C(20)-C(23)	109.74(17)
C(18)-C(15)-C(13)	110.47(18)

C(19)-C(21)-C(24)	110.08(17)
C(34)-C(36)-C(33)	110.04(18)
C(1)-C(13)-C(14)	106.78(18)
C(1)-C(13)-C(15)	106.58(19)
C(14)-C(13)-C(15)	107.53(18)
C(16)-C(18)-C(15)	109.7(2)
C(35)-C(32)-C(31)	110.10(19)
C(31)-C(33)-C(36)	110.01(19)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,y,-z+3/2

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(2)	23(1)	24(1)	28(1)	-2(1)	17(1)	-2(1)
S(1)	35(1)	21(1)	40(1)	-2(1)	30(1)	-3(1)
C(3)	33(3)	36(4)	31(3)	-11(3)	18(2)	0(3)
C(1)	25(1)	26(1)	30(1)	2(1)	17(1)	-2(1)
C(2)	18(1)	31(1)	25(1)	-3(1)	13(1)	-1(1)
C(103)	130(20)	60(20)	68(17)	-32(15)	18(15)	-46(17)
S(101)	25(2)	31(4)	38(3)	-12(3)	25(2)	-14(2)
S(3)	25(1)	25(1)	26(1)	-3(1)	19(1)	-4(1)
C(10)	24(2)	27(4)	23(3)	2(2)	11(2)	-6(2)
C(11)	18(1)	31(1)	21(1)	-3(1)	10(1)	-7(1)
C(12)	20(1)	24(1)	28(1)	-5(1)	14(1)	-3(1)
C(110)	100(20)	60(20)	120(30)	-39(18)	4(19)	-22(16)
S(103)	25(2)	27(4)	27(3)	-5(3)	20(2)	-5(2)
S(4)	27(1)	20(1)	23(1)	1(1)	14(1)	1(1)
C(27)	22(2)	28(4)	34(3)	-8(3)	13(2)	-9(3)
C(127)	47(10)	29(13)	160(30)	27(13)	59(14)	20(10)
S(104)	19(2)	25(3)	16(2)	6(2)	5(2)	-3(2)
S(5)	32(1)	18(1)	24(1)	0	15(1)	0
C(7)	27(1)	30(1)	26(1)	-8(1)	16(1)	-10(1)
C(4)	17(1)	21(1)	17(1)	-3(1)	8(1)	0(1)
C(6)	25(1)	28(1)	25(1)	-7(1)	14(1)	-4(1)
C(19)	28(1)	22(1)	27(1)	4(1)	15(1)	0(1)
C(25)	23(1)	22(1)	32(1)	2(1)	16(1)	-3(1)
C(8)	16(1)	28(1)	21(1)	0(1)	9(1)	-3(1)
C(29)	15(1)	23(1)	24(1)	-2(1)	9(1)	-1(1)
C(5)	16(1)	26(1)	15(1)	-1(1)	7(1)	0(1)
C(28)	16(1)	19(1)	24(1)	-3(1)	11(1)	-1(1)
C(24)	26(1)	27(1)	23(1)	1(1)	14(1)	-2(1)
C(9)	20(1)	24(1)	23(1)	-2(1)	12(1)	-6(1)
C(14)	35(1)	35(2)	32(1)	-1(1)	23(1)	-2(1)
C(34)	35(1)	18(1)	31(1)	-1(1)	18(1)	-2(1)

C(22)	28(1)	20(1)	31(1)	0(1)	20(1)	-2(1)
C(30)	39(1)	20(1)	24(1)	-2(1)	9(1)	-1(1)
C(31)	47(2)	25(1)	39(2)	-8(1)	31(1)	-8(1)
C(17)	29(1)	25(1)	42(2)	6(1)	21(1)	1(1)
C(23)	24(1)	39(2)	34(1)	-12(1)	20(1)	-12(1)
C(35)	35(1)	41(2)	25(1)	9(1)	8(1)	-1(1)
C(16)	29(1)	29(1)	42(2)	-13(1)	23(1)	-9(1)
C(26)	20(1)	24(1)	24(1)	-2(1)	12(1)	-7(1)
C(20)	25(1)	41(2)	28(1)	2(1)	14(1)	4(1)
C(15)	31(1)	63(2)	58(2)	37(2)	33(2)	23(1)
C(21)	31(1)	23(1)	29(1)	-3(1)	18(1)	-2(1)
C(36)	53(2)	29(1)	38(2)	3(1)	28(1)	-8(1)
C(13)	46(2)	19(1)	51(2)	3(1)	37(2)	5(1)
C(18)	23(1)	76(2)	34(2)	1(1)	15(1)	-13(1)
C(32)	48(2)	46(2)	24(1)	-8(1)	19(1)	-19(1)
C(33)	63(2)	38(2)	47(2)	-7(1)	42(2)	-14(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **2**.

	x	y	z	U(eq)
H(3)	6640	6946	1698	40
H(103)	6699	12552	2301	128
H(10)	7926	6981	1401	32
H(110)	7757	12662	786	150
H(27)	5477	1066	8712	35
H(127)	5252	6575	8993	94
H(7)	7663	13757	1709	32
H(6)	7220	13711	2049	31
H(19)	8359	5395	923	31
H(24A)	8202	9120	-348	30
H(24B)	7779	9351	-427	30
H(14A)	5926	8702	2944	38
H(14B)	6393	8827	3193	38
H(34)	5859	-626	9870	35
H(22)	8208	12139	205	30
H(30)	5140	7991	8017	39
H(31)	5628	5941	10337	40
H(17A)	6351	5655	2830	38
H(17B)	5879	5590	2549	38
H(23A)	8824	11141	1093	36
H(23B)	8831	10240	562	36
H(35A)	6371	939	10791	46
H(35B)	6378	2049	10281	46
H(16)	6018	5281	1808	38
H(20A)	8899	6974	896	38
H(20B)	8901	7881	1433	38
H(15A)	5415	9955	1948	56
H(15B)	5546	11073	1563	56
H(21A)	7844	6123	-73	32
H(21B)	8262	5869	-9	32
H(36A)	5729	-292	10622	46

H(36B)	5321	-194	9990	46
H(13)	6053	11817	2559	40
H(18A)	5395	6878	1559	54
H(18B)	5545	7980	1195	54
H(32A)	6280	5140	10549	48
H(32B)	6246	4012	11034	48
H(33A)	5192	3003	10171	52
H(33B)	5587	2843	10815	52

Table 6. Torsion angles [°] for **2**.

C(4)-S(1)-C(1)-C(2)	0.26(19)
C(4)-S(1)-C(1)-C(103)	-2(5)
C(4)-S(1)-C(1)-C(13)	-177.6(2)
C(103)-C(1)-C(2)-C(3)	0.2(13)
C(13)-C(1)-C(2)-C(3)	177.8(4)
S(1)-C(1)-C(2)-C(3)	-0.4(4)
C(103)-C(1)-C(2)-C(16)	-176.6(12)
C(13)-C(1)-C(2)-C(16)	1.0(3)
S(1)-C(1)-C(2)-C(16)	-177.10(16)
C(103)-C(1)-C(2)-S(101)	1.6(13)
C(13)-C(1)-C(2)-S(101)	179.2(5)
S(1)-C(1)-C(2)-S(101)	1.1(5)
C(4)-C(3)-C(2)-C(1)	0.3(7)
C(4)-C(3)-C(2)-C(16)	175.9(3)
C(4)-C(3)-C(2)-S(101)	-175(3)
C(2)-C(1)-C(103)-C(4)	-1(2)
C(13)-C(1)-C(103)-C(4)	-176.9(5)
S(1)-C(1)-C(103)-C(4)	177(7)
C(1)-C(2)-S(101)-C(4)	-1.7(6)
C(3)-C(2)-S(101)-C(4)	4(2)
C(16)-C(2)-S(101)-C(4)	176.3(2)
C(9)-C(10)-C(11)-C(12)	-0.5(6)
C(9)-C(10)-C(11)-C(19)	177.9(3)
C(9)-C(10)-C(11)-S(103)	171(3)
C(10)-C(11)-C(12)-C(110)	-1.0(12)
C(19)-C(11)-C(12)-C(110)	-179.8(11)
S(103)-C(11)-C(12)-C(110)	-3.8(12)
C(10)-C(11)-C(12)-C(22)	177.8(4)
C(19)-C(11)-C(12)-C(22)	-1.0(3)
S(103)-C(11)-C(12)-C(22)	175.0(4)
C(10)-C(11)-C(12)-S(3)	-0.3(4)
C(19)-C(11)-C(12)-S(3)	-179.15(14)
S(103)-C(11)-C(12)-S(3)	-3.1(5)
C(9)-S(3)-C(12)-C(11)	0.77(18)

C(9)-S(3)-C(12)-C(110)	3(4)
C(9)-S(3)-C(12)-C(22)	-177.1(2)
C(11)-C(12)-C(110)-C(9)	2(2)
C(22)-C(12)-C(110)-C(9)	-175.7(5)
S(3)-C(12)-C(110)-C(9)	-175(6)
C(12)-C(11)-S(103)-C(9)	3.4(5)
C(10)-C(11)-S(103)-C(9)	-6.1(18)
C(19)-C(11)-S(103)-C(9)	179.1(2)
C(2)-C(3)-C(4)-C(103)	-0.6(14)
C(2)-C(3)-C(4)-C(5)	-176.8(3)
C(2)-C(3)-C(4)-S(101)	174(4)
C(2)-C(3)-C(4)-S(1)	-0.1(7)
C(1)-C(103)-C(4)-C(3)	1(2)
C(1)-C(103)-C(4)-C(5)	176.9(9)
C(1)-C(103)-C(4)-S(101)	0(3)
C(1)-C(103)-C(4)-S(1)	-177(8)
C(2)-S(101)-C(4)-C(3)	-4(3)
C(2)-S(101)-C(4)-C(103)	1.0(14)
C(2)-S(101)-C(4)-C(5)	-176.7(2)
C(2)-S(101)-C(4)-S(1)	1.9(6)
C(1)-S(1)-C(4)-C(3)	-0.1(4)
C(1)-S(1)-C(4)-C(103)	2(6)
C(1)-S(1)-C(4)-C(5)	177.08(17)
C(1)-S(1)-C(4)-S(101)	-1.5(4)
C(8)-C(7)-C(6)-C(5)	0.0(3)
C(12)-C(11)-C(19)-C(21)	-57.2(2)
C(10)-C(11)-C(19)-C(21)	124.5(5)
S(103)-C(11)-C(19)-C(21)	126.6(4)
C(12)-C(11)-C(19)-C(20)	58.7(2)
C(10)-C(11)-C(19)-C(20)	-119.6(5)
S(103)-C(11)-C(19)-C(20)	-117.5(4)
C(28)-C(127)-C(25)-C(26)	-2.2(17)
C(28)-C(127)-C(25)-C(31)	174.3(5)
C(28)-C(127)-C(25)-S(4)	176(4)
C(28)-S(4)-C(25)-C(26)	-0.35(19)
C(28)-S(4)-C(25)-C(127)	-3(2)

C(28)-S(4)-C(25)-C(31)	176.4(2)
C(6)-C(7)-C(8)-C(9)	177.0(2)
C(6)-C(7)-C(8)-S(2)	0.2(2)
C(5)-S(2)-C(8)-C(7)	-0.27(17)
C(5)-S(2)-C(8)-C(9)	-177.35(18)
C(29)#1-S(5)-C(29)-C(30)	-0.05(12)
C(29)#1-S(5)-C(29)-C(28)	180.0(2)
C(7)-C(6)-C(5)-C(4)	-176.7(2)
C(7)-C(6)-C(5)-S(2)	-0.2(2)
C(3)-C(4)-C(5)-C(6)	173.2(5)
C(103)-C(4)-C(5)-C(6)	-1.7(17)
S(101)-C(4)-C(5)-C(6)	175.4(4)
S(1)-C(4)-C(5)-C(6)	-3.3(3)
C(3)-C(4)-C(5)-S(2)	-3.0(6)
C(103)-C(4)-C(5)-S(2)	-178.0(17)
S(101)-C(4)-C(5)-S(2)	-0.8(5)
S(1)-C(4)-C(5)-S(2)	-179.51(12)
C(8)-S(2)-C(5)-C(6)	0.25(16)
C(8)-S(2)-C(5)-C(4)	177.15(17)
C(25)-C(127)-C(28)-C(27)	2.1(17)
C(25)-C(127)-C(28)-C(29)	-177.4(7)
C(25)-C(127)-C(28)-S(104)	2.0(19)
C(25)-C(127)-C(28)-S(4)	-174(5)
C(26)-C(27)-C(28)-C(127)	-1.1(11)
C(26)-C(27)-C(28)-C(29)	178.4(3)
C(26)-C(27)-C(28)-S(104)	179(100)
C(26)-C(27)-C(28)-S(4)	-0.2(7)
C(30)-C(29)-C(28)-C(127)	17.8(13)
S(5)-C(29)-C(28)-C(127)	-162.2(12)
C(30)-C(29)-C(28)-C(27)	-161.5(5)
S(5)-C(29)-C(28)-C(27)	18.5(5)
C(30)-C(29)-C(28)-S(104)	-161.6(4)
S(5)-C(29)-C(28)-S(104)	18.4(4)
C(30)-C(29)-C(28)-S(4)	16.9(3)
S(5)-C(29)-C(28)-S(4)	-163.11(12)
C(26)-S(104)-C(28)-C(127)	-0.8(10)

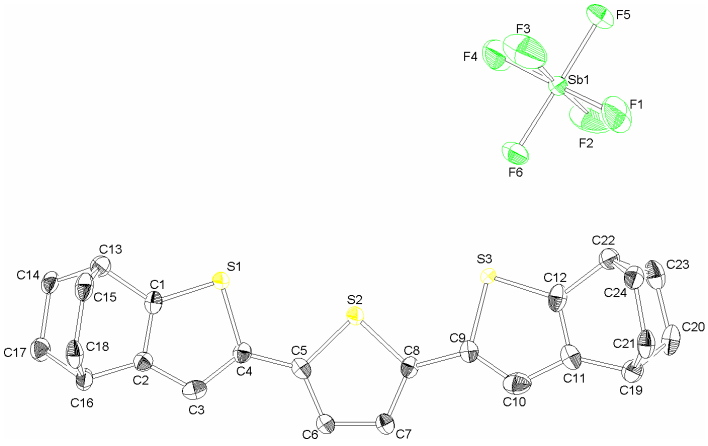
C(26)-S(104)-C(28)-C(27)	-1(2)
C(26)-S(104)-C(28)-C(29)	178.7(2)
C(26)-S(104)-C(28)-S(4)	0.3(4)
C(25)-S(4)-C(28)-C(127)	4(4)
C(25)-S(4)-C(28)-C(27)	0.3(4)
C(25)-S(4)-C(28)-C(29)	-178.45(17)
C(25)-S(4)-C(28)-S(104)	0.0(3)
C(11)-C(10)-C(9)-C(110)	1.7(13)
C(11)-C(10)-C(9)-C(8)	178.1(3)
C(11)-C(10)-C(9)-S(3)	1.0(6)
C(11)-C(10)-C(9)-S(103)	-169(3)
C(12)-C(110)-C(9)-C(10)	-3(2)
C(12)-C(110)-C(9)-C(8)	-179.0(9)
C(12)-C(110)-C(9)-S(3)	175(6)
C(12)-C(110)-C(9)-S(103)	-1(2)
C(7)-C(8)-C(9)-C(10)	150.9(5)
S(2)-C(8)-C(9)-C(10)	-32.6(5)
C(7)-C(8)-C(9)-C(110)	-33.8(15)
S(2)-C(8)-C(9)-C(110)	142.7(15)
C(7)-C(8)-C(9)-S(3)	-32.1(3)
S(2)-C(8)-C(9)-S(3)	144.37(14)
C(7)-C(8)-C(9)-S(103)	147.8(4)
S(2)-C(8)-C(9)-S(103)	-35.7(4)
C(12)-S(3)-C(9)-C(10)	-1.0(4)
C(12)-S(3)-C(9)-C(110)	-4(5)
C(12)-S(3)-C(9)-C(8)	-178.54(17)
C(12)-S(3)-C(9)-S(103)	1.5(4)
C(11)-S(103)-C(9)-C(10)	8(2)
C(11)-S(103)-C(9)-C(110)	-1.3(12)
C(11)-S(103)-C(9)-C(8)	177.4(2)
C(11)-S(103)-C(9)-S(3)	-2.6(5)
C(11)-C(12)-C(22)-C(24)	57.9(2)
C(110)-C(12)-C(22)-C(24)	-124.1(19)
S(3)-C(12)-C(22)-C(24)	-124.3(2)
C(11)-C(12)-C(22)-C(23)	-57.2(2)
C(110)-C(12)-C(22)-C(23)	120.8(19)

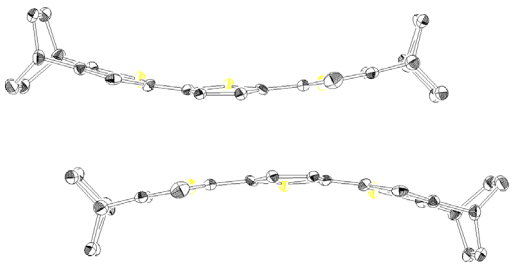
S(3)-C(12)-C(22)-C(23)	120.6(2)
C(21)-C(24)-C(22)-C(12)	-53.5(2)
C(21)-C(24)-C(22)-C(23)	60.8(2)
C(28)-C(29)-C(30)-C(30)#1	-179.9(2)
S(5)-C(29)-C(30)-C(30)#1	0.1(3)
C(26)-C(25)-C(31)-C(33)	-56.8(3)
C(127)-C(25)-C(31)-C(33)	127.1(15)
S(4)-C(25)-C(31)-C(33)	126.4(2)
C(26)-C(25)-C(31)-C(32)	58.1(2)
C(127)-C(25)-C(31)-C(32)	-118.0(15)
S(4)-C(25)-C(31)-C(32)	-118.7(2)
C(13)-C(14)-C(17)-C(16)	3.1(3)
C(12)-C(22)-C(23)-C(20)	55.3(2)
C(24)-C(22)-C(23)-C(20)	-59.5(2)
C(26)-C(34)-C(35)-C(32)	57.6(2)
C(36)-C(34)-C(35)-C(32)	-58.2(2)
C(1)-C(2)-C(16)-C(17)	-57.6(3)
C(3)-C(2)-C(16)-C(17)	126.9(6)
S(101)-C(2)-C(16)-C(17)	124.2(5)
C(1)-C(2)-C(16)-C(18)	57.9(3)
C(3)-C(2)-C(16)-C(18)	-117.6(6)
S(101)-C(2)-C(16)-C(18)	-120.3(5)
C(14)-C(17)-C(16)-C(2)	52.7(2)
C(14)-C(17)-C(16)-C(18)	-62.3(2)
C(127)-C(25)-C(26)-C(27)	1.1(9)
C(31)-C(25)-C(26)-C(27)	-176.9(4)
S(4)-C(25)-C(26)-C(27)	0.3(4)
C(127)-C(25)-C(26)-C(34)	176.6(8)
C(31)-C(25)-C(26)-C(34)	-1.4(3)
S(4)-C(25)-C(26)-C(34)	175.86(15)
C(127)-C(25)-C(26)-S(104)	1.5(9)
C(31)-C(25)-C(26)-S(104)	-176.5(4)
S(4)-C(25)-C(26)-S(104)	0.7(4)
C(28)-C(27)-C(26)-C(25)	-0.1(7)
C(28)-C(27)-C(26)-C(34)	-174.1(3)
C(28)-C(27)-C(26)-S(104)	-179(100)

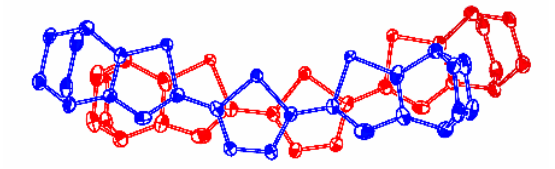
C(36)-C(34)-C(26)-C(25)	57.8(2)
C(35)-C(34)-C(26)-C(25)	-57.7(2)
C(36)-C(34)-C(26)-C(27)	-128.3(5)
C(35)-C(34)-C(26)-C(27)	116.2(5)
C(36)-C(34)-C(26)-S(104)	-126.9(4)
C(35)-C(34)-C(26)-S(104)	117.7(4)
C(28)-S(104)-C(26)-C(25)	-0.6(5)
C(28)-S(104)-C(26)-C(27)	0.8(18)
C(28)-S(104)-C(26)-C(34)	-175.4(2)
C(11)-C(19)-C(20)-C(23)	-54.9(2)
C(21)-C(19)-C(20)-C(23)	60.7(2)
C(22)-C(23)-C(20)-C(19)	-1.0(3)
C(11)-C(19)-C(21)-C(24)	56.0(2)
C(20)-C(19)-C(21)-C(24)	-59.3(2)
C(22)-C(24)-C(21)-C(19)	-1.4(2)
C(26)-C(34)-C(36)-C(33)	-52.6(2)
C(35)-C(34)-C(36)-C(33)	62.1(2)
C(2)-C(1)-C(13)-C(14)	56.9(3)
C(103)-C(1)-C(13)-C(14)	-127(2)
S(1)-C(1)-C(13)-C(14)	-125.3(2)
C(2)-C(1)-C(13)-C(15)	-57.8(3)
C(103)-C(1)-C(13)-C(15)	118(2)
S(1)-C(1)-C(13)-C(15)	120.0(2)
C(17)-C(14)-C(13)-C(1)	-56.2(2)
C(17)-C(14)-C(13)-C(15)	57.8(2)
C(18)-C(15)-C(13)-C(1)	52.9(2)
C(18)-C(15)-C(13)-C(14)	-61.3(2)
C(2)-C(16)-C(18)-C(15)	-57.2(2)
C(17)-C(16)-C(18)-C(15)	58.8(2)
C(13)-C(15)-C(18)-C(16)	2.4(3)
C(34)-C(35)-C(32)-C(31)	-3.2(3)
C(25)-C(31)-C(32)-C(35)	-52.4(2)
C(33)-C(31)-C(32)-C(35)	61.9(2)
C(25)-C(31)-C(33)-C(36)	56.4(3)
C(32)-C(31)-C(33)-C(36)	-58.0(3)
C(34)-C(36)-C(33)-C(31)	-3.3(3)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,y,-z+3/2

X-Ray Crystallography of $2^{\bullet+}SbF_6^-$ (100K).







Packing Structure

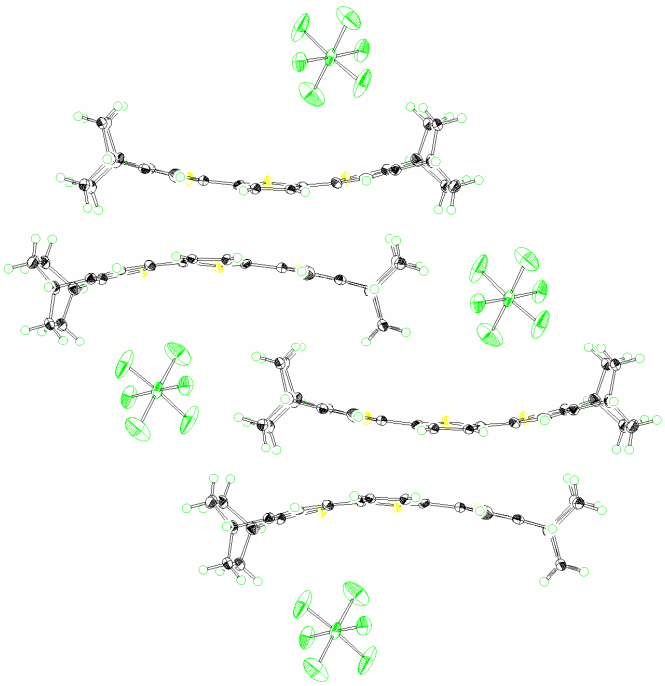


Table 1. Crystal data and structure refinement for $\mathbf{2}^{\bullet+}\mathbf{SbF_6}^-$.

Identification code	100KpD	
Empirical formula	C24 H24 F6 S3 Sb	
Formula weight	644.36	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbcn	
Unit cell dimensions	a = 11.6808(17) Å	α= 90°.
	b = 21.565(3) Å	β= 90°.
	c = 19.163(3) Å	γ = 90°.
Volume	4826.9(12) $Å^3$	
Z	8	
Density (calculated)	1.773 Mg/m^3	
Absorption coefficient	1.461 mm^{-1}	
F(000)	2568	
Crystal size	0.15 x 0.15 x 0.10 mm^3	
Theta range for data collection	1.89 to 25.00°.	
Index ranges	-13<=h<=13, -25<=k<=20, -22<=l<=22	
Reflections collected	23249	
Independent reflections	4244 [R(int) = 0.0586]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	Empirical	
Max. and min. transmission	0.8677 and 0.8106	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4244 / 12 / 340	
Goodness-of-fit on F^2	1.002	
Final R indices [I>2sigma(I)]	R1 = 0.0490, wR2 = 0.1004	
R indices (all data)	R1 = 0.0784, wR2 = 0.1092	
Largest diff. peak and hole	1.741 and -0.444 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $\mathbf{2}^{\bullet+}\mathbf{SbF_6}^-$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(18)	11211(5)	6253(3)	6881(3)	28(1)
C(12)	6647(4)	6237(3)	1628(3)	27(1)
C(17)	13196(5)	6158(3)	6410(3)	27(1)
C(13)	11702(5)	5353(3)	6085(3)	25(1)
C(11)	6561(4)	6879(2)	1569(3)	25(1)
C(15)	10987(5)	5554(3)	6725(3)	29(1)
C(16)	12064(5)	6528(3)	6351(3)	25(1)
C(20)	5793(5)	6816(3)	388(3)	30(1)
C(22)	5760(5)	5888(3)	1203(3)	29(1)
C(7)	9334(4)	7358(2)	3162(3)	20(1)
C(9)	8052(4)	6694(2)	2385(3)	20(1)
C(2)	11589(4)	6410(2)	5653(3)	20(1)
C(23)	5935(5)	6110(3)	445(3)	33(1)
C(6)	10052(4)	7287(2)	3723(3)	18(1)
C(19)	5614(5)	7101(3)	1119(3)	27(1)
C(8)	8870(4)	6790(2)	2919(3)	19(1)
C(14)	12988(5)	5462(2)	6248(3)	24(1)
C(24)	4562(5)	6118(2)	1454(3)	27(1)
C(1)	11378(5)	5798(2)	5496(3)	22(1)
C(5)	10176(5)	6670(2)	3939(3)	20(1)
C(21)	4494(5)	6835(3)	1421(3)	28(1)
C(4)	10760(5)	6436(2)	4527(3)	21(1)
Sb(1)	7261(1)	3978(1)	942(1)	30(1)
S(2)	9380(1)	6178(1)	3411(1)	21(1)
F(6)	7676(3)	4641(2)	1512(2)	51(1)
F(5)	6803(3)	3298(2)	400(2)	44(1)
F(1)	5850(4)	4357(2)	795(3)	84(2)
F(4)	8607(4)	3582(2)	1153(3)	79(2)
F(2)	7859(5)	4355(2)	173(2)	86(2)
F(3)	6595(5)	3580(2)	1724(2)	87(2)
C(10)	7407(12)	7092(5)	2023(7)	34(4)

S(3)	7670(3)	5921(1)	2148(2)	18(1)
S(13)	7429(6)	7374(3)	1998(4)	26(2)
C(110)	7531(17)	6181(6)	2131(12)	26(7)
S(1)	10797(2)	5647(1)	4712(1)	21(1)
C(3)	11244(16)	6770(5)	5084(6)	23(2)
C(103)	10810(100)	5829(8)	4830(30)	70(60)
S(11)	11220(40)	6977(4)	5125(12)	26(7)

Table 3. Bond lengths [Å] and angles [°] for $\mathbf{2}^{\bullet+}\mathbf{SbF_6}^-$.

C(18)-C(16)	1.542(8)
C(18)-C(15)	1.559(8)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(12)-C(11)	1.391(8)
C(12)-C(110)	1.417(15)
C(12)-C(22)	1.518(7)
C(12)-S(3)	1.699(5)
C(17)-C(16)	1.549(8)
C(17)-C(14)	1.553(7)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(13)-C(1)	1.528(7)
C(13)-C(15)	1.546(8)
C(13)-C(14)	1.552(8)
C(13)-H(13)	1.0000
C(11)-C(10)	1.395(13)
C(11)-C(19)	1.483(7)
C(11)-S(13)	1.687(7)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(2)	1.470(7)
C(16)-H(16)	1.0000
C(20)-C(23)	1.536(8)
C(20)-C(19)	1.544(7)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(22)-C(23)	1.543(8)
C(22)-C(24)	1.561(8)
C(22)-H(22)	1.0000
C(7)-C(6)	1.372(7)
C(7)-C(8)	1.419(7)
C(7)-H(7)	0.9500
C(9)-C(10)	1.337(13)

C(9)-C(110)	1.353(15)
C(9)-C(8)	1.415(7)
C(9)-S(3)	1.784(5)
C(9)-S(13)	1.797(6)
C(2)-C(1)	1.375(7)
C(2)-C(3)	1.399(11)
C(2)-S(11)	1.646(10)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(6)-C(5)	1.401(7)
C(6)-H(6)	0.9500
C(19)-C(21)	1.541(8)
C(19)-H(19)	1.0000
C(8)-S(2)	1.727(5)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(24)-C(21)	1.549(8)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(1)-C(103)	1.443(17)
C(1)-S(1)	1.682(5)
C(5)-C(4)	1.411(7)
C(5)-S(2)	1.736(5)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(4)-C(3)	1.405(12)
C(4)-C(103)	1.433(18)
C(4)-S(11)	1.720(11)
C(4)-S(1)	1.738(5)
Sb(1)-F(2)	1.821(4)
Sb(1)-F(4)	1.834(4)
Sb(1)-F(1)	1.861(4)
Sb(1)-F(6)	1.864(3)
Sb(1)-F(5)	1.876(3)
Sb(1)-F(3)	1.894(4)
C(10)-H(10)	0.9500

C(110)-H(110)	0.9500
C(3)-H(3)	0.9500
C(103)-H(103)	0.9500

C(16)-C(18)-C(15)	110.8(4)
C(16)-C(18)-H(18A)	109.5
C(15)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
C(15)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	108.1
C(11)-C(12)-C(110)	101.1(6)
C(11)-C(12)-C(22)	113.6(4)
C(110)-C(12)-C(22)	145.0(7)
C(11)-C(12)-S(3)	119.8(3)
C(110)-C(12)-S(3)	19.0(6)
C(22)-C(12)-S(3)	126.5(4)
C(16)-C(17)-C(14)	110.5(4)
C(16)-C(17)-H(17A)	109.6
C(14)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.6
C(14)-C(17)-H(17B)	109.6
H(17A)-C(17)-H(17B)	108.1
C(1)-C(13)-C(15)	106.1(4)
C(1)-C(13)-C(14)	107.1(4)
C(15)-C(13)-C(14)	108.7(4)
C(1)-C(13)-H(13)	111.6
C(15)-C(13)-H(13)	111.6
C(14)-C(13)-H(13)	111.6
C(12)-C(11)-C(10)	103.1(5)
C(12)-C(11)-C(19)	115.0(4)
C(10)-C(11)-C(19)	141.7(6)
C(12)-C(11)-S(13)	123.1(4)
C(10)-C(11)-S(13)	20.1(5)
C(19)-C(11)-S(13)	121.8(4)
C(13)-C(15)-C(18)	109.4(4)
C(13)-C(15)-H(15A)	109.8

C(18)-C(15)-H(15A)	109.8
C(13)-C(15)-H(15B)	109.8
C(18)-C(15)-H(15B)	109.8
H(15A)-C(15)-H(15B)	108.2
C(2)-C(16)-C(18)	106.7(4)
C(2)-C(16)-C(17)	107.5(5)
C(18)-C(16)-C(17)	107.8(5)
C(2)-C(16)-H(16)	111.6
C(18)-C(16)-H(16)	111.6
C(17)-C(16)-H(16)	111.5
C(23)-C(20)-C(19)	110.2(4)
C(23)-C(20)-H(20A)	109.6
C(19)-C(20)-H(20A)	109.6
C(23)-C(20)-H(20B)	109.6
C(19)-C(20)-H(20B)	109.6
H(20A)-C(20)-H(20B)	108.1
C(12)-C(22)-C(23)	105.1(5)
C(12)-C(22)-C(24)	106.8(5)
C(23)-C(22)-C(24)	108.1(5)
C(12)-C(22)-H(22)	112.2
C(23)-C(22)-H(22)	112.2
C(24)-C(22)-H(22)	112.2
C(6)-C(7)-C(8)	113.3(5)
C(6)-C(7)-H(7)	123.4
C(8)-C(7)-H(7)	123.4
C(10)-C(9)-C(110)	94.8(10)
C(10)-C(9)-C(8)	131.4(6)
C(110)-C(9)-C(8)	133.1(7)
C(10)-C(9)-S(3)	109.1(6)
C(110)-C(9)-S(3)	14.6(6)
C(8)-C(9)-S(3)	119.3(4)
C(10)-C(9)-S(13)	14.8(5)
C(110)-C(9)-S(13)	109.6(6)
C(8)-C(9)-S(13)	116.9(4)
S(3)-C(9)-S(13)	123.8(4)
C(1)-C(2)-C(3)	108.1(6)

C(1)-C(2)-C(16)	115.7(4)
C(3)-C(2)-C(16)	136.2(6)
C(1)-C(2)-S(11)	122.1(5)
C(3)-C(2)-S(11)	14.5(8)
C(16)-C(2)-S(11)	122.0(6)
C(20)-C(23)-C(22)	111.1(5)
C(20)-C(23)-H(23A)	109.4
C(22)-C(23)-H(23A)	109.4
C(20)-C(23)-H(23B)	109.4
C(22)-C(23)-H(23B)	109.4
H(23A)-C(23)-H(23B)	108.0
C(7)-C(6)-C(5)	113.6(5)
C(7)-C(6)-H(6)	123.2
C(5)-C(6)-H(6)	123.2
C(11)-C(19)-C(21)	107.2(4)
C(11)-C(19)-C(20)	107.3(5)
C(21)-C(19)-C(20)	107.8(5)
C(11)-C(19)-H(19)	111.5
C(21)-C(19)-H(19)	111.4
C(20)-C(19)-H(19)	111.5
C(9)-C(8)-C(7)	128.4(5)
C(9)-C(8)-S(2)	121.1(4)
C(7)-C(8)-S(2)	110.4(4)
C(13)-C(14)-C(17)	109.8(4)
C(13)-C(14)-H(14A)	109.7
C(17)-C(14)-H(14A)	109.7
C(13)-C(14)-H(14B)	109.7
C(17)-C(14)-H(14B)	109.7
H(14A)-C(14)-H(14B)	108.2
C(21)-C(24)-C(22)	110.5(4)
C(21)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24A)	109.5
C(21)-C(24)-H(24B)	109.6
C(22)-C(24)-H(24B)	109.6
H(24A)-C(24)-H(24B)	108.1
C(2)-C(1)-C(103)	103.4(6)

C(2)-C(1)-C(13)	113.4(4)
C(103)-C(1)-C(13)	142.9(11)
C(2)-C(1)-S(1)	116.9(3)
C(103)-C(1)-S(1)	14.1(14)
C(13)-C(1)-S(1)	129.7(4)
C(6)-C(5)-C(4)	128.7(5)
C(6)-C(5)-S(2)	110.6(4)
C(4)-C(5)-S(2)	120.4(4)
C(19)-C(21)-C(24)	110.2(5)
C(19)-C(21)-H(21A)	109.6
C(24)-C(21)-H(21A)	109.6
C(19)-C(21)-H(21B)	109.6
C(24)-C(21)-H(21B)	109.6
H(21A)-C(21)-H(21B)	108.1
C(3)-C(4)-C(5)	128.1(5)
C(3)-C(4)-C(103)	98.4(10)
C(5)-C(4)-C(103)	132.0(16)
C(3)-C(4)-S(11)	12.1(7)
C(5)-C(4)-S(11)	116.1(6)
C(103)-C(4)-S(11)	109.8(6)
C(3)-C(4)-S(1)	109.7(5)
C(5)-C(4)-S(1)	121.6(4)
C(103)-C(4)-S(1)	12.0(16)
S(11)-C(4)-S(1)	121.4(5)
F(2)-Sb(1)-F(4)	93.3(3)
F(2)-Sb(1)-F(1)	91.2(3)
F(4)-Sb(1)-F(1)	175.5(3)
F(2)-Sb(1)-F(6)	91.9(2)
F(4)-Sb(1)-F(6)	90.31(17)
F(1)-Sb(1)-F(6)	88.97(18)
F(2)-Sb(1)-F(5)	90.56(18)
F(4)-Sb(1)-F(5)	90.14(17)
F(1)-Sb(1)-F(5)	90.39(18)
F(6)-Sb(1)-F(5)	177.51(18)
F(2)-Sb(1)-F(3)	178.0(2)
F(4)-Sb(1)-F(3)	88.1(3)

F(1)-Sb(1)-F(3)	87.4(3)
F(6)-Sb(1)-F(3)	89.50(19)
F(5)-Sb(1)-F(3)	88.07(18)
C(8)-S(2)-C(5)	92.1(3)
C(9)-C(10)-C(11)	120.7(8)
C(9)-C(10)-H(10)	119.6
C(11)-C(10)-H(10)	119.6
C(12)-S(3)-C(9)	87.1(3)
C(11)-S(13)-C(9)	85.8(3)
C(9)-C(110)-C(12)	120.2(9)
C(9)-C(110)-H(110)	119.9
C(12)-C(110)-H(110)	119.9
C(1)-S(1)-C(4)	90.1(3)
C(2)-C(3)-C(4)	115.0(8)
C(2)-C(3)-H(3)	122.5
C(4)-C(3)-H(3)	122.5
C(4)-C(103)-C(1)	114.7(16)
C(4)-C(103)-H(103)	122.0
C(1)-C(103)-H(103)	122.0
C(2)-S(11)-C(4)	89.2(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3) for $\mathbf{2}^{\bullet+}\mathbf{SbF_6}^-$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(18)	24(3)	44(4)	15(3)	-2(3)	-2(2)	4(3)
C(12)	17(3)	41(4)	22(3)	7(3)	1(2)	2(3)
C(17)	21(3)	31(3)	30(3)	2(3)	-4(3)	-1(2)
C(13)	29(3)	24(3)	21(3)	4(2)	0(3)	-2(2)
C(11)	20(3)	36(3)	18(3)	-3(3)	4(2)	-5(2)
C(15)	25(3)	43(4)	19(3)	11(3)	-1(3)	-2(3)
C(16)	26(3)	27(3)	20(3)	-1(2)	-6(3)	6(2)
C(20)	21(3)	49(4)	22(3)	7(3)	-1(3)	5(3)
C(22)	22(3)	25(3)	39(4)	2(3)	-8(3)	-3(2)
C(7)	18(3)	24(3)	19(3)	-2(2)	0(2)	-1(2)
C(9)	17(3)	27(3)	17(3)	0(2)	2(2)	0(2)
C(2)	19(3)	20(3)	21(3)	2(2)	1(2)	-1(2)
C(23)	28(3)	50(4)	21(3)	-8(3)	-2(3)	2(3)
C(6)	17(3)	22(3)	15(3)	-2(2)	3(2)	-1(2)
C(19)	25(3)	28(3)	27(3)	1(2)	0(2)	2(2)
C(8)	10(3)	25(3)	22(3)	3(2)	1(2)	1(2)
C(14)	27(4)	27(3)	18(3)	8(2)	-3(2)	0(2)
C(24)	20(3)	30(3)	30(3)	10(3)	-4(3)	-8(2)
C(1)	18(3)	29(3)	19(3)	2(2)	-1(2)	2(2)
C(5)	17(3)	26(3)	16(3)	-3(2)	4(2)	-4(2)
C(21)	23(3)	45(4)	16(3)	0(3)	-1(2)	6(3)
C(4)	22(3)	23(3)	16(3)	4(2)	2(2)	-1(2)
Sb(1)	30(1)	21(1)	38(1)	1(1)	-15(1)	-3(1)
S(2)	25(1)	19(1)	19(1)	3(1)	-6(1)	-5(1)
F(6)	55(3)	30(2)	69(3)	-16(2)	-26(2)	2(2)
F(5)	49(2)	36(2)	48(2)	-9(2)	-11(2)	-13(2)
F(1)	49(3)	77(3)	127(5)	-38(3)	-50(3)	26(2)
F(4)	54(3)	56(3)	127(4)	-32(3)	-50(3)	23(2)
F(2)	143(5)	57(3)	57(3)	6(2)	21(3)	-47(3)
F(3)	136(5)	74(3)	50(3)	-8(2)	17(3)	-45(3)
C(10)	42(7)	26(7)	34(6)	4(6)	7(5)	-6(6)

S(3)	21(1)	13(2)	19(1)	2(1)	-6(1)	1(1)
S(13)	13(3)	43(5)	23(3)	3(3)	-5(2)	-3(3)
C(110)	0(11)	42(18)	37(14)	41(15)	6(8)	2(12)
S(1)	27(1)	17(1)	20(1)	2(1)	-7(1)	-3(1)
C(3)	22(5)	20(5)	26(5)	-1(4)	9(3)	4(6)
S(11)	21(11)	35(15)	20(11)	7(10)	2(8)	4(13)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $\mathbf{2}^{\bullet+}\mathbf{SbF_6}^-$.

	x	y	z	U(eq)
H(18A)	10480	6484	6857	33
H(18B)	11522	6298	7359	33
H(17A)	13510	6202	6888	33
H(17B)	13765	6328	6078	33
H(13)	11548	4912	5954	30
H(15A)	11204	5301	7136	34
H(15B)	10163	5487	6631	34
H(16)	12189	6981	6432	29
H(20A)	5126	6913	89	36
H(20B)	6483	6998	170	36
H(22)	5845	5428	1249	34
H(7)	9165	7748	2956	24
H(23A)	6711	5991	286	40
H(23B)	5371	5903	138	40
H(6)	10430	7625	3944	22
H(19)	5592	7565	1098	32
H(14A)	13458	5335	5843	29
H(14B)	13218	5207	6655	29
H(24A)	3958	5936	1155	32
H(24B)	4428	5978	1940	32
H(21A)	3841	6960	1123	34
H(21B)	4365	7004	1895	34
H(10)	7526	7526	2076	41
H(110)	7757	5782	2289	32
H(3)	11330	7208	5074	27
H(103)	10497	5474	4605	86

Table 6. Torsion angles [°] for $\mathbf{2}^{\bullet+}\mathbf{SbF_6}^-$.

C(110)-C(12)-C(11)-C(10)	1.3(14)
C(22)-C(12)-C(11)-C(10)	177.1(8)
S(3)-C(12)-C(11)-C(10)	-2.3(9)
C(110)-C(12)-C(11)-C(19)	-174.5(12)
C(22)-C(12)-C(11)-C(19)	1.3(7)
S(3)-C(12)-C(11)-C(19)	-178.1(4)
C(110)-C(12)-C(11)-S(13)	3.1(13)
C(22)-C(12)-C(11)-S(13)	178.9(5)
S(3)-C(12)-C(11)-S(13)	-0.5(8)
C(1)-C(13)-C(15)-C(18)	-55.3(6)
C(14)-C(13)-C(15)-C(18)	59.6(5)
C(16)-C(18)-C(15)-C(13)	0.3(6)
C(15)-C(18)-C(16)-C(2)	55.5(6)
C(15)-C(18)-C(16)-C(17)	-59.7(6)
C(14)-C(17)-C(16)-C(2)	-54.9(6)
C(14)-C(17)-C(16)-C(18)	59.8(6)
C(11)-C(12)-C(22)-C(23)	57.2(6)
C(110)-C(12)-C(22)-C(23)	-130(2)
S(3)-C(12)-C(22)-C(23)	-123.5(5)
C(11)-C(12)-C(22)-C(24)	-57.5(6)
C(110)-C(12)-C(22)-C(24)	115(2)
S(3)-C(12)-C(22)-C(24)	121.9(5)
C(18)-C(16)-C(2)-C(1)	-57.4(6)
C(17)-C(16)-C(2)-C(1)	58.0(6)
C(18)-C(16)-C(2)-C(3)	120.3(13)
C(17)-C(16)-C(2)-C(3)	-124.4(13)
C(18)-C(16)-C(2)-S(11)	117(2)
C(17)-C(16)-C(2)-S(11)	-128(2)
C(19)-C(20)-C(23)-C(22)	4.6(7)
C(12)-C(22)-C(23)-C(20)	-58.2(6)
C(24)-C(22)-C(23)-C(20)	55.5(6)
C(8)-C(7)-C(6)-C(5)	0.0(7)
C(12)-C(11)-C(19)-C(21)	57.5(6)
C(10)-C(11)-C(19)-C(21)	-115.9(12)

S(13)-C(11)-C(19)-C(21)	-120.1(6)
C(12)-C(11)-C(19)-C(20)	-58.1(6)
C(10)-C(11)-C(19)-C(20)	128.5(12)
S(13)-C(11)-C(19)-C(20)	124.3(6)
C(23)-C(20)-C(19)-C(11)	52.5(6)
C(23)-C(20)-C(19)-C(21)	-62.6(6)
C(10)-C(9)-C(8)-C(7)	-8.6(12)
C(110)-C(9)-C(8)-C(7)	-177.5(17)
S(3)-C(9)-C(8)-C(7)	176.5(5)
S(13)-C(9)-C(8)-C(7)	-5.1(8)
C(10)-C(9)-C(8)-S(2)	167.5(9)
C(110)-C(9)-C(8)-S(2)	-1.4(18)
S(3)-C(9)-C(8)-S(2)	-7.4(6)
S(13)-C(9)-C(8)-S(2)	171.0(4)
C(6)-C(7)-C(8)-C(9)	175.7(5)
C(6)-C(7)-C(8)-S(2)	-0.7(6)
C(1)-C(13)-C(14)-C(17)	54.7(6)
C(15)-C(13)-C(14)-C(17)	-59.5(6)
C(16)-C(17)-C(14)-C(13)	-0.6(6)
C(12)-C(22)-C(24)-C(21)	53.0(6)
C(23)-C(22)-C(24)-C(21)	-59.6(6)
C(3)-C(2)-C(1)-C(103)	-4(5)
C(16)-C(2)-C(1)-C(103)	174(5)
S(11)-C(2)-C(1)-C(103)	0(6)
C(3)-C(2)-C(1)-C(13)	-179.1(9)
C(16)-C(2)-C(1)-C(13)	-0.8(7)
S(11)-C(2)-C(1)-C(13)	-175(2)
C(3)-C(2)-C(1)-S(1)	0.0(10)
C(16)-C(2)-C(1)-S(1)	178.2(4)
S(11)-C(2)-C(1)-S(1)	4(2)
C(15)-C(13)-C(1)-C(2)	59.0(6)
C(14)-C(13)-C(1)-C(2)	-57.0(6)
C(15)-C(13)-C(1)-C(103)	-113(8)
C(14)-C(13)-C(1)-C(103)	131(8)
C(15)-C(13)-C(1)-S(1)	-120.0(5)
C(14)-C(13)-C(1)-S(1)	124.1(5)

C(7)-C(6)-C(5)-C(4)	-174.0(5)
C(7)-C(6)-C(5)-S(2)	0.8(6)
C(11)-C(19)-C(21)-C(24)	-57.1(6)
C(20)-C(19)-C(21)-C(24)	58.1(6)
C(22)-C(24)-C(21)-C(19)	2.4(6)
C(6)-C(5)-C(4)-C(3)	8.3(14)
S(2)-C(5)-C(4)-C(3)	-166.0(11)
C(6)-C(5)-C(4)-C(103)	171(7)
S(2)-C(5)-C(4)-C(103)	-3(7)
C(6)-C(5)-C(4)-S(11)	10(2)
S(2)-C(5)-C(4)-S(11)	-164.5(18)
C(6)-C(5)-C(4)-S(1)	179.0(4)
S(2)-C(5)-C(4)-S(1)	4.8(7)
C(9)-C(8)-S(2)-C(5)	-175.8(4)
C(7)-C(8)-S(2)-C(5)	1.0(4)
C(6)-C(5)-S(2)-C(8)	-1.0(4)
C(4)-C(5)-S(2)-C(8)	174.2(5)
C(110)-C(9)-C(10)-C(11)	-0.9(17)
C(8)-C(9)-C(10)-C(11)	-172.9(7)
S(3)-C(9)-C(10)-C(11)	2.5(14)
S(13)-C(9)-C(10)-C(11)	175(4)
C(12)-C(11)-C(10)-C(9)	-0.3(14)
C(19)-C(11)-C(10)-C(9)	173.6(7)
S(13)-C(11)-C(10)-C(9)	-176(3)
C(11)-C(12)-S(3)-C(9)	3.1(5)
C(110)-C(12)-S(3)-C(9)	-8(4)
C(22)-C(12)-S(3)-C(9)	-176.2(5)
C(10)-C(9)-S(3)-C(12)	-2.9(8)
C(110)-C(9)-S(3)-C(12)	11(5)
C(8)-C(9)-S(3)-C(12)	173.1(5)
S(13)-C(9)-S(3)-C(12)	-5.2(5)
C(12)-C(11)-S(13)-C(9)	-2.5(7)
C(10)-C(11)-S(13)-C(9)	3(2)
C(19)-C(11)-S(13)-C(9)	175.0(5)
C(10)-C(9)-S(13)-C(11)	-4(3)
C(110)-C(9)-S(13)-C(11)	0.8(14)

C(8)-C(9)-S(13)-C(11)	-173.4(5)
S(3)-C(9)-S(13)-C(11)	5.0(6)
C(10)-C(9)-C(110)-C(12)	2(2)
C(8)-C(9)-C(110)-C(12)	173.7(10)
S(3)-C(9)-C(110)-C(12)	-165(7)
S(13)-C(9)-C(110)-C(12)	1(2)
C(11)-C(12)-C(110)-C(9)	-2(2)
C(22)-C(12)-C(110)-C(9)	-175.5(8)
S(3)-C(12)-C(110)-C(9)	168(6)
C(2)-C(1)-S(1)-C(4)	-1.2(5)
C(103)-C(1)-S(1)-C(4)	16(20)
C(13)-C(1)-S(1)-C(4)	177.7(5)
C(3)-C(4)-S(1)-C(1)	2.0(9)
C(5)-C(4)-S(1)-C(1)	-170.3(5)
C(103)-C(4)-S(1)-C(1)	-19(23)
S(11)-C(4)-S(1)-C(1)	-2(2)
C(1)-C(2)-C(3)-C(4)	1.7(16)
C(16)-C(2)-C(3)-C(4)	-176.1(7)
S(11)-C(2)-C(3)-C(4)	-165(11)
C(5)-C(4)-C(3)-C(2)	169.1(8)
C(103)-C(4)-C(3)-C(2)	2(5)
S(11)-C(4)-C(3)-C(2)	163(12)
S(1)-C(4)-C(3)-C(2)	-2.5(16)
C(3)-C(4)-C(103)-C(1)	-5(9)
C(5)-C(4)-C(103)-C(1)	-171(3)
S(11)-C(4)-C(103)-C(1)	-9(10)
S(1)-C(4)-C(103)-C(1)	155(31)
C(2)-C(1)-C(103)-C(4)	6(9)
C(13)-C(1)-C(103)-C(4)	178.0(14)
S(1)-C(1)-C(103)-C(4)	-158(27)
C(1)-C(2)-S(11)-C(4)	-4(3)
C(3)-C(2)-S(11)-C(4)	11(8)
C(16)-C(2)-S(11)-C(4)	-178.0(7)
C(3)-C(4)-S(11)-C(2)	-13(9)
C(5)-C(4)-S(11)-C(2)	172.4(10)
C(103)-C(4)-S(11)-C(2)	7(6)

S(1)-C(4)-S(11)-C(2)	3(3)
C(3)-C(4)-C(5)-C(6)	8.3(14)
C(7)-C(8)-C(9)-C(10)	-8.6(12)
S(1)-C(4)-C(5)-S(2)	4.8(7)
S(2)-C(8)-C(9)-S(3)	-7.4(6)

Symmetry transformations used to generate equivalent atoms:

X-Ray Crystallography of $2^{\bullet+}SbF_6^-$ (298K).

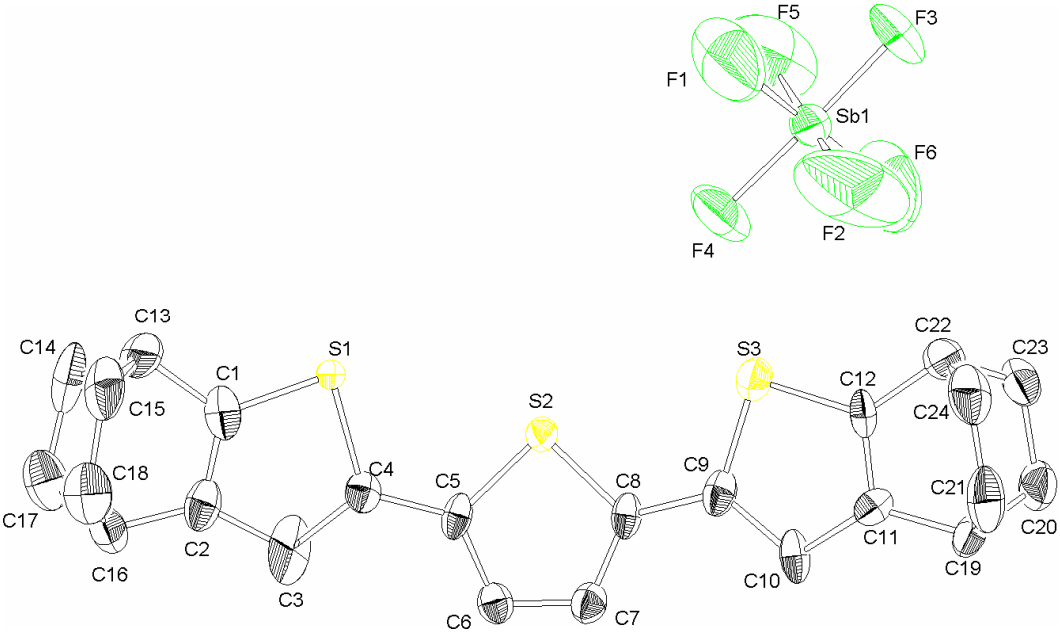


Table 1. Crystal data and structure refinement for $\mathbf{2}^{\bullet+}\mathbf{SbF_6}^-$.

Identification code	RTpD	
Empirical formula	C24 H24 F6 S3 Sb	
Formula weight	644.36	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbcn	
Unit cell dimensions	a = 11.7896(13) Å	α= 90°.
	b = 21.747(2) Å	β= 90°.
	c = 19.296(2) Å	γ = 90°.
Volume	4947.1(10) $Å^3$	
Z	8	
Density (calculated)	1.730 Mg/m^3	
Absorption coefficient	1.426 mm^{-1}	
F(000)	2568	
Crystal size	0.15 x 0.15 x 0.10 mm^3	
Theta range for data collection	1.87 to 25.00°.	
Index ranges	-12<=h<=14, -25<=k<=23, -22<=l<=22	
Reflections collected	23652	
Independent reflections	4357 [R(int) = 0.0695]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	Empirical	
Max. and min. transmission	0.8706 and 0.8146	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4357 / 6 / 326	
Goodness-of-fit on F^2	1.412	
Final R indices [I>2sigma(I)]	R1 = 0.1277, wR2 = 0.2476	
R indices (all data)	R1 = 0.1468, wR2 = 0.2559	
Largest diff. peak and hole	1.790 and -0.496 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $\mathbf{2}^{\bullet+}\mathbf{SbF_6}^-$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Sb(1)	2247(1)	1046(1)	9077(1)	58(1)
S(2)	4376(3)	1162(1)	1589(2)	34(1)
S(3)	5794(3)	648(2)	288(2)	47(1)
S(1)	2653(7)	902(3)	2841(4)	31(2)
C(3)	2430(30)	2098(15)	2964(16)	69(12)
S(101)	2436(15)	2338(7)	2993(13)	63(7)
C(103)	2560(40)	1137(17)	2850(30)	50(20)
F(1)	3519(14)	1444(7)	8838(12)	204(10)
C(4)	3054(9)	1668(4)	2611(6)	31(3)
C(11)	6538(10)	1415(5)	-618(6)	33(3)
C(5)	3865(9)	1769(5)	2076(5)	30(3)
F(3)	1767(10)	1716(5)	9595(6)	109(4)
C(12)	6372(10)	798(6)	-509(6)	38(3)
C(10)	6186(9)	1803(6)	-81(5)	34(3)
C(13)	787(11)	887(6)	3781(8)	50(4)
C(7)	5020(10)	2262(5)	1284(6)	34(3)
F(4)	2647(11)	391(5)	8496(7)	124(5)
C(8)	5145(9)	1652(5)	1068(5)	29(2)
C(22)	6701(12)	371(6)	-1072(6)	44(3)
C(19)	7019(11)	1531(6)	-1335(6)	42(3)
C(6)	4307(9)	2326(5)	1837(6)	32(3)
C(2)	1563(9)	1853(6)	3421(6)	42(3)
C(21)	6173(13)	1254(8)	-1854(7)	60(4)
C(16)	652(11)	2074(6)	3865(6)	44(3)
C(20)	8128(11)	1174(6)	-1410(7)	48(3)
C(17)	818(12)	1805(7)	4586(7)	58(4)
C(9)	5724(10)	1433(5)	476(6)	35(3)
C(1)	1662(10)	1223(6)	3365(6)	46(3)
C(23)	7934(11)	493(6)	-1244(7)	46(3)
C(24)	5977(13)	567(7)	-1692(7)	57(4)
F(2)	2820(20)	676(8)	9803(9)	232(12)

F(6)	885(13)	664(8)	9226(11)	200(10)
C(18)	-450(11)	1818(7)	3575(8)	57(4)
C(15)	-408(11)	1107(7)	3534(8)	60(4)
C(14)	956(12)	1108(8)	4532(7)	66(5)
F(5)	1600(20)	1442(8)	8303(8)	194(9)

Table 3. Bond lengths [Å] and angles [°] for $\mathbf{2}^{\bullet+}\mathbf{SbF_6}^-$.

Sb(1)-F(2)	1.749(15)
Sb(1)-F(1)	1.792(13)
Sb(1)-F(6)	1.830(12)
Sb(1)-F(3)	1.856(9)
Sb(1)-F(4)	1.871(9)
Sb(1)-F(5)	1.888(16)
S(2)-C(8)	1.723(11)
S(2)-C(5)	1.729(11)
S(3)-C(12)	1.715(12)
S(3)-C(9)	1.746(12)
S(1)-C(1)	1.696(12)
S(1)-C(4)	1.788(10)
C(3)-C(4)	1.37(3)
C(3)-C(2)	1.45(3)
S(101)-C(2)	1.689(14)
S(101)-C(4)	1.787(12)
C(103)-C(4)	1.38(3)
C(103)-C(1)	1.46(4)
C(4)-C(5)	1.424(15)
C(11)-C(12)	1.371(16)
C(11)-C(10)	1.399(16)
C(11)-C(19)	1.518(16)
C(5)-C(6)	1.396(15)
C(12)-C(22)	1.481(16)
C(10)-C(9)	1.449(16)
C(13)-C(1)	1.498(15)
C(13)-C(14)	1.54(2)
C(13)-C(15)	1.563(19)
C(7)-C(6)	1.365(15)
C(7)-C(8)	1.398(15)
C(8)-C(9)	1.414(15)
C(22)-C(23)	1.514(18)
C(22)-C(24)	1.530(19)
C(19)-C(20)	1.527(18)

C(19)-C(21)	1.536(19)
C(2)-C(1)	1.378(19)
C(2)-C(16)	1.457(15)
C(21)-C(24)	1.54(2)
C(16)-C(18)	1.520(18)
C(16)-C(17)	1.521(18)
C(20)-C(23)	1.532(18)
C(17)-C(14)	1.53(2)
C(18)-C(15)	1.55(2)

F(2)-Sb(1)-F(1)	96.1(12)
F(2)-Sb(1)-F(6)	90.3(12)
F(1)-Sb(1)-F(6)	173.5(11)
F(2)-Sb(1)-F(3)	92.7(7)
F(1)-Sb(1)-F(3)	90.8(6)
F(6)-Sb(1)-F(3)	90.2(6)
F(2)-Sb(1)-F(4)	91.9(7)
F(1)-Sb(1)-F(4)	90.1(6)
F(6)-Sb(1)-F(4)	88.3(6)
F(3)-Sb(1)-F(4)	175.1(6)
F(2)-Sb(1)-F(5)	178.7(12)
F(1)-Sb(1)-F(5)	85.1(11)
F(6)-Sb(1)-F(5)	88.5(11)
F(3)-Sb(1)-F(5)	86.8(6)
F(4)-Sb(1)-F(5)	88.6(7)
C(8)-S(2)-C(5)	91.6(5)
C(12)-S(3)-C(9)	91.1(6)
C(1)-S(1)-C(4)	86.9(6)
C(4)-C(3)-C(2)	115(2)
C(2)-S(101)-C(4)	86.6(7)
C(4)-C(103)-C(1)	115(2)
C(3)-C(4)-C(103)	100(3)
C(3)-C(4)-C(5)	128.0(15)
C(103)-C(4)-C(5)	131.3(18)
C(3)-C(4)-S(101)	11.7(16)
C(103)-C(4)-S(101)	111.8(15)

C(5)-C(4)-S(101)	116.6(9)
C(3)-C(4)-S(1)	111.7(15)
C(103)-C(4)-S(1)	11.8(17)
C(5)-C(4)-S(1)	120.1(8)
S(101)-C(4)-S(1)	123.3(8)
C(12)-C(11)-C(10)	115.8(11)
C(12)-C(11)-C(19)	110.8(10)
C(10)-C(11)-C(19)	133.3(11)
C(6)-C(5)-C(4)	128.5(10)
C(6)-C(5)-S(2)	110.7(8)
C(4)-C(5)-S(2)	120.7(8)
C(11)-C(12)-C(22)	117.7(11)
C(11)-C(12)-S(3)	112.3(9)
C(22)-C(12)-S(3)	130.0(10)
C(11)-C(10)-C(9)	109.0(11)
C(1)-C(13)-C(14)	105.3(11)
C(1)-C(13)-C(15)	107.9(11)
C(14)-C(13)-C(15)	108.0(11)
C(6)-C(7)-C(8)	113.2(10)
C(7)-C(8)-C(9)	127.8(10)
C(7)-C(8)-S(2)	110.9(8)
C(9)-C(8)-S(2)	121.0(9)
C(12)-C(22)-C(23)	107.6(10)
C(12)-C(22)-C(24)	104.6(11)
C(23)-C(22)-C(24)	108.4(11)
C(11)-C(19)-C(20)	108.8(10)
C(11)-C(19)-C(21)	106.6(10)
C(20)-C(19)-C(21)	107.2(11)
C(7)-C(6)-C(5)	113.5(10)
C(1)-C(2)-C(3)	105.0(14)
C(1)-C(2)-C(16)	115.8(9)
C(3)-C(2)-C(16)	139.1(17)
C(1)-C(2)-S(101)	122.0(6)
C(3)-C(2)-S(101)	17.1(14)
C(16)-C(2)-S(101)	122.1(10)
C(19)-C(21)-C(24)	110.1(11)

C(2)-C(16)-C(18)	107.0(10)
C(2)-C(16)-C(17)	108.5(11)
C(18)-C(16)-C(17)	107.8(12)
C(19)-C(20)-C(23)	110.1(10)
C(16)-C(17)-C(14)	109.4(11)
C(8)-C(9)-C(10)	126.3(11)
C(8)-C(9)-S(3)	121.4(9)
C(10)-C(9)-S(3)	111.8(8)
C(2)-C(1)-C(103)	104.1(14)
C(2)-C(1)-C(13)	112.6(9)
C(103)-C(1)-C(13)	143.0(16)
C(2)-C(1)-S(1)	121.0(5)
C(103)-C(1)-S(1)	17.0(15)
C(13)-C(1)-S(1)	126.4(10)
C(22)-C(23)-C(20)	111.0(11)
C(22)-C(24)-C(21)	110.2(11)
C(16)-C(18)-C(15)	111.0(11)
C(18)-C(15)-C(13)	108.5(10)
C(17)-C(14)-C(13)	111.1(12)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3) for $\mathbf{2}^{\bullet+}\mathbf{SbF_6}^-$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2\, a^{*2}U^{11} + \ldots + 2\, h\, k\, a^*\, b^*\, U^{12}\,]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Sb(1)	54(1)	40(1)	81(1)	4(1)	31(1)	9(1)
S(2)	42(2)	27(1)	34(2)	-6(1)	15(1)	-9(1)
S(3)	62(2)	42(2)	38(2)	-4(1)	18(2)	-10(2)
S(1)	34(3)	20(4)	38(3)	2(3)	18(2)	2(3)
C(3)	90(30)	110(30)	3(11)	-8(15)	-4(12)	-10(20)
S(101)	24(7)	108(15)	58(11)	-20(9)	10(6)	2(7)
C(103)	40(30)	40(40)	60(30)	-50(30)	0(30)	-30(30)
F(1)	136(13)	138(13)	340(30)	-99(15)	137(16)	-60(10)
C(4)	31(6)	38(6)	23(6)	-5(5)	-3(5)	-5(5)
C(11)	34(7)	32(6)	33(6)	5(5)	0(5)	-6(5)
C(5)	20(6)	49(7)	20(5)	0(5)	0(4)	-9(5)
F(3)	129(10)	71(6)	127(9)	-32(6)	52(8)	34(6)
C(12)	32(7)	52(7)	31(7)	-5(6)	15(5)	6(6)
C(10)	23(6)	64(8)	15(5)	-11(5)	-4(4)	2(5)
C(13)	31(7)	47(8)	73(10)	6(7)	18(7)	-8(6)
C(7)	37(7)	38(6)	27(6)	0(5)	3(5)	-4(5)
F(4)	139(10)	60(6)	173(12)	-50(7)	75(9)	-5(6)
C(8)	27(6)	48(7)	14(5)	-1(5)	-1(4)	-2(5)
C(22)	62(9)	38(7)	33(7)	-6(5)	5(6)	-6(6)
C(19)	43(8)	46(7)	36(7)	10(6)	14(6)	-1(6)
C(6)	30(6)	37(6)	28(6)	-5(5)	-1(5)	0(5)
C(2)	40(7)	62(9)	23(6)	0(6)	0(5)	-9(6)
C(21)	53(9)	99(12)	27(7)	-6(7)	3(6)	9(8)
C(16)	48(8)	47(7)	38(7)	-8(6)	7(6)	7(6)
C(20)	38(7)	55(8)	52(8)	-6(7)	15(6)	-7(6)
C(17)	39(8)	80(11)	53(9)	-11(8)	-2(7)	13(7)
C(9)	33(7)	50(7)	23(6)	-1(5)	2(5)	-9(5)
C(1)	41(8)	64(9)	34(7)	-8(6)	6(6)	3(6)
C(23)	44(8)	49(8)	44(7)	-14(6)	7(6)	2(6)
C(24)	60(9)	77(10)	33(7)	-22(7)	-1(7)	-6(8)
F(2)	410(30)	132(13)	151(15)	23(11)	-72(18)	128(17)

F(6)	118(12)	174(14)	310(20)	-98(15)	129(14)	-74(11)
C(18)	34(8)	84(11)	54(9)	-3(8)	-7(6)	5(7)
C(15)	32(7)	88(11)	60(9)	-21(8)	14(6)	-27(7)
C(14)	41(8)	120(14)	35(8)	19(9)	15(6)	6(9)
F(5)	310(30)	152(14)	120(12)	-13(10)	-40(15)	63(16)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $\mathbf{2}^{\bullet+}\mathbf{SbF_6}^-$.

	x	y	z	U(eq)
H(3)	2552	2519	2914	83
H(103)	2782	749	2703	55
H(10)	6241	2230	-81	41
H(13)	872	440	3741	60
H(7)	5385	2592	1073	41
H(22)	6570	-59	-945	53
H(19)	7133	1971	-1419	50
H(6)	4132	2704	2036	38
H(21A)	6466	1298	-2321	71
H(21B)	5459	1474	-1827	71
H(16)	636	2524	3880	53
H(20A)	8692	1342	-1097	58
H(20B)	8411	1215	-1880	58
H(17A)	168	1901	4874	69
H(17B)	1487	1983	4799	69
H(23A)	8155	245	-1640	55
H(23B)	8405	375	-854	55
H(24A)	5182	498	-1589	68
H(24B)	6176	321	-2093	68
H(18A)	-579	1985	3116	69
H(18B)	-1076	1942	3870	69
H(15A)	-541	973	3061	72
H(15B)	-993	930	3827	72
H(14A)	406	908	4830	79
H(14B)	1708	993	4689	79

Table 6. Torsion angles [°] for $\mathbf{2}^{\bullet+}\mathbf{SbF_6}^-$.

C(2)-C(3)-C(4)-C(103)	0(4)
C(2)-C(3)-C(4)-C(5)	172.4(16)
C(2)-C(3)-C(4)-S(101)	-175(14)
C(2)-C(3)-C(4)-S(1)	-2(3)
C(1)-C(103)-C(4)-C(3)	-2(5)
C(1)-C(103)-C(4)-C(5)	-173(2)
C(1)-C(103)-C(4)-S(101)	-1(6)
C(1)-C(103)-C(4)-S(1)	168(18)
C(2)-S(101)-C(4)-C(3)	4(11)
C(2)-S(101)-C(4)-C(103)	-1(3)
C(2)-S(101)-C(4)-C(5)	172.7(10)
C(2)-S(101)-C(4)-S(1)	-4.3(16)
C(1)-S(1)-C(4)-C(3)	2(2)
C(1)-S(1)-C(4)-C(103)	-10(14)
C(1)-S(1)-C(4)-C(5)	-173.3(10)
C(1)-S(1)-C(4)-S(101)	3.6(13)
C(3)-C(4)-C(5)-C(6)	8(3)
C(103)-C(4)-C(5)-C(6)	178(4)
S(101)-C(4)-C(5)-C(6)	4.8(18)
S(1)-C(4)-C(5)-C(6)	-178.1(10)
C(3)-C(4)-C(5)-S(2)	-168(2)
C(103)-C(4)-C(5)-S(2)	2(4)
S(101)-C(4)-C(5)-S(2)	-171.2(11)
S(1)-C(4)-C(5)-S(2)	5.9(13)
C(8)-S(2)-C(5)-C(6)	-0.9(9)
C(8)-S(2)-C(5)-C(4)	175.7(9)
C(10)-C(11)-C(12)-C(22)	178.3(11)
C(19)-C(11)-C(12)-C(22)	1.5(16)
C(10)-C(11)-C(12)-S(3)	-1.6(15)
C(19)-C(11)-C(12)-S(3)	-178.5(8)
C(9)-S(3)-C(12)-C(11)	1.9(10)
C(9)-S(3)-C(12)-C(22)	-178.0(13)
C(12)-C(11)-C(10)-C(9)	0.3(15)
C(19)-C(11)-C(10)-C(9)	176.2(12)

C(6)-C(7)-C(8)-C(9)	173.2(11)
C(6)-C(7)-C(8)-S(2)	-1.5(13)
C(5)-S(2)-C(8)-C(7)	1.4(9)
C(5)-S(2)-C(8)-C(9)	-173.7(10)
C(11)-C(12)-C(22)-C(23)	55.2(15)
S(3)-C(12)-C(22)-C(23)	-124.9(12)
C(11)-C(12)-C(22)-C(24)	-59.9(15)
S(3)-C(12)-C(22)-C(24)	120.0(12)
C(12)-C(11)-C(19)-C(20)	-57.5(14)
C(10)-C(11)-C(19)-C(20)	126.4(14)
C(12)-C(11)-C(19)-C(21)	57.8(14)
C(10)-C(11)-C(19)-C(21)	-118.3(15)
C(8)-C(7)-C(6)-C(5)	0.8(15)
C(4)-C(5)-C(6)-C(7)	-176.0(11)
S(2)-C(5)-C(6)-C(7)	0.3(12)
C(4)-C(3)-C(2)-C(1)	1(3)
C(4)-C(3)-C(2)-C(16)	-175.3(16)
C(4)-C(3)-C(2)-S(101)	176(11)
C(4)-S(101)-C(2)-C(1)	3.3(18)
C(4)-S(101)-C(2)-C(3)	-3(7)
C(4)-S(101)-C(2)-C(16)	-176.1(11)
C(11)-C(19)-C(21)-C(24)	-56.2(14)
C(20)-C(19)-C(21)-C(24)	60.2(13)
C(1)-C(2)-C(16)-C(18)	-58.7(15)
C(3)-C(2)-C(16)-C(18)	118(3)
S(101)-C(2)-C(16)-C(18)	120.8(15)
C(1)-C(2)-C(16)-C(17)	57.4(15)
C(3)-C(2)-C(16)-C(17)	-126(3)
S(101)-C(2)-C(16)-C(17)	-123.2(15)
C(11)-C(19)-C(20)-C(23)	54.3(14)
C(21)-C(19)-C(20)-C(23)	-60.6(14)
C(2)-C(16)-C(17)-C(14)	-51.9(15)
C(18)-C(16)-C(17)-C(14)	63.6(14)
C(7)-C(8)-C(9)-C(10)	-8.6(19)
S(2)-C(8)-C(9)-C(10)	165.6(9)
C(7)-C(8)-C(9)-S(3)	179.9(10)

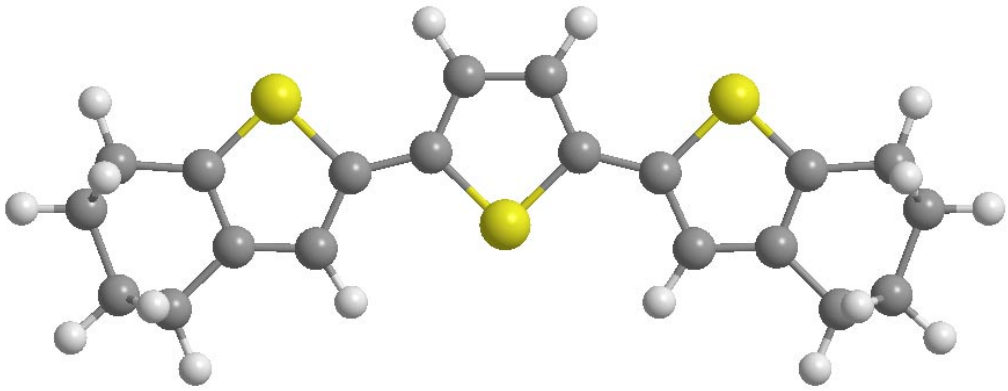
S(2)-C(8)-C(9)-S(3)	-5.9(14)
C(11)-C(10)-C(9)-C(8)	-171.1(11)
C(11)-C(10)-C(9)-S(3)	1.1(12)
C(12)-S(3)-C(9)-C(8)	170.9(10)
C(12)-S(3)-C(9)-C(10)	-1.7(9)
C(3)-C(2)-C(1)-C(103)	-2(3)
C(16)-C(2)-C(1)-C(103)	175(3)
S(101)-C(2)-C(1)-C(103)	-4(3)
C(3)-C(2)-C(1)-C(13)	-177.3(19)
C(16)-C(2)-C(1)-C(13)	0.2(17)
S(101)-C(2)-C(1)-C(13)	-179.2(14)
C(3)-C(2)-C(1)-S(1)	0(2)
C(16)-C(2)-C(1)-S(1)	177.7(10)
S(101)-C(2)-C(1)-S(1)	-2(2)
C(4)-C(103)-C(1)-C(2)	3(5)
C(4)-C(103)-C(1)-C(13)	175.2(19)
C(4)-C(103)-C(1)-S(1)	-171(14)
C(14)-C(13)-C(1)-C(2)	-57.9(15)
C(15)-C(13)-C(1)-C(2)	57.3(15)
C(14)-C(13)-C(1)-C(103)	130(5)
C(15)-C(13)-C(1)-C(103)	-115(5)
C(14)-C(13)-C(1)-S(1)	124.9(13)
C(15)-C(13)-C(1)-S(1)	-120.0(13)
C(4)-S(1)-C(1)-C(2)	-1.1(12)
C(4)-S(1)-C(1)-C(103)	6(9)
C(4)-S(1)-C(1)-C(13)	176.0(12)
C(12)-C(22)-C(23)-C(20)	-54.1(14)
C(24)-C(22)-C(23)-C(20)	58.5(14)
C(19)-C(20)-C(23)-C(22)	1.4(15)
C(12)-C(22)-C(24)-C(21)	56.1(14)
C(23)-C(22)-C(24)-C(21)	-58.4(14)
C(19)-C(21)-C(24)-C(22)	-0.9(15)
C(2)-C(16)-C(18)-C(15)	56.9(15)
C(17)-C(16)-C(18)-C(15)	-59.6(14)
C(16)-C(18)-C(15)-C(13)	-2.2(16)
C(1)-C(13)-C(15)-C(18)	-53.6(15)

C(14)-C(13)-C(15)-C(18)	59.8(14)
C(16)-C(17)-C(14)-C(13)	-4.7(16)
C(1)-C(13)-C(14)-C(17)	58.6(14)
C(15)-C(13)-C(14)-C(17)	-56.5(14)

Symmetry transformations used to generate equivalent atoms:

Calculated Results

Optimized Strucuture



Cartesian coordinates and absolute energies

2$^{\bullet+}$ (all-anti), C1, no negative frequencies

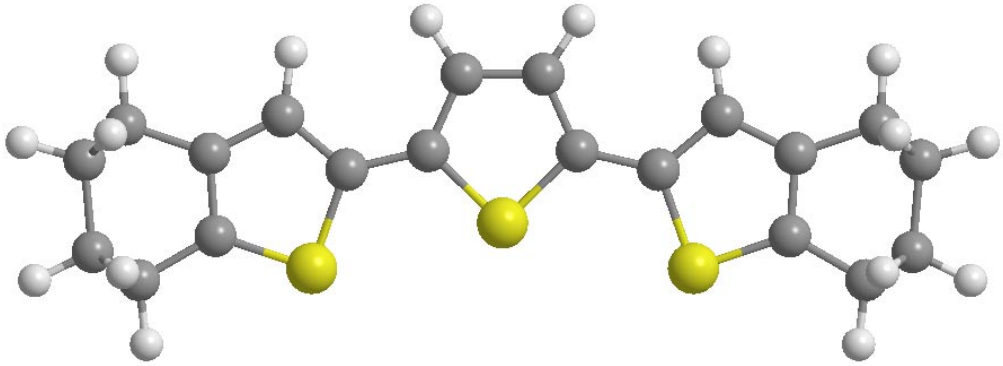
B3LYP/6-31G(d) -2123.3519065 hartree

51

C	6.610503	0.604412	0.000456
C	5.121772	0.494551	0.000123
C	4.607330	-0.804161	-0.000123
S	3.893547	1.698200	0.000279
C	5.680682	-1.859275	-0.000365
C	3.211169	-0.832531	-0.000251
C	2.632499	0.448680	-0.000087
H	2.617821	-1.741554	-0.000466
C	1.264795	0.796372	-0.000168
C	0.692026	2.086024	-0.000181
S	0.000009	-0.428566	-0.000226
C	-0.692024	2.086020	-0.000203
H	1.291600	2.989526	-0.000135
C	-1.264787	0.796365	-0.000205
H	-1.291603	2.989518	-0.000168
C	-2.632493	0.448671	-0.000124
C	-3.211170	-0.832538	0.000018
S	-3.893540	1.698191	-0.000176

C	-4.607333	-0.804164	0.000069
H	-2.617824	-1.741563	0.000107
C	-5.121771	0.494550	-0.000054
C	-5.680691	-1.859273	0.000072
C	-6.610503	0.604417	0.000133
H	-5.265123	-2.871172	0.000046
C	-6.565189	-1.623213	1.258216
C	-6.564973	-1.623071	-1.258209
C	-7.114275	-0.164773	1.260946
C	-7.114884	-0.164944	-1.260313
H	-6.968138	1.637248	0.000154
H	-8.209349	-0.156934	1.243411
H	-6.805549	0.368483	2.165237
H	-6.807366	0.368547	-2.164872
H	-7.386199	-2.347483	-1.249298
H	-5.980807	-1.816816	2.163200
H	-7.386832	-2.347144	1.248537
H	-8.209947	-0.157747	-1.241698
H	-5.980091	-1.815793	-2.163063
H	5.265108	-2.871172	-0.000702
C	6.565139	-1.623588	1.257877
C	6.565003	-1.622707	-1.258548
H	6.968141	1.637242	0.000787
C	7.114997	-0.164612	-1.260150
C	7.114150	-0.165120	1.261110
H	6.805264	0.367854	2.165513
H	8.209226	-0.157216	1.243733
H	8.210057	-0.157483	-1.241383
H	5.980754	-1.817528	2.162787
H	6.807635	0.369162	-2.164596
H	7.386816	-2.347477	1.247963
H	5.980116	-1.815087	-2.163472
H	7.386186	-2.347169	-1.249877

Optimized Strucuture



Cartesian coordinates and absolute energies

2$^{\bullet+}$ (all-syn), C1, no negative frequencies

B3LYP/6-31G(d) -2123.3497717 hartree

51

C	6.158181	-1.448264	-0.000002
C	4.865244	-0.702270	0.000013
C	4.964908	0.690125	0.000034
S	3.233038	-1.251112	-0.000080
C	6.390236	1.175371	0.000154
C	3.720740	1.322817	-0.000012
C	2.641015	0.418185	-0.000068
C	1.265233	0.737937	-0.000104
C	0.691350	2.029209	-0.000123
S	0.000005	-0.482740	-0.000155
C	-0.691346	2.029207	-0.000133
C	-1.265227	0.737933	-0.000114
C	-2.641011	0.418181	-0.000093
C	-3.720738	1.322814	-0.000112
S	-3.233039	-1.251115	-0.000088
C	-4.964908	0.690124	-0.000019
C	-4.865246	-0.702271	0.000027
C	-6.390236	1.175372	0.000099
C	-6.158185	-1.448263	0.000070
C	-7.085169	0.578909	-1.257339
C	-7.084860	0.578919	1.257714

C	-6.946311	-0.973356	-1.260326
C	-6.946343	-0.973378	1.260453
C	7.085149	0.578968	-1.257324
C	7.084875	0.578856	1.257730
C	6.946354	-0.973441	1.260395
C	6.946290	-0.973297	-1.260386
H	6.032089	-2.533923	-0.000063
H	6.454593	2.267435	0.000212
H	3.583900	2.398547	0.000009
H	1.289754	2.932198	-0.000110
H	-1.289752	2.932195	-0.000125
H	-3.583897	2.398544	-0.000140
H	-6.454592	2.267436	0.000105
H	-6.032096	-2.533922	0.000058
H	-6.644062	1.007041	-2.162919
H	-8.139773	0.873950	-1.246327
H	-8.139401	0.874200	1.247158
H	-6.643287	1.006836	2.163168
H	-7.929215	-1.456334	-1.242498
H	-6.436962	-1.319462	-2.164899
H	-6.437215	-1.319760	2.165044
H	-7.929359	-1.456123	1.242394
H	6.644029	1.007144	-2.162875
H	8.139754	0.874008	-1.246312
H	6.643316	1.006729	2.163211
H	8.139417	0.874134	1.247173
H	7.929368	-1.456190	1.242300
H	6.437235	-1.319866	2.164974
H	6.436926	-1.319358	-2.164968
H	7.929194	-1.456277	-1.242598

Explanation for the formation of all-syn conformer of $2^{\bullet+}SbF_6^-$

The KS-SOMO of radical cation $\mathbf{2}^{\bullet+}$ is shown in Figure S3. Apparently the MO coefficients on carbon atoms of the π-systems are much larger than those on sulfur atoms.

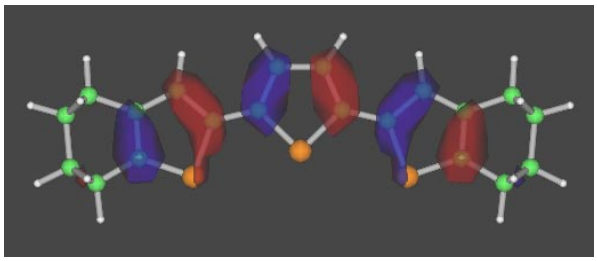


Figure S3. The KS-SOMO of radical cation $\mathbf{2}^{\bullet+}$.

In the case of the all-syn conformer, effective overlaps of SOMOs are possible mainly at the three central areas as shown in Figure S4.

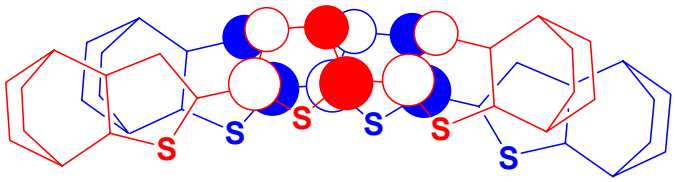


Figure S4. Schematic representation of SOMOs of the central areas of all-syn conformers of the π-dimer. The phase of the MOs are expressed by filling the circles.

In the case of the all-anti conformer, the area, in which effective overlap of SOMOs is possible, is limited only to the central position as schematically shown in Figure S5.

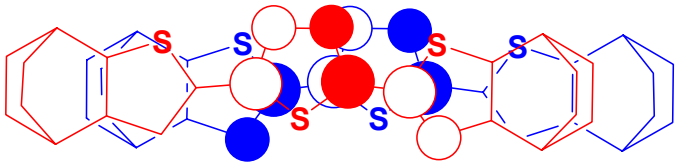


Figure S5. Schematic representation of SOMOs of the central areas of all-anti conformers of the π-dimer. The phase of the MOs are expressed by filling the circles.